8.051: Quantum Physics II

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Introduction

An MITx page for this class will be up by this afternoon. That's where most of the content for this class will come from (regular class meetings are recitations).

Lecture videos on the MITx page are divided into 7 to 25 minute sections, each covering some particular topic. After each block, there are some "lecture exercises:" this class is structured in a way so that before each recitation, we should have finished going over the material designated for it. We'll also have real problems in problem sets – there are about 11 of these over the semester, and they're also going to be online.

Homework is the best predictor of how we're going to do in this course – if we basically understand the homework completely, we're extremely likely to do very well. Homework on the MITx page is given to us problem by problem, part by part, but we'll also be given a PDF of the problems that we can complete like a regular problem set. And we'll have some tests in the evenings of the exams instead of recitations on those days.

This class also has a graduate TA (Matt Hodel) and an MITx site administrator (Michelle Tomasik), and we should ask them if we have questions.

Grading is 10 percent lecture questions, 30 percent online homework, 15 percent for each of the two midterms (March 11 and April 22), and 25 percent from the final. It's pretty likely we'll be able to drop one problem set. Because this is an online course, we have a bit more flexibility - if we need a one-day extension, it's easy for the system to give that. Beyond that, we should go through S^3.

In principle, no textbook is required for this class, but Griffiths and Shankar are good references – it's good to read things in a different way. There will be lecture notes, and students seem to like them.

MIT has been a bit reluctant to accept that online classes are equivalent to normal lecture-based classes, so in general, coming to recitation is generally mandatory. When this class runs in previous years, a rule has not had to be imposed, but attendance sheets are passed around. It will make a difference, and it's important!

Scheduled office hours will be posted by the end of today – there will be about 2 to 3 hours per week. Other times are also welcome by appointment.

1 February 3, 2020

8.05 is being changed a bit. The issue being corrected is that the addition of angular momentum is usually the last topic of the semester, and it's always a little rush even though it's a bit difficult. So we'll shift it a bit forward, and there will be at least three more lectures at the end about the density matrix (which is a topic that jumped between 8.05 and 8.06 and eventually got dropped from both). So the aspects of 8.05 that were 8.04 review will go away: there

will be an 8.04 review section in the MITx page, but it won't be covered anymore. We can use it at our discretion, or we can proceed to unit 1.

Fact 1

This class assumes pretty good knowledge of 8.04, so we'll move to new material very quickly.

Wednesday's exercises will not be due, but next week's Monday, Wednesday, and Friday lectures will be graded. We're really hitting the ground running.

Fact 2

8.051 is a class based on **online lectures**, so we go through the lectures at our own pace. However, I will still transcribe notes from each lecture and insert them in the appropriate spots of the class: lectures 1 and 2 will be placed in the notes after this recitation (that is, before recitation 2), and all future lectures will be placed before their corresponding recitations. This means that the flow of the class material approximately corresponds to the flow of the notes.

With the last half hour or so of this first recitation, we'll talk a bit about **states** in quantum mechanics.

Example 3 (Two-state system)

Consider a quantum system with two **basis states** ψ_+ and ψ_-.

This means that any state in this system can be written as a **superposition** of the two basis states. (Recall that the ψ notation tells us that these are [complex-valued] wavefunctions.) Because these are wavefunctions, they are normalized in such a way so that

$$\langle \psi_+, \psi_+ \rangle = 1, \quad \langle \psi_-, \psi_- \rangle = 1$$

and it's nice if the two basis states are **orthonormal**, so that

$$\langle \psi_+, \psi_- \rangle = 0.$$

Recall that we often define the inner product between two wave functions as

$$\langle \phi(x), \psi(x) \rangle = \int dx \phi^*(x) \psi(x),$$

so that $\langle \phi, \phi \rangle = \int dx |\phi|^2 = 1$.

Question 4. *How many* **real parameters** *do I need to characterize a general state in this quantum system? That is, how many real parameters are needed to describe the* **inequivalent states** *(that is, states that aren't proportional by some complex constant)?*

(Survey: 1, 3, 6, 3 votes for 1, 2, 3, and 4.) Let's go through and solve this: a general superposition looks like

$$\psi(x) = c_+ \psi_+ + c_- \psi_-, \quad c_+, c_- \in \mathbb{C}.$$

But many of these states are physically equivalent: right now, we have two complex numbers, which means four real parameters. But a state like ψ is equivalent to 2ψ, which is equivalent to $(1+3i)\psi$, and so on: we **normalize the state** to get the physics! So we need $\langle \psi, \psi \rangle = 1$, which means

$$\langle c_+ \psi_+ + c_- \psi_-, c_+ \psi_+ + c_- \psi_- \rangle = 1.$$

We can expand out the inner product, noticing that constants from the left term come out with a conjugate, to find that

$$c_+^* c_+ \langle \psi_+, \psi_+ \rangle + c_+^* c_- \langle \psi_+, \psi_- \rangle + c_-^* c_+ \langle \psi_-, \psi_+ \rangle + c_-^* c_- \langle \psi_-, \psi_- \rangle = 1.$$

And now using our orthonormality conditions, this tells us that

$$|c_+|^2 + |c_-|^2 = 1.$$

This is a real constraint, so it removes one parameter.

But are we done? Let's use our new information to rewrite

$$\psi = e^{i\alpha_+} a\psi_+ + e^{i\alpha_-} b\psi_-$$

where $a, b \geq 0$ and α_+, α_- are real. So now our condition tells us that $a^2 + b^2 = 1$, and $a, b \geq 0$, but now we can see another constraint: remember that we can normalize in the phase direction as well! So this is actually equivalent to

$$\psi = a\psi_+ + e^{i(\alpha_- - \alpha_+)} b\psi_-,$$

which means we really only have $\boxed{2}$ free parameters: one for the phase difference and one for the magnitude of ψ_+.

In summary, let's rewrite this in a slightly nicer way:

$$\psi = a\psi_+ + e^{i\beta} b\psi_-,$$

where $a, b \geq 0$, $a^2 + b^2 = 1$, which can also be written as

$$\psi = \cos(\chi)\psi_+ + e^{i\beta} \sin(\chi)\psi_-,$$

where $\beta \in [0, 2\pi]$ and $\chi \in \left[0, \frac{\pi}{2}\right]$ (because both cos and sin have to be positive).

Here's one way to never forget the characterization of this state: think about **spherical coordinates**. Every point has a coordinate θ and ϕ, and in spherical coordinates we have $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$. So we could write

$$\psi = \left(\cos\frac{\theta}{2}\right)\psi_+ + e^{i\phi}\left(\sin\frac{\theta}{2}\right)\psi_-.$$

So we can think of the space of states as the surface of a 2-sphere in 3-dimensional space: for every direction of our 2-sphere, we have a state, which is a linear combination of our "up state" ψ_+ and "down state" ψ_-.

2 The Variational Method and Introduction to Stern-Gerlach

We'll start this class by discussing the **variational problem**, which might be new to some of us. This is connected to a field called the **calculus of variations** – this is a pretty complicated topic, and we won't get into a lot of the difficulties. The main idea of calculus of variations is to look at maxima and minima of a **functional** instead of a function. (In ordinary calculus, we try to find a point where some quantity is maximized, but here we'll be trying to find a **function** that maximizes some quantity.) So things are a bit more challenging!

Fact 5

Calculus of variations seemed to have originated from Newton. The question he considered was to start with a cross-sectional area and try to taper it in a way such that the resistance from a viscous fluid flowing through is minimized. And this is complicated, because our ultimate goal is to find a shape rather than just a single number or point (as we do in ordinary calculus).

Fact 6

Another famous problem, called the **Brachistochrone problem**, asks for us to design a curve from point A to point B in a plane such that an object (under the influence of gravity) traverses the path the fastest. This was a difficult problem for many mathematicians back then, including Leibniz, Newton, andthe Bernoullis!

So how is this calculus of variations idea related to quantum mechanics? It seems that special functions are often the minimizer of some important quantity, and we have some special functions in quantum mechanics: the **energy eigenfunctions**. It's then natural to ask whether there's a quantity that they minimize, and indeed the answer is yes.

So let's start setting up our problem: we're trying to solve the energy eigenstate equation

$$\hat{H}\psi = E\psi,$$

where $\hat{H}$ is some (any-dimensional) Hamiltonian and ψ is a wavefunction (which can be of a vector $\vec{x}$ or just a single x in one dimension). It'll take a while for us to get to the "minimum or maximum" answer, so we'll start with a simpler question – determining something about the **ground state energy**.

Theorem 7 (Variational principle)

Let $\psi(x)$ be an **arbitrary** normalized wavefunction (it doesn't need to solve the Schrodinger equation), meaning that $\int |\psi|^2 d\vec{x} = 1$. Then we have the upper bound on the ground state energy

$$\int \psi^*(x)\hat{H}\psi(x) = \langle \hat{H} \rangle_\psi \geq E_{\text{gs}}.$$

This equation doesn't tell us the exact value of the ground state energy, but it gives us an upper bound for **any** arbitrary function that we try putting in! And the strategy when we apply this principle is to plug in functions that we think **look like the wave function of a bound state**. (Those $\psi(\vec{x})$ functions that we plug in are called **trail wavefunctions**.)

Remark 8. *Unfortunately, there isn't a very good way of determining how good our bound is just from this equation – we'll develop some better tools later on.*

"Proof". We'll make a few assumptions, which basically says that we don't have a **continuous spectrum** of energy eigenvalues. This is only used so that the proof is easier to write down – it means we can write down our energies

$$E_{\text{gs}} = E_1 \leq E_2 \leq E_3 \cdots,$$

and we know that our Hamiltonian acts on the energy eigenstates via

$$\hat{H}\psi_n = E_n\psi_n.$$

By **completeness of the energy eigenstates**, we can write our trial wave function

$$\psi(x) = \sum_{n \geq 1} b_n \psi_n(x)$$

as a superposition of energy eigenstates. It's important to note that ψ here **does not solve the Schrodinger equation** – it's just something invented out of our head. Now, we know that ψ is normalized, so

$$1 = \int |\psi|^2 dx = \sum_{n \geq 1} |b_n|^2,$$

where we've used **orthonormality** of the energy eigenstates. And expanding out the expression for the expectation value of the Hamiltonian $\langle H \rangle_\psi$ will yield

$$\boxed{\int \psi^* \hat{H} \psi} = \sum_{n \geq 1} |b_n|^2 E_n.$$

(This takes a few lines, but we're basically using orthonormality again.) But we're now almost done: the above expression is lower bounded by

$$\geq \sum_{n \geq 1} |b_n|^2 E_1 = E_1 \cdot 1 = \boxed{E_{\text{gs}}},$$

as desired. □

Our next step is to make a more general statement for the variational principle – it's not always convenient for us to have normalized wave functions. But we know that for an unnormalized wave function ψ, we can create the **normalized** wave function

$$\frac{\psi(x)}{\sqrt{\int |\psi|^2 dx}},$$

and this should satisfy the equation in the variational principle. Thus, we find that

$$E_{\text{gs}} \leq \frac{\int \psi^* \hat{H} \psi dx}{\int \psi^* \psi dx},$$

and this is actually nicer because we don't need to work with such a restricted set of functions.

Fact 9

It is true that our trial function ψ cannot be completely arbitrary – it must be **normalizable** so that the denominator here is well-defined and finite.

We can introduce the notation

$$\mathcal{F}[\psi] = \frac{\int \psi^* \hat{H} \psi dx}{\int \psi^* \psi dx},$$

and this $\mathcal{F}$ is called a **functional** (which inputs a function and outputs a number). Basically, given a trial wave function $\psi(x)$, which is a function, we compute a number, which is an upper bound on the energy ground state.

So we want to find the "critical point" of a functional – it seems that the ground state energy will be the minimum value of the functional. And in fact, this functional is minimized exactly by the **ground state wave function!** (This might seem dizzying, because a function can be specified by infinitely many numbers – critical points are hard to visualize.) But it turns out that **every eigenstate is actually a critical point of the functional** (though the non-ground states are saddle points), which we'll show in our homework.

Example 10

Consider the delta function potential

$$V(x) = -\alpha\delta(x), \quad \alpha > 0.$$

The ground state energy is well-known here, since we've solved this problem in 8.04 already: we have

$$E_{\text{gs}} = -\frac{m\alpha^2}{2\hbar^2}.$$

But let's assume we don't know what the ground-state wave function should look like, and we use some kind of Gaussian as our trial function:

$$\psi(x) = e^{-\frac{1}{2}\beta^2 x^2}.$$

(The reason for the β is to reap more of the benefits of our calculation to get a better bound – we can adjust our parameter β to get the best possible bound on our energy.) So let's start calculating: we can find the denominator (from a standard Gaussian integral) to be

$$\int |\psi|^2 dx = \frac{\sqrt{\pi}}{\beta},$$

and then we need to find

$$\int \psi^*(x)\hat{H}\psi(x) = \int e^{-\frac{1}{2}\beta^2 x^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x)\right)e^{-\frac{1}{2}\beta^2 x^2},$$

where we've substituted in the Hamiltonian with the given potential. This is not so fun, and **in general in 8.05, we can use Mathematica or Maple or MATLAB to make our life easier**, as long as we think we could theoretically find it ourselves. Well, the delta function part of the integral just gives us a $-\alpha$, because we pick out the value at 0 with the delta function, and we actually want to **integrate by parts** for the term with the second derivative. This is because our integral reduces to

$$\frac{\hbar^2}{2m}\int dx \left[\frac{d}{dx}e^{-\frac{1}{2}\beta^2 x^2}\right]^2,$$

which is an easier integral to evaluate. And if we carry out all of the calculations, the **final answer** we get is that (remembering to bring in the term from the denominator)

$$F[\psi] = -\frac{\beta}{\sqrt{\pi}}\alpha + \frac{\beta^2\hbar^2}{4m}.$$

This expression is 0 at $\beta = 0$, and it's 0 at some other positive value of β – specifically, this is some quadratic function, and we can find the minimum to get the best possible upper bound on the energy ground state. Explicitly, the variational principle tells us that

$$E_{\text{gs}} \leq \min_{\beta}\left\{-\frac{\beta}{\sqrt{\pi}}\alpha + \frac{\beta^2\hbar^2}{4m}\right\} = -\frac{m\alpha^2}{\pi\hbar^2} = \frac{2}{\pi}\left(-\frac{m\alpha^2}{2\hbar^2}\right).$$

And the term in parentheses on the right is the **true** ground state energy, so our bound is just off by a factor of $\frac{2}{\pi}$, which is somewhat close!

With that, we'll move on to a new topic: that of **Stern-Gerlach devices** and the **spin 1/2** system. Spin 1/2 will keep us busy for a good chunk of the semester, and we'll go into a lot of detail – today, we'll just give the beginning of the story, and our descriptions will become more elaborate as time goes on. We'll start with the experiment which led to the discovery of spin, and we'll then describe how to construct a physical theory out of that. Afterwards, we'll spend some time on **linear algebra**, which will provide us with some mathematical tools for studying this physical model.

Fact 11

The **Stern-Gerlach experiment** was done in 1922 in Frankfurt, and it wasn't clear for a while why it was being done. The background is that Pauli thought electrons had two degrees of freedom but didn't know what they were. Kronig suggested that it had to do with some kind of rotation, but Pauli thought this made no sense. Meanwhile, Uhlenbeck and Goudsmit (in 1925) had the same idea, and Ehrenfest (their advisor) also thought this made no sense but still let them publish it. So that's why they have credit for discovering the spin of an electron.

Stern and Gerlach were atomic physicists who were actually interested in measuring **speed of thermal motion of ions** by using magnetic fields to deflect beams of these ions. Then experts who heard of Bohr, who said that an electron might have angular momentum, and they tried to detect it. When the experiment was run, they did see something, but the electrons in the silver atoms of those experiments actually had no angular momentum, only spin! So there was a lot of confusion – let's try to describe what exactly they saw and extract the quantum mechanics out of that.

First of all, **we don't see spin directly** in an experiments: we see magnetic moments.

Definition 12

A magnetic moment μ is the magnetic analog of an electric dipole, and it is given by the formula

$$\mu = I\vec{A}.$$

Roughly what's going on here is that we can imagine a loop in the plane with some current I, and there is some normal vector $\vec{A}$ corresponding to the area enclosed by that loop. Looking at units, it turns out that μB has units of energy, so we can define the units

$$[\mu] = \frac{\text{Joules}}{\text{Tesla}}.$$

Let's consider another situation in which a magnetic moment might come up: say we have a **ring of charge** of radius R with some total charge Q, which means we have a linear (uniform) charge density λ. In addition, say that this ring is rotating with some velocity v and has some mass M. Then we want to measure this magnetic moment, because there happens to be a fundamental relation between angular momentum and magnetic moments!

To understand that, first note that the current satisfies

$$I = \lambda v = \frac{Q}{2\pi R} v$$

(the rotating ring creates a charge "moving" through the wire in our frame), and thus the magnetic moment is

$$\mu = IA = \frac{Q}{2\pi R} v\pi R^2 = \frac{1}{2} QvR.$$

This is an okay answer, but it depends on the radius and velocity of our ring. So let's compare it to the magnitude of the angular momentum, which is $\mathbf{r} \times \mathbf{p}$ for each individual part of the ring. Thus,

$$L = MvR = \frac{1}{2}\frac{Q}{M}(MvR) \implies \boxed{\mu = \frac{Q}{2M} L}.$$

And all of the "incidentals" like the radius and velocity of the ring have dropped out – the relation is thus universal for any ring, and thus it also holds for any axially symmetric object, like a hollow sphere or ellipsoid!

With this in mind, we can now speculate that **a particle might have a magnetic moment if there is a little ball of charge rotating inside it**. This was exactly what Pauli didn't like about the model, though, so let's take a

more quantum mechanical approach to this. We'll consider a single particle, and now we'll replace L with S, the **spin angular momentum** of the particle (since this particle is no longer rotating around another object). So if this particle is, for instance, an electron, it's natural to ask whether we have

$$\mu \stackrel{?}{=} \frac{e}{2m_e} = \frac{e\hbar}{2m_e}\left(\frac{S}{\hbar}\right).$$

If this were true, it would be a quantum analog of the classical statement. (The second equality is just to make the $\frac{S}{\hbar}$ term unitless.) It turns out this equation isn't quite true, but it's very close! The actual answer turns out to be that

$$\mu = g\frac{e\hbar}{2m}\frac{S}{\hbar},$$

where g is sometimes called the **Landé factor**. We can usually calculate g – it turns out that the electron's g-factor is equal to 2. So the magnetic moment is twice what we predict in the classical case (and this is predicted by the Dirac equation, the relativistic equation of the electron). Defining $\mu_B = \frac{e\hbar}{2m_e} \approx 9.3 \times 10^{-24}$J/Tesla (here B stands for **Bohr magneton**), we have

$$\boxed{\vec{\mu} = -2\mu_B\frac{\vec{S}}{\hbar}},$$

where the negative sign comes from the negatively charged electron.

Remark 13. *Protons and neutrons have a more complicated system, because they are made up of quarks interacting in odd ways. (And the magnetic moment of a proton or neutron is much smaller, because the mass in the denominator of μ_B is much larger.*

With this, our next question is to think about how these magnetic moments behave under magnetic fields.

Example 14

Suppose we have a loop of charge in the plane, rotating counterclockwise, and magnetic field lines are coming up out of the plane and diverging (so that the magnetic field is weaker above the loop). Does the loop feel a force up or down?

To solve this, we look at two diametrically opposite points and calculate the force $I \times \vec{B}$ at both points. Both have a vertical component pointing down and the horizontal components cancel out, so the net force is pointing down, and in fact

$$\vec{F} = \nabla(\vec{\mu} \cdot \vec{B})$$

(which was derived in 8.02). We can indeed see that this equation is consistent: **the force goes in the direction that makes $\vec{\mu} \cdot \vec{B}$ largest**. And this problem becomes simpler if the magnetic field is mostly in the z-direction.

But with that, let's return to the Stern-Gerlach experiment. Recall that silver atoms have 47 electrons – 46 of these fill out the lower energy levels, and there is a **lone 5s electron** which is out in its own spherical shell. An s state electron has zero orbital angular momentum, so throwing a silver atom through an apparatus is essentially like throwing a single electron (that is, throwing spins), because everything else cancels out!

As far as we're considered experimentally, what we're actually throwing is **dipole moments**: magnetic fields push these dipole moments up and down. So here's the apparatus that was being used: silver atoms are shot in a beam, and we **insert a magnet** such that the magnetic field lines, mostly in the z-direction, have a slight gradient. Then these silver atoms hit a screen after the magnet, and we can track where they land.

In such an apparatus, we can assume that the force will be approximately in the z-direction:

$$\vec{F} = \nabla(\vec{\mu} \cdot \vec{B}) \approx \mu_z \frac{\partial B_z}{\partial z} \hat{z}.$$

(It turns out that the gradient in the other directions averages out!) So it seems like the magnetic moments will all be distributed in random directions, so we'll get a smudge of z-components when the silver hits the screen.

But the shock was that there were actually two separate peaks! The magnetic field being used in this experiment was about 0.1 Tesla, and the **space quantization** that was seen between the two peaks was about 0.2 millimeters. So this was clear enough for everyone to observe it, and this caused a bit of confusion.

At the end of the day, people realized that this didn't come from angular momentum of the electron around the atom, and the concept of spin came back. It took a while for the details to be resolved, but the idea is that

$$\mu_z = -2\mu_B \frac{S_z}{\hbar},$$

and experiments suggested that the true value of the dimensionless term was

$$\frac{S_z}{\hbar} = \pm \frac{1}{2}.$$

Such a particle is known as a **spin 1/2 particle**! With our 8.04 knowledge, we can think of this quantum mechanically as our states being a **superposition** of a "spin up" and a "spin down" state. And when the particle goes through the magnetic field, it splits into these two beams, and the wavefunction collapses when we observe it (that is, when the silver atom hits a screen).

To finish this lecture, let's do a few thought experiments with our Stern-Gerlach apparatus. We can represent this with a box: a beam (an inward arrow) goes in, and two beams (represented by outward arrows) come out, with values $S_z = \frac{\hbar}{2}$ and $S_z = -\frac{\hbar}{2}$. This box **measures the value of** S_z, and it splits our beam.

Example 15

Take a Stern-Gerlach device and block the lower beam (so only the $S_z = \frac{\hbar}{2}$ beam passes through). Feed that beam into another Stern-Gerlach (z) device – what happens?

We see experimentally that nothing comes out from the bottom of the second Stern-Gerlach device: all particles have $S_z = \frac{\hbar}{2}$. Quantum mechanically, we can think of this as having the **quantum states**

$$|z;+\rangle\,, \quad |z;+z;-\rangle\,.$$

We'll be thinking of these as our **basis states**: any other state, even a state that points along the x-direction, is a superposition of these two states. And this is a big assumption to make: we're saying that the set of spin states is a **two-dimensional complex vector space**, where linear combinations of $|z;+\rangle$ and $|z;+z;-\rangle$ can represent all configurations. So in algebra, this means that measuring a $|z;+\rangle$ state will have no minus component, or equivalently that

$$\langle z;-|z;+\rangle = 0.$$

(These are **orthogonal basis states**.) We can also similarly write that

$$\langle z;+|z;-\rangle = 0, \quad \langle z;+|z;+\rangle = 1.$$

This might seem a little strange to us, because there's a bit of a conflict with "orthgonality" here – it turns out that "up" and "down" are orthogonal, not antiparallel! And this is one of the most confusing parts of working with spin 1/2

particles – we shouldn't think of this **overlap** expression above as a regular dot product.

Example 16

Again, start with a z-filter Stern-Gerlach device with the bottom beam blocked, and feed this into an x-filter Stern-Gerlach device. This turns out to give us $S_x = \frac{\hbar}{2}$ and $S_x = -\frac{\hbar}{2}$ with equal probability.

This means that spin states along the x and z directions do have some overlap – they aren't orthogonal! In particular, we get the expression

$$\langle x; +|z; +\rangle = \langle x; -|z; +\rangle \neq 0.$$

(We'll be more precise with all of this notation later.)

Example 17

Take the system from the previous example, and this time **block particles with** $S_x = \frac{\hbar}{2}$. So the exiting beam has all particles satisfying $S_x = -\frac{\hbar}{2}$: what happens when we feed this into a z-filter Stern-Gerlach machine?

It seems possible that all of these particles that we've filtered have both $S_x = -\frac{\hbar}{2}$ **and** $S_z = \frac{\hbar}{2}$, since we've filtered for both qualities. **But that doesn't happen**! We get both $S_z = \pm\frac{\hbar}{2}$, so the "memory of the state" from the first Stern-Gerlach device has been destroyed. We'll talk more formally about all of this next time, and we'll try to discuss more about the relations about our different states.

3 Spin One-Half, Bras, Kets, and Operators

Last time, we spoke about the Stern-Gerlach experiment, and we discussed how a sequence of Stern-Gerlach boxes could help us extract properties of the spin 1/2 system. The biggest surprise was that these Stern-Gerlach devices split our magnetic moments into two beams (basically forcing them to point in one of two opposite directions). Today, we'll talk more about how to represent the set of states as a two-dimensional vector space, and we'll set up all of the machinery that will be necessary. Even though we haven't quite discussed all of the linear algebra concepts, we'll assume some vague ideas today – mathematical formalism will come soon.

Recall that the possible states of the silver atom (really, an electron) can be described by the two states $|z; +\rangle$ and $|z; -\rangle$, corresponding to angular momenta $S_z = \frac{\hbar}{2}$ and $-\frac{\hbar}{2}$, respectively. (The z-label here indicates that we've passed our atoms through a z-filter Stern-Gerlach device.) We can ask whether the state $|z; +\rangle$ have an angular momentum in the x- or y-direction, and we'll be able to answer that soon.

Proposition 18

Saying that $S_z = \frac{\hbar}{2}$ really means that there is an **operator** $\hat{S}_z$ with

$$\hat{S}\,|z; +\rangle = \frac{\hbar}{2}\,|z; +\rangle\,.$$

Operators often come up in quantum mechanics because they represent measurement of some sort! And here $\hat{S}_z$ also acts on the other state and gives

$$\hat{S}\,|z; -\rangle = -\frac{\hbar}{2}\,|z; -\rangle\,.$$

Operators on a state give another state, and the nice thing in this case is that the operators on the left and right are just scalar multiples of each other. This is known as an **eigenstate**, and such eigenstates have corresponding **eigenvalues** (such as the $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ above).

As mentioned last time, the underlying assumption we're using here is that **these two states are enough**. In other words, if we do this experiment again with an x-filter Stern-Gerlach device, $|x;+\rangle$ and $|x;-\rangle$ are also valid states. But we're postulating a theory of spin in which $|z;+\rangle$ and $|z;-\rangle$ are basis states, so

$$|\psi\rangle = c_1 |z;+\rangle + c_2 |z;-\rangle$$

(for some complex numbers c_1, c_2) **for any spin state** ψ. This is called a two-dimensional complex vector space, because we have two basis vectors and complex coefficients. (The $|z;+\rangle$ object doesn't quite look like a vector, but it's what we call a **ket**. and we'll make the correspondence clear in subsequent lectures.)

Letting $|z;+\rangle$ be the first basis state and $|z;-\rangle$ be the second, we should be clear that these vectors are not "complex:" a complex vector space means the coefficients, not the vectors, are complex numbers. To be more concrete, we'll use a **representation** (that is, some way of exhibiting a vector in a more familiar way). Then if we define $|z;+\rangle = |1\rangle$ and $|z;-\rangle = |2\rangle$, we will **represent**

$$|z;+\rangle = |1\rangle \iff \begin{bmatrix}1\\0\end{bmatrix}, \quad |z;-\rangle = |2\rangle \iff \begin{bmatrix}0\\1\end{bmatrix},$$

and now our states look like column vectors! In particular, we can now represent any state as a two-dimensional column vector

$$|\psi\rangle = c_1 |1\rangle + c_2 |2\rangle \iff \begin{bmatrix}c_1\\c_2\end{bmatrix}.$$

To proceed, we'll return to an example of the Stern-Gerlach experiment. One thing we did was filter the first machine so that all particles are in a $|z;+\rangle$ state – if we feed this beam into another z-filter Stern-Gerlach apparatus, then all of the states will be in the + state. (There's zero probability of being in the - state.) The way we'll represent this in mathematical terms is that those two states are **orthogonal**, and to explain that, we'll need to talk about bras and kets. For now, though, we'll just explain the basics.

What we're saying is that the **bra-ket** or **overlap** of the + and - states is zero:

$$\langle z;-|z;+\rangle = 0.$$

Similarly, the states are "well-normalized," so

$$\langle z;+|z;+\rangle = 1.$$

We can make analogous equations when the right entry is $z;-$, and we can now use the notation $|1\rangle$ and $|2\rangle$ usefully by summarizing all four equations as

$$\langle i|j\rangle = \delta_{ij}.$$

We haven't really defined what these "bras" are yet – let's start with a working definition. We associate the **ket** $|1\rangle$ with the column vector $\begin{bmatrix}1\\0\end{bmatrix}$, and similarly we'll associate the **bra** $\langle 1|$ with the row vector $\begin{bmatrix}1 & 0\end{bmatrix}$. (This means the bra $\langle 2|$ will be thought of as the row vector $\begin{bmatrix}0 & 1\end{bmatrix}$.) In slightly more generality, we can write a state

$$|\alpha\rangle = \alpha_1 |1\rangle + \alpha_2 |2\rangle \iff \begin{bmatrix}\alpha_1\\\alpha_2\end{bmatrix}.$$

Similarly, we can associate

$$|\beta\rangle = \beta_1 |1\rangle + \beta_2 |2\rangle \iff \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}.$$

And now we can define the corresponding bra for α to be

$$\langle\alpha| = \alpha_1^* \langle 1| + \alpha_2^* \langle 2| = \begin{bmatrix} \alpha_1^* & \alpha_2^* \end{bmatrix},$$

where α_1^* denotes the complex conjugate of α_1.

Fact 19

We'll make all of these definitions more axiomatically soon – this is all just to give us some intuition.

And now we can define the **bra-ket** $\langle\alpha|\beta\rangle$, which is a **number** – ultimately the reason for the complex conjugation above is to make sure $\langle\alpha|\alpha\rangle$ is a positive number (it's a "length squared"). And the reasonable way for us to get a definition of this is to take the matrix multiplication of the representatives

$$\langle\alpha|\beta\rangle = \begin{bmatrix} \alpha_1^* & \alpha_2^* \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \alpha_1^* \beta_1 + \alpha_2^* \beta_2.$$

We'll soon see that this is actually an **inner product** – vectors that satisfy the above $\langle i|j\rangle = \delta_{ij}$ inner product relation are known as **orthonormal** (because they're normal with respect to each other, and they're also orthogonal).

Example 20

We can check, for example, that taking inner products like $\langle 1|2\rangle$ give the same value as our explicit definition.

With this, we can now return to the idea of representing our states as column vectors by thinking about our operator again. The only object that naturally acts on two-component vectors is a 2×2 **matrix**, so we're going to claim that our spin operator can be written as

$$\hat{S}_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

And this can be verified now that we're writing our states as column vectors: for example,

$$\hat{S}_z |1\rangle = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{\hbar}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

as desired. And we can also check that the action $\hat{S}_z |2\rangle = -\frac{\hbar}{2} |2\rangle$ is correct, and the idea is that **we don't need to check any more vectors**: since the operator behaves correctly on basis vectors, it will behave correctly on any arbitrary vector in this space.

But we're not quite done yet: remember that in one of the experiments from last time, we wanted to know about what happens when we measure the spin states along the x-direction. In other words, how do we know that we can come up with numbers c_1, c_2 such that $c_1 |z;+\rangle + c_2 |z;-\rangle$ points along the x-direction? So we need to invent something new – this is always a difficult process, and there's many different approaches we can take. We won't be using Feynman's approach of rotating Stern-Gerlach machines: instead, we'll think about angular momentum again.

Basically, we'll compare spin angular momentum with **orbital angular momentum**: what we really care about is the operators $\hat{S}_x$ and $\hat{S}_y$. Remember that we have, in the classical case, the angular momenta $\hat{L}_x, \hat{L}_y, \hat{L}_z$. And these

are a lot easier to work with: they look like $\hat{x}\hat{p}_y - \hat{y}\hat{p}_x$, and we know how that kind of object works on wave functions. (This is a lot nicer than $\hat{S}_z$, which is working in a different kind of space.)

The key idea is that $\hat{L}_z$ is a Hermitian operator – this is good, because it means we have a good observable. And $\hat{S}_z$ is Hermitian as well, which means that its complex conjugate transpose is equal to itself (we'll talk a lot more about this later). One useful property of the L's is that we have the commutator relation

$$[\hat{L}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}\hat{L}_k$$

(where $[A, B] = AB - BA$), if we denote $\hat{L}_x, \hat{L}_y, \hat{L}_z = \hat{L}_1, \hat{L}_2, \hat{L}_3$ respectively. This is called the **algebra of angular momentum**, and in the relation above we're using **index notation**, meaning that we're summing over $k = 1, 2, 3$, and ε_{ijk} is 1 for an even permutation, -1 for an odd permutation, and 0 otherwise (we'll get more practice with this later). So we can write these formulas out explicitly:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y.$$

So our goal will be to find an analogy of this for $\hat{S}_x, \hat{S}_y, \hat{S}_z$. Specifically, our goal will be that

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \quad [\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x, \quad [\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y.$$

So we need to determine what our Hermitian 2×2 matrices look like – by definition, we need them to look like $\begin{bmatrix} 2c & a+ib \\ a-ib & 2d \end{bmatrix}$, where a, b, c, d are real (this is because we take the complex conjugate of all entries and then flip the off-diagonal entries to each other). So being hermitian is some kind of "reality" condition – the $2c$ and $2d$ are just for convenience later on.

To make progress, note that we're trying to find matrices $\hat{S}_x, \hat{S}_y$ that satisfy commutation relations. If there's any identity matrix terms, that will commute with everything (so it doesn't contribute at all). So we'll remove the "identity matrix" part from this:

$$\begin{bmatrix} 2c & a+ib \\ a-ib & 2d \end{bmatrix} - (c+d)1_{2\times 2} = \begin{bmatrix} c-d & a+ib \\ a-ib & d-c \end{bmatrix}.$$

Remember that we already have the Hermitian matrix $\hat{S}_z$: it has a number on the top diagonal entry and the opposite number on the bottom diagonal entry. We want $\hat{S}_x, \hat{S}_y$ to be "independent" from $\hat{S}_z$, so we should kill the diagonal terms. This leaves us with just $\begin{bmatrix} 0 & a-ib \\ a+ib & 0 \end{bmatrix}$, which we can rewrite as

$$a\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + b\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},$$

where a and b are real numbers.

Proposition 21

What's funny here is that we can think of Hermitian spaces as **forming a vector space** – adding two Hermitian matrices still gives a Hermitian matrix, and multiplying a Hermitian matrix by a real number still gives us something Hermitian.

So the set of Hermitian matrices is a **real vector space** with four basis vectors:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}.$$

So these four matrices are the "linearly independent Hermitian matrices" – these are quite famous, but let's first finish up our problem. It sounds like we've found two potential matrices for $\hat{S}_x$ and $\hat{S}_y$, but we don't know what the scale factor is. So we need a bit of physics: the eigenvalues of the other two operators should also be $\frac{\hbar}{2}$, because we could have done all of the Stern-Gerlach experiment by thinking of a different direction.

So there are some sign issues – the answer isn't completely unique – but luckily, **everyone uses the same convention** for these matrices $\hat{S}_x, \hat{S}_y$ (though the identities would be preserved if we used slightly different matrices as well). And from here, our attention should turn to **eigenvalues and eigenvectors**. The matrix $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ has two eigenvalues: $\lambda = 1$ for the eigenvector $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\lambda = -1$ for the eigenvector $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$. Similarly, $\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ has $\lambda = 1$ for the eigenvector $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$ and $\lambda = -1$ for $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$. The $\frac{1}{\sqrt{2}}$s here are to make sure our column vectors are **normalized** – their lengths should be 1, where length is defined in terms of the bra-ket inner product. And now that our eigenvalues are ± 1 for these matrices, it's natural to try

$$\hat{S}_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{S}_y = \frac{\hbar}{2} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}.$$

(Multiplying matrices by numbers multiplies the eigenvalues by those numbers as well.) And to check that these indeed work, we check that commutator relations. Let's do an example:

Example 22
What is the commutator of $\hat{S}_x$ and $\hat{S}_y$?

We can pull out the $\frac{\hbar}{2}$ factors to get

$$\frac{\hbar^2}{4}\left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right) = \frac{\hbar^2}{4}\left(\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} - \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}\right).$$

Simplifying this indeed yields

$$\frac{\hbar}{2}\frac{\hbar}{2}\begin{bmatrix} 2i & 0 \\ 0 & -2i \end{bmatrix} = i\hbar\frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = i\hbar\hat{S}_z.$$

And we can double check that the other commutator relations hold, and now we've found our three matrices for our spin states along the x, y, and z directions! These are extremely important, and they're important enough that we have the definition

$$\hat{S}_i = \frac{\hbar}{2}\sigma_i,$$

where the σ_i are the **Pauli matrices**

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

This is enough to give us the answer to almost all experiments we could do with the Stern-Gerlach apparatus! For example, we said that

$$\hat{S}_x \left|x;\pm\right\rangle = \pm\frac{\hbar}{2}\left|x;\pm\right\rangle,$$

but we also already know the eigenstates for this operator! And thus

$$|x;+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} = \frac{1}{\sqrt{2}}\left(|z;+\rangle + |z;-\rangle\right)$$

corresponds to the eigenvector with eigenvalue 1 in σ_1, and

$$|x;-\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} = \frac{1}{\sqrt{2}}\left(|z;+\rangle - |z;-\rangle\right)$$

corresponds to the eigenvector with eigenvalue -1 in σ_1. So these aren't new states that we need to add to the state space – they're linear combinations of the states we already have! (And similarly, this means that we can write $|z;+\rangle$ in terms of $|x;+\rangle$ and $|z;-\rangle$ if we want to.)

So let's return to one of the questions: what happens to a $|z;+\rangle$ state under an x-filter? The overlap of an $|x;+\rangle$ state with the $|z;+\rangle$ is just going to be

$$\langle x;+|z;+\rangle = \frac{1}{\sqrt{2}},$$

and the same number comes up for $\langle x;-|z;+\rangle$. These amplitudes are equal, so the probabilities are indeed $\frac{1}{2}$ each, which is what we want!

And of course, we can construct the y-states in a very similar way: S_y has eigenstates $|y;\pm\rangle$ such that

$$\hat{S}_y\,|y;\pm\rangle = \pm\frac{\hbar}{2}\,|y;\pm\rangle\,,$$

and this will give us

$$|y;\pm\rangle = \frac{1}{\sqrt{2}}\left(|z;+\rangle \pm i\,|z;-\rangle\right).$$

It's very important here that we're working with complex numbers: that's the only way we can get so many linear combinations that are all orthogonal!

So we've described a theory, and our goal will be to expand it now. We're now able to produce a state along the x, y, and z-directions; let's see if we can expand this to producing states along any unit vector $\vec{n} = (n_x, n_y, n_z)$. To make some progress on this question, **consider the triplet of operators** $(\hat{S}_x, \hat{S}_y, \hat{S}_z)$. (We could write this out as $\hat{S}_x\vec{e}_x$ and so on, but that doesn't really make any sense other than as an accounting procedure.) The idea now is to consider the spin operator

$$\hat{S}_{\hat{n}} = \vec{n}\cdot\vec{S} = n_x\hat{S}_x + n_y\hat{S}_y + n_z\hat{S}_z.$$

Indeed, if this vector $\hat{n}$ points in the z-direction, we have $(n_x, n_y, n_z) = (0, 0, 1)$ and we do recover $\hat{S}_z$. A similar thing holds for x and y, so this is the **spin operator in the direction of the vector** $\vec{n}$.

We're going to want $\hat{S}_{\hat{n}}$ to have the same eigenvalues of $\pm\frac{\hbar}{2}$ as our fundamental spin operators: to make that clear, we'll use spherical coordinates

$$n_z = \cos\theta, \quad n_x = \sin\theta\cos\phi, \quad n_y = \sin\theta\sin\phi.$$

Then we can just do some computation:

$$\hat{S}_{\hat{n}} = \vec{n}\cdot\vec{S} = \frac{\hbar}{2}\left(n_x\sigma_1 + n_y\sigma_2 + n_Z\sigma_3\right) = \frac{\hbar}{2}\begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z\end{bmatrix}.$$

And now plugging in the spherical coordinates makes this simplify very nicely: we actually just have

$$\hat{S}_{\vec{n}} = \frac{\hbar}{2}\begin{bmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i}\phi\sin\theta & -\cos\theta \end{bmatrix}.$$

For completeness, let's calculate the eigenvectors and eigenvalues here: remember that in order to find an eigenvalue λ of a matrix A, we solve the equation $\det(A - \lambda I) = 0$. So we want

$$\det\begin{bmatrix} \frac{\hbar}{2}\cos\theta - \lambda & \frac{\hbar}{2}e^{-i\phi}\sin\theta \\ \frac{\hbar}{2}e^{i}\phi\sin\theta & -\frac{\hbar}{2}\cos\theta - \lambda \end{bmatrix} = 0.$$

This turns out to not be very bad – the phases cancel out, and we indeed do get $\lambda = \pm\frac{\hbar}{2}$. But the eigenvectors are more nontrivial: to find an eigenvector in the $\vec{n}$-direction, we need to find vectors $|\vec{n};\pm\rangle$ such that

$$\hat{S}_{\vec{n}}\,|\vec{n};\pm\rangle = \pm\,|\vec{n};\pm\rangle\,.$$

In other words, we want to find a vector $\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$ such that

$$\left(\hat{S}_n - \frac{\hbar}{2}\right)\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0.$$

We can factor out the $\frac{\hbar}{2}$, and what we end up needing to solve is that

$$\begin{bmatrix} \cos\theta - 1 & \frac{\hbar}{2}e^{-i\phi}\sin\theta \\ \frac{\hbar}{2}e^{i}\phi\sin\theta & -\cos\theta - 1 \end{bmatrix}\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0.$$

This gives two equations that relate c_1 and c_2, and they actually tell us the same information (this is exactly the purpose of having our eigenvalues)! Either way, what we find is that

$$c_2 = e^{i\phi}\frac{1-\cos\theta}{\sin\theta}c_1,$$

and we can simplify this by using the half-angle identities on both the numerator and denominator of our fraction. We end up finding that

$$c_2 = e^{i\phi}\frac{\sin\frac{\theta}{2}}{\cos\frac{\theta}{2}}c_1,$$

and if we want a normalized eigenvector with $|c_1|^2 + |c_2|^2 = 1$, it turns out that we need $|c_1|^2 = \cos^2\frac{\theta}{2}$. And it doesn't really matter what phase we choose, so let's keep it simple:

$$c_1 = \cos\frac{\theta}{2}, \quad c_2 = \sin\frac{\theta}{2}e^{i\phi},$$

and we've found our state

$$\boxed{|\vec{n};+\rangle = \cos\frac{\theta}{2}\,|z;+\rangle + \sin\frac{\theta}{2}e^{i\phi}\,|z;-\rangle}.$$

In other words, we've found the spin state that points in the $\vec{n}$-direction as a linear superposition as our basis states! And we can check that setting $\theta = 0$ gives us the z-axis, and this does indeed recover the $|z;+\rangle$ state.

A similar calculation **seems to** tell us that

$$|\vec{n};-\rangle = \sin\frac{\theta}{2}\,|z;+\rangle - \cos\frac{\theta}{2}e^{i\phi}\,|z;-\rangle\,.$$

But now if we take $\theta = 0$, we're supposed to end up with the minus state along the direction of the z-axis, which is the $|z;-\rangle$ state. But now the second term is not so well-defined, because ϕ can be anything! So instead it's better to multiply through by the phase so that

$$\boxed{|\vec{n};-\rangle = \sin\frac{\theta}{2}e^{-i\phi}|z;+\rangle - \cos\frac{\theta}{2}|z;-\rangle}.$$

We've now basically done everything that's possible to do without reviewing linear algebra – that's what we'll do soon.

Fact 23

Notice that $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = 1$, and this actually tells us something about the eigenvalues of these matrices.

In general, if a matrix M satisfies a **matrix equation** like $M^2 + \alpha M + \beta I = 0$, then the eigenvalues also satisfy the same equation. This is because we can let both sides of this equation act on an eigenvector v of eigenvalue λ: notice that $M^2 v = M\lambda v = \lambda^2 v$, so

$$0 = (M^2 + \alpha M + \beta I)v = \lambda^2 v + \alpha\lambda v + \beta v.$$

Since this is true for a eigenvector v, which is defined to be nonzero, we must have $\lambda^2 + \alpha\lambda + \beta = 0$, which is the same equation as we had for our matrix equation!

So what this tells us is that σ_1's eigenvalues satisfy $\lambda^2 = 1$, and thus we have eigenvalues of ± 1. It's possible that they're both 1 or both -1, but now we can use the **trace**: the sum of the diagonal entries of our matrix is also the sum of the eigenvalues! Since this trace is 0, we must have one eigenvalue be 1 and the other be -1, as we calculated earlier.

Let's talk some more about these Pauli matrices now: remember that our spin operators are $\frac{\hbar}{2}$ times the Pauli matrices, and we have the algebra for angular momentum

$$[\hat{S}_i, \hat{S}_j] = i\hbar\varepsilon_{ijk}\hat{S}_k.$$

Plugging in the corresponding Pauli matrices, we find that

$$\boxed{[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k}.$$

It also turns out that there's a nice property with **anticommutators**: we have

$$\sigma_1\sigma_2 = -\sigma_2\sigma_1,$$

so the two matrices actually **anticommute**. We denote this with the anticommutator, and the general form of this identity is that

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}I_{2\times 2}.$$

Since we can write any matrix product as

$$AB = \frac{1}{2}[A, B] + \frac{1}{2}\{A, B\}$$

(by direct expansion), we can plug in the Pauli matrices to find that

$$\boxed{\sigma_i\sigma_j = \delta_{ij}I + i\varepsilon_{ijk}\sigma_k}.$$

To make this look even nicer, we consider the "vector" $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$. Then we can take the dot product with a

vector $\vec{a} = (a_1, a_2, a_3)$

$$\vec{a} \cdot \vec{\sigma} = a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3 = a_i\sigma_i$$

with the repeated index notation. Now, if we multiply the boxed equation above by $a_i b_j$, we find that

$$a_i\sigma_i b_j\sigma_j = a_i b_j \delta_{ij} I + i\varepsilon_{ijk} a_j b_k \sigma_k.$$

And now we can write this in a neater form: we have

$$(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = a_i b_i I + i\varepsilon_{ijk} a_i b_j \sigma_k,$$

and now the right hand side actually have to do with dot and cross products:

$$\boxed{(\vec{a} \cdot \vec{\sigma})(\vec{b} \cdot \vec{\sigma}) = (\vec{a} \cdot \vec{b})I + i(\vec{a} \times \vec{b}) \cdot \vec{\sigma}}.$$

This has now represented a product of Pauli matrices in a geometric way, and this is very useful for doing calculations!

Example 24

Let's say that $\vec{a} = \vec{b} = \vec{n}$ is a unit vector – how does the above equation simplify?

Plugging everything in, we find that

$$(\vec{n} \cdot \vec{\sigma})^2 = 1.$$

This is useful, because it makes it easier for us to understand the operator $\hat{S}_{\vec{n}}$ from last time (which we defined to be $\vec{n} \cdot \vec{S} = \frac{\hbar}{2}\vec{n} \cdot \vec{\sigma}$). If we square this, we end up with $\left(\frac{\hbar}{2}\right)^2 I$. Note that the **trace of the $\vec{S}_n$ operator is also zero** – this is because we're adding a linear combination of $\sigma_1, \sigma_2, \sigma_3$, which are all traceless – and thus by the same argument, we know that the eigenvalues of the matrix $\hat{S}_{\vec{n}}$ have to be $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$. We didn't need to calculate the eigenvalues directly!

And this is fundamental because we've now discovered a **key property** of spin: if we measure it along any arbitrary direction, we'll always find $\frac{\hbar}{2}$ or $-\frac{\hbar}{2}$. (And this makes sense – the universe is isotropic, so the direction should not matter here.)

We'll finish with a bit of an aside: if we have two triplets of **operators** $\vec{X} = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$ and $\vec{Y} = (\hat{y}_1, \hat{y}_2, \hat{y}_3)$, we can define their dot product

$$\vec{X} \cdot \vec{Y} = \hat{S}_i \hat{Y}_i,$$

where we sum over i. (Such a dot product may not commute, because operators don't always commute.) And we can similarly define the cross-product

$$(\vec{X} \times \vec{Y})_k = \varepsilon_{ijk} \hat{X}_i \hat{Y}_j,$$

just like we do with number-valued vectors. Again, this cross product does not need to satisfy the same properties as the normal cross product – even $\vec{X} \times \vec{X}$ may be nonzero! So one thing we'll be asked to compute is the value of $\vec{S} \times \vec{S}$ – it'll be an interesting result.

4 February 5, 2020

We'll talk a bit about the axioms of quantum mechanics today, which will be pretty important for us in connection with the 8.051 material. And we'll do some practice with the variational principle as well.

As a reminder, lecture questions are due 9 am before every Monday and Wednesday (except for today). We'll be moving now into spin 1/2, and there's the issue of manipulating indices – we should watch the index manipulation video if we haven't worked with this before. Starting next way, there will be a lot of emphasis on linear algebra.

Fact 25

Tentative office hours have been announced (Wednesday 11-12 and Thursday 1:30-2:30).

Here are the axioms of quantum mechanics:

- States exist. A **state** is a **complete** description of a physical system, and it is a **ray** in Hilbert space.

A Hilbert space is a complex vector space – it does not mean the vectors are complex numbers, only the scalars! Geometrically, a **ray** in Hilbert space represents a one-dimensional subspace (the collection of all vectors along a specific line), because ψ and $c\psi$ represent the same state for any complex number c. But we'll mostly work with normalized wavefunctions, so we'll pick c so that our vectors have length 1.

We'll talk more about Hilbert spaces later, but one important thing is that there is an **inner product**

$$(\phi, \psi) \in \mathbb{C}$$

which satisfies the properties

$$(\phi, \phi) \in \mathbb{R}_{\geq 0}, \quad (\phi, \phi) = 0 \implies \phi = 0.$$

This means that the norm

$$||\phi|| = \sqrt{(\phi, \phi)}$$

of any state is nonnegative (and only zero if ϕ itself is zero). One last important property is that $(\phi, \psi) = (\psi, \phi)^*$ (conjugates of each other). Hilbert spaces can be finite-dimensional or infinite-dimensional, and the latter makes things a bit more difficult to work with.

- Observables exist. An **observable** is a Hermitian operator, meaning that $A^\dagger = A$.

We'll discuss the **spectral theorem** later in this class, which is important: **eigenstates of Hermitian operators give an orthonormal basis for the Hilbert space!** Basically, we can write any such operator in a finite-dimensional vector space of dimension N as

$$A = \sum_{n=1}^{N} a_n E_n,$$

where a_n are actually the eigenvalues of A and E_n are called the **orthogonal projectors**. (A projector P satisfies $P^2 = P$.)

- Measurement postulate. Measurement of an observable A results in the system becoming an **eigenstate** of A.

We'll end up in a new state

$$\frac{E_n \psi}{||E_n \psi||}$$

for some fixed n (though we don't know what n is). Remember that E_n is a **projector**, so it moves us to an eigenstate, and then the denominator normalizes us to unit norm. One important note is that the probability that A measure a_n (the eigenvalue for E_n) is the **inner product** $(\psi, E_n \psi)$.

This is a shocking admission that we can't really know things in quantum mechanics! Supopse we throw linearly polarized photons into a polarizer at an angle. Then some fraction of the photons will go through, but who decides

which ones go through and which don't? There seems to be some irreducible unpredictability in the universe, which people have trouble with.

- Dynamics. The evolution of any state ψ **in time** is governed by a unitary operator $\mathcal{U}(t)$

$$\psi(t) = U(t)\psi(t=0).$$

(A unitary operator is an operator that preserves lengths of vectors.) We'll see in a few weeks that even though we know the Schrödinger equation governs dynamics, this postulate alone is actually enough to show where the equation $i\hbar\frac{\partial\psi}{\partial t} = H\psi$ comes from (we'll build H from $\mathcal{U}$ – it's Hermitian and has units of energy).

- Composite systems. Say we have two quantum systems A and B in Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ – if we want to describe the two systems together, we live in the **tensor product** $\mathcal{H}_A \otimes \mathcal{H}_B$.

No one has found a logical problem or experimental situation that has contradicted these axioms yet, and so discussions and attempts at interpretation have been ongoing – no good consensus has been found yet!

We'll finish today by briefly talking about the variational principle:

Proposition 26 (Variational principle)
If we know the Hamiltonian H for a system, we can use **any** normalized trial wavefunction $\psi(\vec{x})$. Then the ground state energy satisfies

$$E_{gs} \leq (\psi, H\psi).$$

(Equality holds when ψ is the ground state eigenstate.)

So we can try better and better trial wavefunctions and get better and better bounds for the energy ground state! The proof is fairly nice, and there are generalizations that will be explored soon.

5 Linear Algebra – Vector Spaces and Operators, Part 1

We'll be doing linear algebra slightly differently from how it's been done in 8.05 in the past: MIT uses a book called **Linear Algebra Done Right** (by Sheldon Axler) for the 18.700 linear algebra class. It's a bit difficult to learn things this way if we haven't heard of a matrix or determinant or eigenvalue before, but the book is a very nice way of learning if we've heard those words before!

Fact 27
We need to study this book pretty seriously if we want to grab the results that we want out of it. This is because the book builds up from **basic properties** and develops theorems and ideas in a logical progression.

So we'll be introducing linear algebra in the same way in this class – it's not too clear how much detail we'll need, but we'll try to make the main points about **structure in a vector space** clear. Otherwise, we might miss some important basic ideas! (For example, many physicists don't quite realize that in the matrix representations, we don't need bras and kets. And also, there is a big difference between a real and complex vector space, which is a detail that we might miss otherwise.)

We'll begin by talking about **vector spaces and dimensionality**. Throughout this part of the class, we should remember that the **end result** is a vector space of states in our physical system, where observables are linear operators. So we'll need to understand all of those individual properties to make some more progress.

In a **vector space**, we have two kinds of objects: **numbers** and **vectors**. If the numbers are real (resp: complex), we have a real (resp: complex) vector space. (Vectors aren't "real" or "complex" or anything like that.) There are two key operations: we can add vectors, and we can multiply vectors by numbers.

It turns out that the set of numbers we'll be using in this class, often either the real numbers $\mathbb{R}$ or complex numbers $\mathbb{C}$, form a **field**. We won't define what this is, but we'll use the notation $\mathbb{F}$ to denote either kind of field. Let's now set up our formal definition:

Definition 28

A **vector space** V is a set of vectors equipped with an **addition** operation $+$, which takes in two vectors $u, v \in V$ and gives us a vector $u + v \in V$. We also have a **scalar multiplication** operation by elements of $\mathbb{F}$, such that $av \in V$ for any $a \in \mathbb{F}$ and $v \in V$. In addition, these operations must follow the **axioms** defined in Definition 29.

Here, the vector space is **closed** under addition: we can't get out of it if we just keep adding vectors. (And similarly, it's also closed under scalar multiplication.)

Definition 29 (Vector space axioms)

A vector space V must satisfy the following properties:

- $u + v = v + u$ (addition is commutative) and $u + (v + w) = (u + v) + w$ (addition is associative) for any $u, v, w, \in V$.
- $a(bv) = (ab)v$ for any $a, b \in \mathbb{F}$ and $v \in V$.
- There is an **additive identity** $0 \in V$ such that $v + 0 = v$ for all $v \in V$, and a **multiplicative identity** $1 \in \mathcal{F}$ such that $1 \cdot v = v$ for all $v \in V$.
- **Additive inverses** exist: for any $v \in V$, there is a $u \in V$ such that $u + v = 0$.
- We have **distributivity** between multiplication and addition: $a(u + v) = au + av$ and $(a + b)v = ab + bv$ for $a, b \in \mathbb{F}$ and $u, v \in V$.

Remark 30. *There can often be a bit of confusion between the* 0 *number and the* 0 *vector, so we should watch out for that.*

This seems like a lot of properties, but it's a good set of "minimal requirements" – from this, we can show lots of things with little proofs pretty immediately. Here's a quick example:

Lemma 31

The additive identity $0 \in V$ is unique.

Proof. Suppose there were two zero vectors $0, 0'$. Then $0 = 0 + 0' = 0'$, so we must have $0 = 0'$. □

Similarly, we can show that $0v = 0$ for any vector v. Here, we should be careful – the 0 on the left side is in $\mathbb{F}$, and the 0 on the right side is in V. We can also find that $a0 = 0$ and so on: basically, the zero vector and zero number do exactly what we expect them to do.

It also turns out that the additive inverse of v, which we denote $-v$, is unique and is equal to $(-1) \cdot v$. This might seem silly, but it's worth trying to prove them – these results are not completely trivial!

Let's do a few examples: the main thing to keep in mind is that **vectors are not real or complex**.

Example 32

The N-component vectors $\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix}$, with all entries $a_i \in \mathbb{R}$, form a vector space over $\mathbb{R}$ (a real vector space).

We have to think for a second to see if we believe all of the axioms for vector spaces here, but the definition of addition and multiplication are pretty easy: we just do everything component-wise. And then it's easy to find the zero vector – it's just the one with all components 0 – and the additive inverse – it's where we take the negative of each entry. So if we understand addition and multiplication, the rest is not too difficult.

Example 33

The $M \times N$ matrices with complex entries, $\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{M1} & a_{M2} & \cdots & a_{MN} \end{bmatrix}$, form a complex vector space.

Addition and multiplication also look pretty familiar here, because everything is done entry by entry again.

Example 34

The set of 2×2 Hermitian matrices form a **real** vector space.

This might look a bit surprising, because Hermitian matrices have is in the entries: remember that the most general matrix looks like $\begin{bmatrix} c+d & a+ib \\ a-ib & c-d \end{bmatrix}$, where a, b, c, d are real numbers. The reason that we must have a real vector space is that multiplying by complex numbers doesn't preserve Hermiticity (for instance, multiplying by i is not allowed). So this might feel a bit weird: something like $\begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$ is a vector over the real numbers!

Example 35

The set of all **polynomials**, each of the form $p(z) = a_0 + a_1 z + \cdots + a_n z^n$ for $a_i \in \mathbb{F}$ and some nonnegative integer n, form an $\mathbb{F}$-vector space.

To verify this, note that we sum polynomials by combining terms of the same exponent, and we multiply a polynomial by a number by multiplying each term by a number. (And we don't need to worry about multiplying two polynomials together, because that's not a thing we need to do with this vector space.)

This vector space looks like it is **infinite dimensional**: we have the constant, linear, quadratic, cubic, quartic polynomials, and so on. And we'll soon see that this is indeed the case.

Example 36

The set of infinite sequences $\mathbb{F}^\infty = (x_1, x_2, \cdots)$ (where $x_i \in \mathbb{F}$) is an $\mathbb{F}$-vector space.

Addition and multiplication are defined the same way as we usually do.

Example 37

The set of complex-valued functions $f(x)$ on an interval $x \in [0, L]$ is a complex vector space.

These last three examples seem to be infinite dimensional, and now we're going to try to formalize the ideas around that. We'll start by understanding the concept of a subspace:

Definition 38

A **subspace** of a vector space V is a subset W of the vectors of V in which W is also a vector space.

There are some conditions that are necessary for such a subspace to exist: it must contain the **zero vector**, because every vector space has a zero vector. In general, we also need to check that our subspace is closed under vector addition and scalar multiplication – the extra axioms will automatically follow, because W is just a subset.

Example 39

Let's consider a two-dimensional real vector space $V = \mathbb{R}^2$: vectors here can be written as (v_1, v_2), where $v_1, v_2 \in \mathbb{R}$. Consider the subset W of vectors where $3v_1 + 4v_2 = a$ for some real number a.

When is such a collection of vectors a subspace? First of all, W must contain the zero vector $(0, 0)$, so $3{\cdot}0+4{\cdot}0 = 0$ – this means W is **only a subspace** if $a = 0$. And now we just need to check the closure properties, and those are pretty easy. For example, if we have a vector $(v_1, v_2) \in W$ and we multiply by λ, then $(\lambda v_1, \lambda v_2)$ is indeed in W, because

$$3(\lambda v_1) + 4(\lambda v_2) = \lambda(3v_1 + 4v_2) = 0$$

by the assumption that (v_1, v_2) is in W.

So once we have the concept of a subspace, we might ask whether we can understand a large, complicated vector space by just understanding its subspaces? The answer is yes, and the main idea is to "break up the space" as much as possible. Our goal is to fill up the full vector space with a bunch of different subspaces, and this will become much more important when we talk about eigenvectors and eigenvalues later!

Definition 40

A vector space V is a **direct sum** of subspaces $U_1, \cdots, U_m$, denoted

$$V = U_1 \oplus U_2 \oplus \cdots \oplus U_m,$$

if any vector in v can be written uniquely as a sum $u_1 + u_2 + \cdots + u_m$, where each $u_i \in U_i$.

One way to think about this decomposition is that picking a vector in V is equivalent to picking a unique representative $u_1, \cdots, u_m$ from each of the subspaces $U_1, \cdots, U_m$. So one important property is that **the vector spaces cannot overlap** except at the zero vector: we must have

$$U_i \cap U_j = \{\vec{0}\}$$

for all $i \neq j$. It's worth thinking through why this is true, but the basic idea is that any vector that is in both U_i and U_j could be put in either one, and we would not have a unique way of writing down v as a sum $u_1 + \cdots + u_m$. (Then we would have a **sum**, but not a **direct sum**.)

Example 41

Let's look at the subspaces of $V = \mathbb{R}^2$.

We have a two-dimensional subspace, and there's no way to get a two-dimensional subspace of V other than the whole space itself – we can convince ourselves that we need the rest of the space if we have two vectors in different dimensions. So the only other subspaces are one-dimensional, which are just **lines through the origin**, and zero-dimensional, which is **just the zero vector**. Indeed, lines are subspaces, because adding two vectors on the line gives us another on the line, and so does scaling a vector by a real number.

So now let's pick U_1 to be the "horizontal" axis and U_2 to be the "vertical" axis in $\mathbb{R}^2$: both of these are one-dimensional subspaces. And indeed, every vector in $\mathbb{R}^2$ can be written uniquely as a sum of a horizontal part and a vertical part, so we have

$$\mathbb{R}^2 = U_1 \oplus U_2.$$

But we can change things a little bit: instead of using the vertical axis U_2, let's use the subspace of vectors (v_1, v_2) where $v_1 = v_2$, which is a "diagonal line" U_2'. This is a little bit more complicated, but the **parallelogram law** tells us that we can indeed decompose any vector in $\mathbb{R}^2$ as a sum of a vector in U_1 and a vector in U_2', so we again have

$$\mathbb{R}^2 = U_1 \oplus U_2'.$$

In general, **any two lines through the origin** (that don't coincide) will direct sum to $\mathbb{R}^2$, but if we try to add in a third line, we will no longer get a unique representation of a vector in $\mathbb{R}^2$. So this is the first step to understanding the concept of dimension – we can't have three lines that direct sum to $\mathbb{R}^2$, and indeed we're now going to figure out why we can call $\mathbb{R}^2$ two-dimensional.

Remark 42. *This kind of logic will be necessary for understanding dimensionality better in more complicated vector spaces. For example, the space of states for a particle in a central potential is infinite-dimensional, but we can break it down into easier-to-understand subspaces to talk about the evolution of the wavefunction!*

To understand dimension, we're going to introduce a few more concepts for rigor, so that we can also talk about infinite-dimensional vector spaces. Consider a **list of vectors**, which is just a list $(v_1, \cdots, v_n)$ (which must be of **finite length**) where $v_1, \cdots, v_n \in V$. Then there's a few useful concepst we can extract:

Definition 43

The **span** of a list of vectors $(v_1, \cdots, v_n)$ is the set of linear combinations of the form

$$a_1 v_1 + a_2 v_2 + \cdots + a_n v_n, \quad a_i \in \mathbb{F}.$$

A list **spans** the vector space if the span of the list is the whole vector space.

This is basically the set of vectors that we can reach by taking some combination in our list.

Definition 44

A vector space V is **finite-dimensional** if it's spanned by some list of vectors. (Otherwise, it is **infinite-dimensional**, which means no list spans the whole space.)

This definition has been made in a nice way so that we can work with it:

Proposition 45

The space of polynomials is infinite-dimensional.

Proof. Suppose otherwise; then there is a list of polynomials that spans our space. But because we have a finite list, there is some highest degree (perhaps $z^{1000000}$) in all of our polynomials. And then we can't use a linear combination of our polynomials to get anything of higher degree (say $z^{2000000}$), which is a contradiction. Thus the space must be infinite-dimensional. □

Proposition 46

In contrast, our first example – the set of N-component vectors – is finite-dimensional.

Proof. We just need to produce a list that spans the whole space: we just use

$$e_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad e_2 = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \cdots, e_N = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}.$$

And then a general vector is just of the form $a_1 e_1 + a_2 e_2 + \cdots + a_N e_N$. □

Definition 47

A list of vectors $(v_1, v_2, \cdots, v_n)$ is **linearly independent** if

$$a_1 v_1 + a_2 v_2 + \cdots + a_n v_n = 0$$

only has the solution $a_1 = a_2 = \cdots = a_n = 0$.

In other words, if we want to represent the zero vector with our list, we have to set all of the coefficients to 0.

Definition 48

A **basis** of a vector space V is a list of **linearly independent** vectors which **spans** V.

Basically, we need to have enough vectors to span all of V, but we shouldn't have any "extra vectors" that just give us redundant information.

It turns out that **any finite dimensional vector space has a basis** – this is easy to show – and also that **any two bases have the same length**. So the length is some quantity independent of our basis, and that's what we'll call our dimension:

Definition 49

The **dimension** of a vector space V is the length of any basis of V.

Remark 50. *At the moment, we don't have an inner product on our vector space yet: we're putting the least amount of structure that is necessary. There's a lot of properties that we can already extract without needing an inner product!*

So returning to the example above where we created a list that spans our vector space, this list is also linearly independent: each entry needs to be 0, so all a_is are zero. Thus **the space of N-component vectors has dimension N.** Similarly, we can prove that the space of $M \times N$ matrices has dimension MN.

Example 51

Let's find the dimensionality of the space of Hermitian matrices.

We'll use the following list of four "vectors:"

$$(I, \sigma_1, \sigma_2, \sigma_3).$$

This is indeed a list of vectors in our space, because all four of these matrices are Hermitian. It also spans our space by an argument we made earlier on – we can get $\begin{bmatrix} c+d & a+ib \\ a-ib & c-d \end{bmatrix}$ with the linear combination $cI + a\sigma_1 + b\sigma_2 + d\sigma_3$. And to show that this list is linearly independent, we just set our matrix to 0: then we need $c + d = c - d = 0$, so $c = d = 0$, and we also need $a + ib = a - ib = 0$, so $a = b = 0$. So indeed, we have a linearly independent list which also spans, and thus **the vector space of Hermitian matrices has dimension 4.**

Remark 52. *We can try proving that the space $\mathbb{F}^\infty$ of infinite sequences is infinite-dimensional: it requires a bit of work!*

We'll now move on to something else: we want to talk about **linear maps** from a vector space V to another vector space W. A special case of these is a **linear operator**, where we map from V to the vector space V again.

Definition 53

A **linear operator** T on a vector space V is a function $T : V \to V$ with the properties

$$T(u+v) = T(u) + T(v), \quad T(av) = aT(v)$$

for any $u, v \in V$ and $a \in \mathbb{F}$.

The quantum mechanical motivation for this is that **observables are represented by operators**: expectation values, symmetries, and unitary time-evolution all come from these linear operators.

It's important for us to realize that $T(u) = Tu$ (both notations are okay) is a **vector** which is in the image of our linear operator. In some sense, we can think of T as doing some kind of multiplication – Tu is basically matrix multiplication on a vector!

The key idea here is that we only need to know how the linear operator works on basis vectors, and that gives us everything we need to know about the operator! This is because every vector can be obtained by putting together a linear combination of the basis vectors, the "linearity" of the linear operator tells us the value of $T(v)$ for all other vectors.

Lemma 54

We have $T(\vec{0}) = \vec{0}$ for any linear operator T.

Proof. We know that

$$T(u) = T(u + \vec{0}) = T(u) + T(\vec{0})$$

for any vector u, and now subtracting $T(u)$ from both sides yields $T(\vec{0}) = 0$. (We're allowed to subtract because that's basically adding the additive inverse!) □

The best way to understand such operators is to give some examples, so that's what we'll do now.

Example 55

Let V be the real vector space of polynomials on a real variable x – that is, vectors are real polynomials $p(x)$. Define the **derivative operator** T which sends a polynomial p to its derivative: $T(p) = p'$. Also define the operator S which multiplies a polynomial by x: $S(p) = xp$.

It's indeed true that the derivative of a sum is the sum of the derivatives, and also that we can "take out" constants from a derivative. So T is indeed a linear operator! Similarly, we can check that S is linear by distributivity.

Example 56

Consider the vector space of infinite sequences $\mathbb{F}^\infty$ of the form $(x_1, x_2, x_3 \cdots)$. Define the **left shift** operator L, which sends such a sequence to $(x_2, x_3, x_4, \cdots)$, and similarly define the **right shift** R which sends the sequence to $(0, x_1, x_2, \cdots)$.

We should try writing out the properties: indeed, L and R are both linear operators if we check all of the properties. But it's very important that we need to put the number 0 in the first spot for the right shift R, or else we wouldn't have a linear operator!

Remark 57. *This is tangentially related to the famous Hilbert's Hotel problem – doing a right shift opens up a room.*

L and R look a little bit like inverse operators, but they're not quite the same: we lose information about x_1 when we do a left shift.

Example 58

These are the "trivial operators:" the **zero operator** sends everything to the zero vector, and the **identity operator** sends a vector to itself.

The main idea here is that even though our linear operator sends V to itself, it doesn't have to be one-to-one! And the zero operator is just an extreme case of this where everything is sent to the same vector in V.

6 February 10, 2020

Hopefully we're starting to get accustomed to the pace of this class – it's a bit fast, especially at the beginning, depending on how much we remember from previous classes. So there's quite a bit that we need to remember about bound states and the Schrodinger equation and square wells, but some of us might have just not seen very much of this. We've had a few ideas introduced – spin 1/2, the variational principle, and now we have about a two-week mathy interlude where we're talking about linear algebra so that we can do physics precisely.

Some people have said that in 8.05, there's too much math. It's a valid viewpoint, but that criticism sometimes comes from other faculty that already understand quantum mechanics – math just didn't play much of a role in their understanding. Professor Zwiebach, though, felt that some parts of his understanding remained fuzzy until he had the mathematical formalism. So there might be a 10 percent excess of math, but it will be necessary to help us think about projectors, measurements, tensor products, and so on. And with the ideas of quantum information, linear algebra's role has become even more important!

Fact 59

Lectures 1 and 2 were never due – we have to do them, but there is no associated deadline. But lecture 3 questions were due today (at 9am) – if we were confused about due dates or had trouble, we should let the 8.051 team know. (And there's lecture 4 questions due on Wednesday and pset 1 due on Friday.)

Questions are graded for accuracy, but don't agonize over grading. These are supposed to help us understand the material.

The homework has a lot of parts, so we should get started early on. The advantage of this homework is that it's all based on 8.04 and last week's material. On our first problem set, there's a variational problem where we have a quartic potential

$$H = \frac{p^2}{2m} + \alpha \hat{x}^4.$$

If the quartic were a quadratic term, it would be a simple harmonic oscillator and we'd know how to solve it. But with this new potential (α assumed to be positive, by the way), we get a strange oscillator which doesn't even have the usual harmonicity. With the harmonic oscillator, the energy levels are equally separated and multiples of the lowest energy, which tells us that frequencies are also multiples of each other. But adding a quartic term breaks the harmonicity – energy levels will not be multiples any more.

Is that good or bad? It turns out that for quantum computation, harmonic oscillators are not good – $|0\rangle$ and $|1\rangle$ usually take up the lowest two energy levels, but the energy difference between those two is the same as the difference to the next energy level! So the qubit will not be in the $|0\rangle$ or $|1\rangle$ state anymore, which is bad – that's one motivation for why we study different potentials like in this homework problem.

If the Hamiltonian had a harmonic oscillator term

$$H = \frac{p^2}{2m} + \alpha \hat{x}^4 + \frac{1}{2} m\omega^2 \hat{x}^2,$$

the $\hat{x}^4$ term would be a small correction to the harmonic oscillator potential, and then we calculate things using **perturbation theory** (this is an 8.06 idea). But for our original problem, we need to use variational methods – the differential equation can't be solved analytically. We'll need to calculate some of the energy eigenstates numerically, and we do this with the **shooting method**.

Specifically, we're trying to solve the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V(x)\Psi = E\Psi,$$

and we want to first get rid of the $\hbar, m, \alpha$ before plugging this into a computer (because the energies depend on those quantities in a predictable way). Once we do this, we integrate the differential equation from 0 to some distance, exxpressed in **dimensionless units** u – for example, we can integrate from 0 to 3.5 and that's probably enough – and there are Mathematica instructions on how to do this in the pset PDF.

Fact 60

Energy eigenstates are normalizable, so we can tweak the parameters and look at when the wavefunction "blows up" or "blows down" and look in between those.

Question 61. *On Piazza, there was a question about the axioms of vector spaces – our lecture has the axiom $1v = v$ (for all vectors v in the vector space), but Shankar doesn't have this. So what's going on here?*

Mathematical objects called **fields** have two special numbers, 0 and 1. They're the additive and multiplicative

identity, respectively: this means that $a+0=a$ and $1a=a$ for any $a \in F$. With this, it's also simple to show that $0 \cdot a = 0$, so we don't need this as an axiom.

Well, the statement $1v = v$ is completely different, because v is a vector, not an element of our field $\mathbb{F}$! We can try to prove this statement from the other axioms, but it really doesn't work out – the best hope is to try using $(ab)v = a(bv)$, and that isn't enough. So we need to include it in our set of linear algebra axioms. The main point here is that **we need to keep vectors and scalars separate in our mind**.

We can, however, prove that $0 \cdot v = 0$, where the 0 on the left side is a **scalar** and the 0 on the right side is the zero **vector**. So we can think about all of this a bit more if we like the mathematical formalism.

Let's do some examples with the variational principle:

Example 62

Consider two potentials $V_1(x)$ and $V_2(x)$ which satisfy $V_2(x) \leq V_1(x)$ for all x. Can we show that the ground state energy for V_2 is always lower than the ground state energy for V_1?

The intuition we have is that "the energy is always higher for V_1," and while this might seem clear, it gives us the following result. Consider an **attractive potential** $V(x)$ which is bounded – specifically, it's nowhere positive, piecewise continuous, asymptotically zero, and not zero everywhere. Then there's a famous result that V always has a bound state – this is true in one dimension but not in three dimensions!

How do we show that? We can try to find the bound state, but if V is an arbitrary potential, this is very difficult. Instead, we can just "sandwich" a finite square well potential between $V(x)$ and 0 – since the finite square well potential has a bound state, this example problem would tell us that the attractive potential $V(x)$ has a bound state (with lower energy).

Okay, so let's try to show that the ground state energies satisfy $E_2^{gs} \leq E_1^{gs}$. We have our two Hamiltonians

$$H_1 = \frac{p^2}{2m} + V_1(x), \quad H_2 = \frac{p^2}{2m} + V_2(x),$$

and consider the overlap

$$(\psi, H_1\psi), \quad (\psi, H_2\psi).$$

Both of these are numbers – they're the inner products $(\psi_1, \psi_2) = \int \psi_1^* \psi_2 dx$ – and specifically, because

$$(\psi, H_1\psi) = \boxed{\left(\psi, \frac{p^2}{2m}\psi\right)} + \int \psi^* V_1 \psi \geq \boxed{\left(\psi, \frac{p^2}{2m}\psi\right)} + \int \psi^* V_2 \psi = (\psi, H_2\psi)$$

(after all, the boxed $\frac{p^2}{2m}$ terms cancel out, the left integral is $\int V_1(x)|\psi|^2$, and the right integral is $\int V_2(x)|\psi|^2$), we have

$$\boxed{(\psi, H_1\psi) \geq (\psi, H_2\psi)}.$$

So now we want to use this to look at the energy ground states: the variational principle says that

$$E_2^{gs} \leq (\psi, H_2\psi) \leq (\psi, H_1\psi).$$

Remember that this holds for **any** ψ, so we can now pick ψ to be the ground state wavefunction for V_1! And that tells us that

$$E_2^{gs} \leq (\psi_{gs,1}, H_1\psi_{gs,1}) = E_1^{gs},$$

and we've indeed shown that the ground state energies are related in the way that we expect – the lower potential has a lower energy ground state.

In the remaining time, we'll talk a bit about the concept of a **direct sum** in linear algebra. Recall that a vector space V is the direct sum

$$V = V_1 \oplus V_2$$

if we can write any vector V **uniquely** as a vector in V_1 plus a vector in V_2. One way we can think about this is that we're **increasing the dimension of the vector space by adding more axes**. In principle, the first vector space V_1 has some basis vectors, and V_2 adds some more – the total dimension

$$\dim V = \dim V_1 + \dim V_2.$$

(Soon, we'll consider the other operation $V = V_1 \otimes V_2$, in which case the total dimension

$$\dim V = \dim V_1 \cdot \dim V_2.)$$

One note – just because $V_1 \oplus V_2 = V_1 \oplus V_3$, this doesn't necessarily mean that $V_2 = V_3$. (For example, if V_1 is the x-axis, V_2 can be the y-axis and V_3 can be the line $y = x$, and both sides give us the xy-plane.)

So as an example, the energy eigenstates provide a basis for the whole space in the simple harmonic oscillator. We have a vector $|0\rangle$, the ground state, and we have another vector $|1\rangle = a^\dagger|0\rangle$, the first excited state – in general, we have

$$|k\rangle = \frac{(a^\dagger)^k}{\sqrt{k!}}|0\rangle,$$

defined in such a way that these are all orthonormal. Well, let U_0 be the 1-dimensional vector space which is the span of $|0\rangle$, let U_1 be the span of $|1\rangle$, and define U_k in general. Then what we're saying is that the whole state space

$$\mathcal{H} = U_0 \oplus U_1 \oplus U_2 \cdots = \bigoplus_{k=0}^{\infty} U_k.$$

And this is true because the general wavefunction is a linear combination (unique superposition) of our energy eigenstates – we can write

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle + \cdots.$$

7 Linear Algebra – Vector Spaces and Operators, Part 2

Now that we've begun to see a few properties and examples of linear operators, let's try to extract some structure out of the **set of linear operators**.

Definition 63

For a vector space V, let $\mathcal{L}(V)$ denote the set of linear operators on V.

It turns out that this set actually forms a **new vector space**! This is because we can take two operators $S, T \in \mathcal{L}(V)$ and define their sum $S + T$, which is the operator satisfying

$$(S + T)v = Sv + Tv.$$

Similarly, we define a scalar multiple of a linear operator by defining that

$$(aS)v = a \cdot (Sv).$$

With this definition, we already have all of the properties that we need in a vector space for our linear operators: we just need to check that $S+T$ and aS are indeed linear operators by confirming statements of the form

$$(S+T)(u+v) = (S+T)u + (S+T)v,$$

but it all works out. In addition, we do have an additive operator – it's the zero operator. So $\mathcal{L}(V)$ is a new vector space that we've created, and it's over the same field $\mathbb{F}$ as our vector space V.

Remember that in all of our definitions so far, there hasn't been an obvious way to multiply vectors together. We know that there's a cross product in three dimensions for our ordinary vectors, but there is no such thing in two or four dimensions. On the other hand, these operators have a very natural multiplication: for two operators S and T, define their product via

$$(ST)u = S(Tu).$$

In other words, we let T act on our vector first, and then apply S to the result of that. This is a new structure we've added to our vector space! We now need to show that ST is indeed a linear operator – it's pretty simple to verify, but it's worth working it out on our own. And the point now is that we can **multiply operators**.

There are now a few questions we can ask: is this multiplication commutative or associative, and is there an identity or inverse element?

- It turns out that associativity is true: this is because $S(TU) = (ST)U$ holds for any three linear operators S, T, U, and in both cases we just apply U, then T, then S to our vector.
- There is an identity element: it's the identity operator, which sends every vector to itself. Call this operator I.
- Operators do not always have inverses (for example, consider the zero operator).
- Finally, operators are not always commutative (ST and TS are not always the same).

This last point is pretty important for quantum mechanics, and it'll relate to the concept of a **commutator**, which measures the difference between the two operators AB and BA. Basically, we define the quantity

$$[A, B] = AB - BA,$$

and this can often have important physical implications.

Let's study an illustrative example:

Example 64

Consider the two operators from before on our vector space of polynomials: T differentiates the polynomial, and S multiplies it by x.

The product of T and S is some linear operator, which we can't figure out until we see how it acts on a polynomial. We can try to have it act on a general polynomial, but we don't need to do that: acting on the simple **basis elements** is enough. So let's apply this on x^n:

$$TS(x^n) = T(x^{n+1}) = (n+1)x^n.$$

On the other hand, we can also look at the other way around: we evaluate the product ST to be

$$ST(x^n) = S(nx^{n-1}) = nx^n.$$

Indeed, TS and ST are not the same, and the commutator $[T, S] = TS - ST$ is an operator such that

$$[T, S]x^n = (TS - ST)x^n = (n+1)x^n - nx^n = x^n.$$

In other words, the commutator $[T, S]$ is actually the identity operator I, because we can repeat this argument for any x^n! And this commutation relation has to do with the usual quantum mechanics commutation relation between $\hat{x}$ and $\hat{p}$, which are indeed multiplication by x and an x-derivative (up to constant factors).

So in summary, we've now put an extra structure on our linear operators. As a nice exercise, we can try computing the commutator $[L, R]$ between the left and right shifts on our interesting sequences.

With that out of the way, we'll now move on to some more linear algebra: we're going to extract a few more basic properties out of our operators. There's always a few basic questions to ask when we encounter a new object, and in this case knowing these answers tells us a lot about the linear operator!

There are basically two ways to characterize our linear operators $T \in \mathcal{L}(V)$, related to **injectivity** and **surjectivity**, respectively.

Definition 65

The **null space** of a linear operator T is the set of vectors $v \in V$ such that $T(v) = 0$.

These are the objects that are being "nullified" by T, and it turns out this set of vectors is a **subspace of** V! So there's a bit more here than just having a set of vectors. Indeed, we can check that if $u, v \in \text{null}(T)$, then $u + v \in \text{null}(T)$ as well, and so is au. This is closely related to the next definition here:

Definition 66

A linear operator T is **injective** or **one-to-one** if different vectors end up in different places under T: that is, if $T(u) = T(v)$, then $u = v$.

But there might be a more useful way of representing this idea: "one-to-one" might not represent injectivity very well, because of course T takes in a vector and outputs another vector. So Sean Carroll, a professor at Caltech, has suggested using the word "two-to-two" instead. Indeed, another way to phrase the above idea is that

$$u \neq v \implies T(u) \neq T(v).$$

So let's take the two definitions we've just made and link them together:

Theorem 67

A linear operator T is injective if and only if $\text{null}(T) = \{\vec{0}\}$.

We know that the null space always contains the zero vector, and this theorem says that injectivity forces that to be the entire null space!

Proof. We need to show both directions here. If T is injective, then for any vector u in the null space, $T(u) = T(\vec{0})$ implies that $u = \vec{0}$. And thus the only vector that can be in the null space is $\vec{0}$, as desired.

On the other hand, suppose that we know that the null space is just the zero vector. Then

$$T(u - v) = \vec{0} \implies u - v = 0,$$

because $u - v$ is in the null space. But now $T(u - v) = T(u) - T(v)$, so we can restate the above statement as

$$T(u) = T(v) \implies u = v,$$

which is indeed the definition of injectivity. □

With this, we've now related the words "null space" and "injective," and it's clear how the two are related.

Definition 68

The **range** of a linear operator T is the set of vectors of the form Tv, where $v \in V$.

Basically, we try applying T to everything, and we see which vectors we get. This set of vectors again has some additional structure: **it is also a subspace of V!** This requires a little bit of thinking: if two vectors u', v' are in the range of T, then there are vectors u, v such that $T(u) = u'$ and $T(v) = v'$, so $T(u + v) = u' + v'$. Thus the sum of two vectors in the range of T is also in the range of T, and the scalar multiplication closure follows similarly.

Definition 69

A linear operator is **surjective** if range $T = V$.

In other words, our operator reaches the whole vector space.

Example 70

Consider the left and right shift operators from earlier in the class, defined via

$$L(x_1, x_2, \cdots) = (x_2, x_3, \cdots), \quad R(x_1, x_2, \cdots) = (0, x_1, \cdots).$$

Let's try to extract a few of the elementary properties of these operators.

First of all, what is the nullspace of L? We need the final vector to be 0, which means that $x_2, x_3, \cdots$ must all be 0, but x_1 can be anything:

$$\text{null}(L) = (x_1, 0, 0 \cdots).$$

In other words, L is **not injective**, because the null space is nonzero. (For instance, both $(1, 0, 0, \cdots)$ and $(3, 0, 0, \cdots)$ are sent to the same thing.) However, L is **surjective**, because we can get any vector $(a, b, \cdots)$ by starting with $(0, a, b, \cdots)$.

Similarly, we can find the null space for R: it is just the zero vector, because we need all of $x_1, x_2, \cdots$ to be zero. In other words, R is **injective**. However, R is **not surjective**: it's not possible to end up with the vector $(1, 0, 0, \cdots)$. In other words, the range of R is smaller than V.

This might seem reasonable, but it is actually pretty counterintuitive: in finite-dimensional vector spaces, we won't have a situation like this where the operator is surjective but not injective, or injective but not surjective!

Now that we've introduced a lot of these ideas, we're going to introduce a fundamental result which we'll come close to proving. The key idea is that the null space null T and the range range T are both vector spaces (subspaces of V), so they have a dimension.

Theorem 71 (Rank-nullity theorem)

For any linear operator T on a **finite-dimensional** vector space V,

$$\dim(\text{null } T) + \dim(\text{range } T) = \dim V.$$

This theorem actually turns out to hold in a more general sense too: this still holds if we have a linear map that goes from V into a different vector space W! So this is a powerful result, and it's important to keep in mind.

The key idea for proving this theorem is to think about the **basis vectors** at play here. Since null T is a vector subspace, there is a basis $(u_1, u_2, \cdots, u_m)$ for that null space. But this isn't the full basis – the null space is often much smaller than V – it's just a linearly independent set in V. But now we can extend this to a basis for the whole vector space by adding some elements $v_1, v_2, \cdots, v_n$. It now suffices to show that $Tv_1, Tv_2, \cdots, Tv_n$ actually form a basis for range T: then we'd know that $\dim(\text{null } T)$ is m, $\dim(\text{range } T)$ is n, and $\dim V$ is $(m+n)$.

Instead of going through the whole proof there, we'll just do a simple case for illustration.

Example 72

Consider the linear operator $T = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ on a two-dimensional vector space $V = \mathbb{R}^2$.

To find the null space, we just need to find the set of vectors that are killed by T: we need

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \boxed{\begin{bmatrix} b \\ 0 \end{bmatrix}}$$

to be the zero vector, so we need b to be zero (but there are no restrictions on a). Thus the null space is the set of vectors spanned by $e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$.

On the other hand, the range of T is the set of vectors that come out of applying T: it's the same boxed expression above, so it turns out that the range of T is actually spanned by the same vector e_1. That might seem a bit confusing, but remember that the rank-nullity theorem above tells us that some of our basis vectors of V should form a basis for the null space (in this case just e_1), and T **applied on** the rest of them (in this case just e_2) should form a basis for the range. And indeed, $Te_2 = e_1$ is a basis for the range, and we've verified that the rank-nullity theorem holds in this specific case.

With this, we're now ready to move on to something more concrete: the **matrix representation** of our linear operators. This is an interesting phrase – one important idea is that our linear operators already exist, **independent of whether or not we're representing them**. One analogy is that we can take a picture of some object which already exists, which makes it easier to describe and work with. But we can also take pictures from different angles to get different pictures, and that corresponds to different matrix representations of the same operator. So mathematicians don't always like matrix representations, but they're practically very helpful.

Fact 73

We need to **choose a basis** in a vector space before we can construct a matrix representation. And our result does depend on the basis that we pick.

We'll abuse some notation here and often say that our linear operators T are "equal" to some matrix. But this is just a warning that whenever we do this, we should make sure we understand what basis we're using!

What's perhaps most confusing about matrices when they are first introduced in a math class is that while we do add matrices component by component, we don't do the same for multiplication. So one of the goals of today is to show why the weird, complicated expression for matrix multiplication (taking the ith row and jth column and multiplying component-wise there) makes sense!

So we'll start by considering some basis $\{v\}$ to be a basis for our vector space V. We know that for any vector v_j in our basis, Tv_j must still live in our vector space, so we can write it as some **linear combination of the basis vectors**:

$$\boxed{Tv_j} = T_{1j}v_1 + T_{2j}v_2 + \cdots + T_{mj}v_m = \boxed{\sum_i T_{ij}v_i}.$$

These numbers T_{ij} are going to be the numbers that go into our matrix representation for T, because they carry all of the information about our operator: we just need to know where all of our basis vectors go! So we'll write that

$$T = \begin{bmatrix} T_{11} & T_{12} & \cdots & T_{1N} \\ T_{21} & T_{22} & \cdots & T_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ T_{M1} & T_{M2} & \cdots & T_{MN} \end{bmatrix},$$

where T_{ij} goes in the ith row and jth column of our matrix. The whole point of this is that knowing the basis and knowing the operator will give us the matrix representation, and this might clear up some confusion: we do not need to know anything about a dual basis or bras and kets to define a matrix representation for T!

Remark 74. *If we want to mention that these matrix entries depend on our basis, we may denote the entries as* $T_{ij}(\{v\})$.

Let's use this to start understanding matrix multiplication: first of all, consider some vector

$$v = \sum_i a_i v_i = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix}.$$

Suppose we have a linear operator T: this will send our vector v to some other vector

$$b = Tv = T\sum_i a_i v_i.$$

Since T is a linear operator, we can break this up into each of the individual parts: thus

$$b = \sum_i a_i(Tv_i) = \sum_i a_i \sum_p T_{pi}v_p,$$

where in the last equality we've written out the expression for Tv_i. And now we can just switch the order of summation so that this looks more familiar to us:

$$b = \sum_p \sum_i T_{pi}a_i v_p.$$

So now we've figured out a way to write down b as a linear combination of the basis vectors! So the coefficients must satisfy

$$b_p = \sum_i T_{pi}a_i,$$

and now we've derived the familiar expression for **multiplication of a matrix by a vector**.

Fact 75

By the way, note that the **identity operator** has a nice matrix representation: because $Iv_i = v_i$ for any basis vector T_{ij} is 1 when $i = j$ and 0 otherwise, and thus the operator is a diagonal matrix with 1s on the diagonal and 0s everywhere else. And the zero operator has a simple matrix representation as well: it just has zeros everywhere.

So now we're ready for the more general case: multiplying two matrices together. Suppose we have two linear operators T, S acting on the basis vector v_j. We can start writing this out: since TS is an operator, we know that (by definition)

$$\sum_p (TS)v_j = (TS)_{pj} v_p.$$

Our goal is to show that this entry $(TS)_{pj}$ can be written in the usual matrix-multiplication form. To do that, note that

$$TSv_j = T\sum_k S_{kj} v_k,$$

where we've done the action of S on v_j, and now we can bring the T inside the sum by linearity: this is thus equal to

$$\sum_k S_{kj} T v_k = \sum_k S_{kj} \sum_p T_{pk} v_p.$$

We now use the same trick as before: swap the order of summation, and we find that

$$TSv_j = \sum_p \boxed{\sum_k T_{pk} S_{kj}} v_p.$$

(We flipped the order of T_{pk} and S_{kj}, which is fine because they're both numbers.) But the boxed expression here serves the same purpose as $(TS)_{pj}$, and thus we have a formula for the entries of TS:

$$(TS)_{pj} = \sum_k T_{pk} S_{kj}.$$

And this is indeed matrix multiplication: we're looking at the pth row of T and the jth row of S and multiplying component-wise there! And notice that we've now given a natural explanation, using linear algebra, of why matrix multiplication is defined the way it is: this is the only way to make sure the operator TS is consistent with applying S, then T.

Our last topic for this lecture will be that of a **change of basis**. We said earlier that matrices provide a representation of linear operators on a vector space, but we may want to pick different bases in different scenarios, which lead to different matrices – thus, we need a way of converting between the bases. And in this study, we'll find that there is some information in our matrix that is independent of the basis that we choose!

As we said earlier, we have

$$Tv_j = \sum_i T_{ij}(\{v\}) v_j,$$

where this result depends on the basis $\{v\}$ we've chosen for the situation. So now we'll have **two different bases**: $\{v\} = (v_1, \cdots, v_n)$ and $\{u\} = (u_1, \cdots, u_n)$, and now we need to define some new operators. We'll let A take $\{v\}$ to $\{u\}$, and we'll let B take $\{u\}$ to $\{v\}$: we can write this as

$$u_k = Av_k, \quad v_k = Bu_k$$

for all $1 \leq k \leq n$. Here A and B are linear operators – for example, they take the third basis vector in $\{v\}$ to the third

basis vector in $\{u\}$, and vice versa. So now we can calculate

$$BAv_k = Bu_k = v_k,$$

and similarly

$$ABu_k = Av_k = u_k,$$

so BA and AB are the identity operators, which means that A and B are in fact **inverses** of each other.

The point of introducing these operators A and B to see **how we can relate the matrix elements** $T_{ij}(\{v\})$ and $T_{ij}(\{u\})$ – that is, how can we calculate the entries of matrices in one basis, given the entries in the other basis?

First of all, notice that we've defined our basis-changing linear operators A and B, and we might want to write down matrix representations for them. But we have two bases – which one should we use for the representations? Wonderfully, **it doesn't actually matter**:

Proposition 76

The matrix representations of A, B (our basis-changing operators) are the same in $\{v\}$ and in $\{u\}$.

Proof. We know that

$$Av_k = \sum_i A_{ik}(\{v\})v_i$$

and

$$Au_k = \boxed{\sum A_{ik}(\{u\})u_i}$$

by definition, and we want to show that these coefficients A_{ik} are the same. To do this, note that

$$Au_k = A(Av_k) = A\sum_i A_{ik}(\{v\})v_i$$

(by plugging in the definition of Av_k from earlier), and now $A_{ik}(\{v\})$ are just numbers, so we can bring the A inside the sum to get

$$Au_k = \sum_i A_{ik}(\{v\})(Av_i) = \boxed{\sum_i A_{ik}(\{v\})u_i}.$$

But looking at the two boxed expressions for Au_k, they are identical except for the basis that we're using, so we indeed have that A_{ik} is the same in both bases, as desired. (The same argument works for B.) □

In the same spirit, we know that A and B are inverses of each other, so we know that

$$\sum_j B_{ij}A_{jk} = \delta_{ik} = \sum_j A_{ij}B_{jk}.$$

And in this kind of statement, we again don't need to write down the basis that we're using!

So now we're ready to answer the main question. We'll find the matrix entries $T(\{u\})$ in terms of $T(\{v\})$ and the matrix A (we could also use the entry B). To unclutter notation, we'll use the repeated index convention (where a repeated index means we sum over that index). We'll need to do a bit of computation: we have the sum

$$Tu_k = \boxed{T_{ik}(\{u\})u_i}$$

by definition, and we need to involve the v-vectors somehow: replacing $u_k = Av_k$ on the left hand side, we note that

this expression is also equal to TAv_k. And now letting A act on v_k, we find that

$$= TAv_k = TA_{jk}v_j,$$

and now we can have the operator T act on the v_js to find

$$= \boxed{A_{jk}T_{pj}(\{v\})v_p}.$$

This isn't quite what we want, though – we have v vectors in the second expression, so we need to rewrite this in terms of the u vectors. And because $v_p = B_{ip}u_i$ (rewriting so that we match up the indices on the u vectors), this means that

$$T_{ik}(\{u\})u_i = A_{jk}T_{pj}(\{v\})B_{ip}u_i,$$

and finally using the fact that B is the inverse matrix of A, we arrive at our result (also reshuffling our numbers a bit):

$$T_{ik}(\{u\})u_i = A^{-1}_{ip}(\{v\})A_{jk}T_{pj}u_i.$$

But this means that the matrix $T(\{u\})$ in the u-basis is just $A^{-1}T(\{v\})A$, since all of the ik-entries line up! And thus we've arrived at our main result:

$$\boxed{T(\{u\}) = A^{-1}T(\{v\})A},$$

where A is the basechange matrix such that $u_k = Av_k$. (And this operation of multiplying with the inverse on the left and the matrix on the right is called **conjugation**: it'll come up again.)

With this, we can prove some interesting properties about **invariant properties** of our linear operators.

Proposition 77
The **trace** of a matrix representing a linear operator, which is define to be the sum of the diagonal entries of that matrix, is basis-independent.

Proof. To show this, we need to know a few important properties of trace: in particular, we have

$$\mathrm{tr}(T_1T_2) = \mathrm{tr}(T_2T_1),$$

and more generally the trace is actually **cyclic** – we can show by computing some coefficients of matrix multiplication that

$$\mathrm{tr}(T_1T_2\cdots T_n) = \mathrm{tr}(T_nT_1\cdots T_{n-1}).$$

So we can apply this to our base change formula above:

$$\mathrm{tr}(T\{u\}) = \mathrm{tr}(A^{-1}T\{v\}A) = \mathrm{tr}(AA^{-1}T\{v\}) = \mathrm{tr}(T\{v\}),$$

where we've used cyclicity in the middle equality. □

Proposition 78
The **determinant** of a matrix representating a linear operator is basis-independent.

Proof. For this, we also need to remember the property that

$$\det(AB) = \det A \det B$$

for two matrices A and B. (In particular, this shows that $\det A \det A^{-1} = \det I = 1$.) This generalizes easily to show that

$$\det(A_1 \cdots A_m) = \det A_1 \cdots \det A_m,$$

and thus we can plug this into our base change formula again:

$$\det T\{u\} = \det(A^{-1} T\{v\} A) = \det A^{-1} \det T\{v\} \det A = \det T\{v\},$$

as desired. □

We'll see soon that the trace and determinant, along with a few other invariants, carry intrinsic information about our operators!

8 February 12, 2020

We're doing a bit more linear algebra now – we'll practice some of the ideas about matrix representation and linear operators today during class. (As a reminder, we also have a homework assignment due on Friday.)

Last time, we talked about direct sums of vector spaces, and we'll illustrate that idea again with the **central potentials**. This is a typical situation in three dimensions, where the potential only depends on the magnitude of the position vector:

$$V(\vec{r}) = V(r), \quad r = |\vec{r}|.$$

This means we have a spherical symmetry – the most famous example is the hydrogen atom, but the spherical square well and Morse potential are key ideas in physics as well. These have all been studied, and the way they work out is that the basic separable solutions follow the ansatz

$$\psi_{E\ell m}(\vec{r}) = \frac{u_{\ell E}(r)}{r} \cdot Y_{\ell m}(\theta, \phi).$$

This is called a **basic solution**, and it's indexed by E, ℓ, m. Here, the function u satisfies the Schrodinger equation

$$-\hbar^2 2m \frac{d^2 u}{dr^2} + \left(\frac{\hbar^2}{2mr^2} \ell(\ell+1) + V(r) \right) u = Eu$$

(basically, we have an effective potential, which serves as a centrifugal barrier). This is now a one-dimensional problem, and that's the advantage of working in this system! There's only one confusion we should be careful about – the indexing by m is the quantum number, not the mass. And this holds for any kind of central potential – the general solution is going to be a superposition of these energy eigenstates.

Remark 79. *Where does the centrifugal term come from? The actual Schrodinger equation we want to solve in general has a Laplacian operator*

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi,$$

and if we expand out the Laplacian in spherical coordinates, the angular part act on the $Y_{\ell m}$s in a particularly nice way.

By the way, what are our bounds for E, ℓ, m? ℓ can be any nonnegative integer $0, 1, \cdots$, and for any fixed ℓ, m is an integer between $-\ell$ and ℓ. And to find the energy, we need to solve the wave equation – this will quantize the allowed energy states, and it will tell us the indices for E.

One more comment – the reason we have a $\frac{1}{r}$ term is that $u_{\ell E}$ satisfies a nicer wave equation than $\frac{u(r)}{r}$. A nice bonus is that when we're trying to normalize our wavefunction, the r^2 in the denominator from $|\psi|^2$ cancels out with the $r^2 dr$ term from the spherical d^3x, so the wavefunction almost "normalizes itself!"

So let's go back to the linear algebra here – we were looking at direct sums. If we fix different values of ℓ, we get slightly different wave equations, and they each give slightly different allowed (quantized) values of E. We know that the energy levels will be higher for larger values of ℓ (because the effective potential is larger), but the point is that if we draw a diagram with ℓ on one axis and E on the other axis, we get the spectrum of all energy eigenstates.

Sometimes, different values of ℓ will give the same value of E, and those give us **degeneracies** which need to be explained. But regardless, if we want to represent our total state space, we can write it as

$$\mathcal{H} = \mathcal{H}_{\ell=0} \oplus \mathcal{H}_{\ell=1} \oplus \cdots = \bigoplus_{\ell=0}^{\infty} \mathcal{H}_\ell,$$

which means that the whole set of basis vectors (energy eigenstates) can be decomposed into those from $\ell = 0$, those from $\ell = 1$, and so on, and they're all linearly independent. But we can further decompose each $\mathcal{H}_\ell$ into its different energy eigenstates:

$$\mathcal{H}_\ell = \mathcal{H}_{\ell,E_0} \oplus \mathcal{H}_{\ell,E_1} \oplus \cdots = \bigoplus_{k=0}^{\infty} \mathcal{H}_{\ell,E_k}.$$

This means that we can write the whole energy space

$$\mathcal{H} = \bigoplus_{\ell=0}^{\infty} \bigoplus_{k=0}^{\infty} \mathcal{H}_{\ell,E_k},$$

but we're still not done breaking everything up: for example, $\ell = 1$ allows the quantum number m to be $-1, 0$, or 1. So really,

$$\mathcal{H}_{\ell,E_k} = \bigoplus_{m=-\ell}^{\ell} \mathcal{H}_{\ell,E_k,m},$$

and now $\mathcal{H}_{\ell,E_k,m}$ generates a one-dimensional vector-space – it's just one basis, and if we substitute this back into our equation for $\mathcal{H}$, we've completely decomposed our state space

$$\mathcal{H} = \bigoplus_{\ell=0}^{\infty} \bigoplus_{k=0}^{\infty} \bigoplus_{m=-\ell}^{\ell} \mathcal{H}_{\ell,E_k,m}.$$

One question: what if we have an energy degeneracy, so two different eigenstates (with different numbers ℓ, m) have the same energy E? That doesn't matter: the $\mathcal{H}_{\ell_i,E,m_i}$ and $\mathcal{H}_{\ell_j,E,m_j}$ states are still linearly independent, because they're different vectors. It's just important to remember that degenerate states do differ in some way – otherwise, they'd be indistinguishable from each other!

We'll now move on to talking about Pauli matrices: we'll probably have them memorized by the end of 8.051 with all of the exercises we're doing with them. We have the universal conventions

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Note that these matrices have a few properties:

- Pauli matrices are **Hermitian**, which means they are equal to their (complex) conjugate transpose. In fact, $\sigma_x, \sigma_y, \sigma_z$, and the identity matrix I form an $\mathbb{R}$-basis for the set of 2×2 Hermitian matrices (it's good to think of these as an $\mathbb{R}$-vector space, because multiplying Hermitian matrices by real numbers still give us Hermitian matrices, but this is not true for complex numbers). To show that this is true, note that the most general 2×2

Hermitian matrix can be written as

$$\begin{bmatrix} a_0 + a_3 & a_1 + a_2 i \\ a_1 - a_2 i & a_0 - a_3 \end{bmatrix} = a_0 I + a_1 \sigma_x + a_2 \sigma_y + a_3 \sigma_z.$$

(The diagonal entries should be real, and the off-diagonal entries should be complex conjugates.) We often refer to $\sigma_x, \sigma_y, \sigma_z$ as $\sigma_1, \sigma_2, \sigma_3$, respectively. By the way, the reason we write the diagonal entries as $a_0 + a_3$ and $a_0 - a_3$ instead of just using two numbers b_0 and b_3, because we want to write everything as a linear combination of Hermitian matrices.

It's important to re-emphasize that this is a **real vector space** of dimension 4, even though the matrices are full of imaginary numbers! That's why we don't say that the "vectors" (matrices in this case) are real or complex.

- Pauli matrices are **traceless** – the trace is the sum of the diagonal entries. They all have **determinant** -1 as well. Why is it important that these matrices are traceless? we should think of Pauli matrices as spin-1/2 operators, and they have two kinds of states (spin up and spin down). This means we should have two eigenvalues, and the trace (which is also the sum of the eigenvalues) being zero tells us that the eigenvalues are $+\lambda$ and $-\lambda$.
- What happens when we square the Pauli matrices? It turns out that $\sigma_i^2 = I$, which is a fundamental property as well. The importance of this property is that **if we have a matrix equation, the eigenvalues satisfy the same equation**: this tells us that $\lambda^2 = 1$.
- Finally, the Pauli matrices are **unitary**, which means that $U^\dagger U = I$. There are more pictorial properties of this, but this is a good one to start with. Indeed, we can check that

$$\sigma_i^\dagger \sigma_i = \sigma_i \sigma_i = I$$

(because σ_i are Hermitian, $\sigma_i^\dagger = \sigma_i$).

One fundamental property of the Pauli matrices that we should internalize is that the product

$$\boxed{\sigma_i \sigma_j = \delta_{ij} I + i \varepsilon_{ijk} \sigma_k},$$

where the repeated index k on the right-hand side is summed.

So let's think about an operator $\mathcal{O}$ acting on spin states $|+\rangle$ and $|-\rangle$: we can represent them as $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, respectively. Suppose the operator satisfies

$$\mathcal{O} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \mathcal{O}|+\rangle = \alpha|+\rangle + \beta|-\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

and

$$\mathcal{O} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \mathcal{O}\,|+\rangle = \gamma\,|+\rangle + \delta\,|-\rangle = \begin{bmatrix} \gamma \\ \delta \end{bmatrix}.$$

Because $|+\rangle$ and $|-\rangle$ are the basis vectors and $\mathcal{O}$ is a linear operator, this tells us everything we want about the operator. But perhaps we want a formula that tells us how to act on every vector in our vector space: that's where the matrices come in. It's dangerous, though, to say explicitly what the operator does to every vector, because we need to check linearity! For example, we can prove that **no operator exists which reverses every single spin state**, because that would violate linearity. So the representation of an operator should generally just be **on our basis vectors**.

The best way to write $\mathcal{O}$ as a matrix is to just look at the two equations above and see what we need to satisfy:

we'll find that we basically put the images of the basis vectors down as our column vectors:

$$\boxed{\mathcal{O} = \begin{bmatrix} \alpha & \gamma \\ \beta & \delta \end{bmatrix}}.$$

As a challenge for next time, we can try to write down a matrix representation for the operator

$$|\vec{n}; +\rangle\langle\vec{n}; +|.$$

9 Linear Algebra – Vector Spaces and Operators, Part 3

We started talking about linear operators on vector spaces last time, and the main things we discussed were its rough features – for instance, we've discovered a few things about the operator's null space and range. We now want to ask a few more questions, primarily centered around **eigenvalues** and **eigenvectors**.

The physics motivation here is that our operators are observables, and eigenvalues tell us a specific **possible value of a measurement of that observable**. Since these are crucial properties in quantum mechanics, we should make sure we understand the mathematics here too.

As before, we'll be working with linear operators $T \in \mathcal{L}(V)$ on a vector space V.

Definition 80

A subspace U of a vector space V is an **invariant subspace** if $T(u) \in U$ for all vectors $u \in U$. (Another way to write this is that the set $T(U) \subseteq U$.)

The idea here is that applying T keeps us inside a subspace, so we have a more degenerate (but still interesting) representation of our linear operator. We should remember that being an invariant subspace is an idea connected to an operator – it doesn't just exist on its own!

Example 81

We always have two trivial examples of invariant subspaces: the **zero vector** is an invariant subspace (because it's sent to itself), and the **whole vector space** is also invariant (because T takes a vector space to itself).

These aren't very interesting, so let's try to construct an example of a more interesting invariant subspace. We know that the zero vector is a subspace of dimension 1, while the whole vector space V has full dimension $\dim V$: let's try to get something in between by considering **one-dimensional invariant subspaces**.

Every one-dimensional subspace can be generated by a single vector $u \in V$: the space generated by this vector is the set $U = \{cu : c \in \mathbb{F}\}$ (we can scale the vector by any number, so we have a line through the origin). Because the basis has one vector, this does indeed have dimension 1 by definition.

Fact 82

It's important that u is not the zero vector: otherwise, we won't actually generate a one-dimensional subspace.

So if we want U to be invariant, that means that

$$Tu \in U \implies \boxed{Tu = \lambda u}$$

for some number $\lambda \in \mathbb{F}$. It turns out this is an extremely important equation: such vectors are invariant up to a scalar factor under the action of T.

Definition 83

Let T be a linear operator on an $\mathbb{F}$-vector space V. If there is a vector $u \in V$ and a scalar $\lambda \in \mathbb{F}$ such that

$$Tu = \lambda u, \quad u \neq 0,$$

then λ is an **eigenvalue** of T, and u is its associated **eigenvector**.

The reason we don't allow $u = 0$ is because that's satisfied for any λ: it's not an interesting equation. So eigenvalues need to correspond to **nonzero vectors**, though **it is okay for eigenvalues themselves to be zero**. In fact, 0 is often an interesting eigenvalue – that means that we have some nonzero vector u which is killed by T, and that tells us something about the null space.

So suppose we have such an eigenvector u: then every vector in the span of u, which is the set of vectors of the form cu (for $c \in \mathbb{F}$), is an eigenvector. After all, if $Tu = \lambda u$, it's okay for us to multiply both sides of the equation by any constant c. That means that we'll often say that "the span of u is an eigenvector" (even though we don't actually want to include the zero vector)

Sometimes we'll actually get a funny situation: we might have a particular value of λ for which **more than one independent vector** solves the equation $Tu = \lambda u$. Then we have a **degeneracy** – where a given eigenvalue has more than one eigenvector – and then our invariant subspace is larger than one dimension! For example, if u_1 and u_2 both have eigenvalue λ, then every vector in the span of u_1 and u_2 will also have eigenvalue λ, and then some interesting complications will occur. But there's a lot of physics associated with this idea, so we should keep it in mind.

Definition 84

The **spectrum** of an operator is its set of eigenvalues.

We will want to find a way to solve for the eigenvalues λ: notice that we can rewrite the equation

$$Tu = \lambda u \implies (T - \lambda I)u = 0.$$

So the eigenvalue condition actually tells us that there is a nonzero vector u that is killed by the operator $T - \lambda I$, and in particular this means that $T - \lambda I$ **is not injective** – its null space is not just the zero vector. And when we have a finite-dimensional vector space, this actually means that $T - \lambda I$ is also not surjective and not invertible. And the eigenvectors of T correspond exactly to the **null space of** $T - \lambda I$. (And this explains that since we want the null space to always include the zero vector, it's convenient to just include it as a "soft" eigenvector.)

Example 85

When is $\lambda = 0$ an eigenvalue of an operator T?

The eigenvectors of eigenvalue 0 are those vectors for which $Tu = 0u = 0$: thus, the null space of T is the eigenvectors of eigenvalue 0.

Example 86

We've been talking about properties of matrix representations that are **basis-independent**: are the eigenvalues and eigenvectors basis-independent? Are invariant subspaces basis-independent?

All of these concepts do not need to be defined by a basis, so they are indeed basis-independent. However, we should be careful to note that eigenvectors might be **represented** differently in different bases.

To summarize this first pass through eigenvectors and eigenvalues, we got to this idea by exploring **invariant subspaces**, particularly those with one dimension. Then the **eigenvector** spans our invariant subspace, and the **eigenvalue** tells us how the subspace behaves under the action of our operator T: everything is just scaled. And when we're working in complex vector spaces, knowing all of the eigenvalues and eigenvectors tells us a lot of information!

Remark 87. *The next few pages are optional material.*

Let's try to gain some intuition for what's happening geometrically with eigenvalues and eigenvectors:

Example 88

Consider an operator in $V = \mathbb{R}^3$ which rotates vectors: explicitly, consider a rotation around the z-axis. What are the eigenvalues and eigenvectors of this operator?

We know that all vectors that are not along the z-axis will be rotated (so they end up in a different direction), but all vectors along the z-axis are left invariant. So in $\mathbb{R}^3$, there is only **one eigenvector**: the one along the z-direction (or more precisely, the **span** of $(0, 0, 1)$). This eigenvector has $\lambda = 1$, because there is no scaling on the z-axis.

But are there other eigenvectors? The answer is **no**, as long as we're working in the real numbers. If we try calculating eigenvectors and eigenvalues mathematically here, we'll find that the other potential vectors end up with **complex coefficients**: those aren't allowed when we have a real vector space! Similarly, if we use the example $V = \mathbb{R}^2$ and do a rotation T in the plane, we will actually have **no invariant vectors** and thus **no eigenvectors** at all! So real vector spaces have this kind of complication, and that's a reason why we like **complex vector spaces** better. We'll get some better results – there's always at least one eigenvalue and often many more if our operators are nice – and if we restrict ourselves to a special class of operators, the eigenvalues will be **real**, which is what we need for physical observables to make sense!

Here's an important piece of intuition: **eigenvectors of different eigenvalues are linearly independent**, and we'll actually make a stronger statement soon: they'll be orthogonal once we define an **inner product**. But let's prove what we can for now:

Theorem 89

Let $T \in \mathcal{L}(V)$ be a linear operator, and let $\lambda_1, \cdots, \lambda_n$ be distinct eigenvalues with corresponding (nonzero) eigenvectors $u_1, \cdots, u_n$. Then the eigenvectors are linearly independent.

The reason we care about this is that we often want our eigenvectors to span our vector space, which can be a useful thing to have! Again, note that we can't define orthogonality yet because we don't have an inner product on our space yet.

Remark 90. *Sometimes, it's possible that a given eigenvalue λ has more than one eigenvector. Then we can pick any of those eigenvectors to put in our theorem here. Also, since a dimension n vector space can have at most n linearly independent vectors, this means that T can have* **at most** *n* **different eigenvalues**.

Proof. We'll work by contradiction. Assume that $u_1, \cdots, u_n$ are linearly dependent: then there exists some **smallest** $k \leq n$ such that

$$u_k = a_1 u_1 + \cdots + a_{k-1} u_{k-1}.$$

Basically, follow the following procedure. We look at the first vector – is it linearly independent by itself? Yes. Then look at the first two vectors together – are they linearly independent? If not, then set $k = 2$ above, otherwise look at the first three vectors together and continue on. And in the first place we stop, the contribution from u_k must be nonzero (another way to say this is that u_k is in the span of u_1 through u_{k-1}), and so the equation above is indeed valid.

But now u_k is nonzero by definition, so some of the a_ks must be nonzero. Now apply the operator $T - \lambda_k I$ to this equation: since λ_k is the eigenvalue of u_k, the left hand side becomes 0. We can also simplify the right hand side: $T - \lambda_k I$ doesn't kill any of the other u_is, because they all have distinct eigenvalues. Specifically, we'll get the equation

$$0 = a_1(\lambda_1 - \lambda_k)u_1 + a_2(\lambda_2 - \lambda_k)u_2 + \cdots + a_{k-1}(\lambda_{k-1} - \lambda_k)u_{k-1} = 0.$$

But remember that u_1 through u_{k-1} were assumed to be linearly independent, so for this equation to hold, we must have all coefficients be zero, which means $a_1 = a_2 = \cdots = a_{k-1} = 0$. And this is a contradiction with the defining equation for u_k above! Thus the eigenvectors must be linearly independent, as desired. □

This is a pretty unorthodox proof, but we can now connect this with more standard discussions. We said earlier that

$$Tu = \lambda u \implies T - \lambda I \text{ is not invertible.}$$

And a useful way to restate this is that

$$\boxed{\det(T - \lambda I) = 0}$$

(here we're using a fact from linear algebra that an operator that is not invertible has determinant 0). And the best way to work with such a statement is to find a matrix representation and calculate the determinant explicitly. That basically looks something like

$$\det \begin{bmatrix} T_{11} - \lambda & T_{12} & \cdots & T_{1N} \\ T_{21} & T_{22} - \lambda & \cdots & T_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ T_{N1} & T_{N2} & \cdots & T_{NN} - \lambda \end{bmatrix} = 0.$$

Basically, we put $-\lambda$s on the diagonal, and then the determinant $f(\lambda)$ will be an nth degree **polynomial** in λ. So our defining equation will look something like

$$(-\lambda)^N + b_{N-1}\lambda^{N-1} + \cdots + b_0 = 0.$$

Such equations will have solutions over the complex numbers $\mathbb{C}$, and this is why we like to work with complex vector spaces – we can guarantee that this has at least one solution! And most of the time, we will indeed have N solutions, but occasionally there are repeats: we can always factor this polynomial, called the **characteristic polynomial**, as

$$f(\lambda) = (-1)^N(\lambda - \lambda_1)(\lambda - \lambda_2)\cdots(\lambda - \lambda_N),$$

where it's possible that λ_i and λ_j are the same. (That would correspond to a **degeneracy**.)

Definition 91

If all eigenvalues of an operator are distinct, then we say that the spectrum is **non-degenerate**. On the other hand, if the characteristic polynomial has $(\lambda - \lambda_i)$ appearing k_i times, then λ_i is a **degenerate eigenvalue** with **multiplicity** k_i.

And now we have a typical strategy for calculating eigenvalues and eigenvectors: use this equation $\det(T-\lambda I)=0$ to find solutions for λ, and then we will definitely have corresponding eigenvectors (because the operator is not injective). But to make any more progress at this point, we're going to need to introduce some additional structure.

In particular, the next question that we might be asked about our vectors in our vector space is their **length**. And the object that we'll now introduce – the inner product – helps us talk about lengths, but it also helps us define lots of other things that are coming up in the next few lectures – Hermitian, unitary, and orthogonal operators, among many other things. We'll start by talking about this for **real vector spaces** $\mathbb{R}^n$, because that's what might be more familiar. In this vector space, we'll denote vectors in the form

$$a=(a_1,a_2,\cdots,a_n),\quad a_i\in\mathbb{R}.$$

Recall from geometry that the length of a vector is

$$|a|=\sqrt{a_1^2+a_2^2+\cdots+a_n^2}.$$

This motivates the definition of a **dot product**: perhaps we want

$$|a|^2=a\cdot a=a_1^2+a_2^2+\cdots+a_n^2.$$

So this length squared is now some kind of operation of a with itself, so we can generalize this a bit:

Definition 92

The (real) **dot product** between two vectors $a,b\in\mathbb{R}^n$ is the number

$$a\cdot b=a_1b_1+a_2b_2+\cdots+a_nb_n\in\mathbb{R}.$$

This is a nice definition, because we can explicitly calculate it and also discover some properties. Our goal will be to do this more axiomatically: find some properties that an inner product should satisfy so that it gives us the appropriate structure. This way, we know that all inner products, no matter how they're constructed, will have certain desirable properties.

Let's go ahead and state those axioms for a **real vector space** now:

1. For any vector a, $a\cdot a\geq 0$. (Then it's well-defined to say that we have a length defined by $a\cdot a=|a|^2$.)
2. If $a\cdot a=0$, then $a=0$. This means that the only vector with zero length is the zero vector.
3. We have distributivity: $a(b+c)=ab+ac$ for vectors a,b,c.
4. $a\cdot(\alpha b)=\alpha(a\cdot b)$ for vectors a,b and real numbers α.
5. $a\cdot b=b\cdot a$.

The second property is very important – it will help us with maybe half of the proofs that we'll be doing in this class related to operators! Indeed, it's true for the dot product we've already defined: the only way for a sum of real squares to be zero is if they're all zero.

These dot products **do not** uniquely determine the definition of a dot product: we can actually define

$$a\cdot b=c_1a_1b_1+c_2a_2b_2+\cdots+c_na_nb_n,$$

as long as all of the c_is are positive. We can check that it does indeed satisfy all of the above properties.

Remark 93. *It is not okay for the c_is to be negative or zero, though – this violates one of the axioms, and it's good for us to figure out which one that is.*

Theorem 94 (Schwarz inequality)
For any two vectors a, b, we have

$$|a \cdot b| \leq |a| \cdot |b|.$$

This is not an obvious result, and we need to understand what it says. Note that the bars on the right side give us the **lengths** of the vectors a and b, but the bars on the left side give us the **absolute value** of the number $a \cdot b$. So bars can mean different things – we should be careful!

One way we might have seen this explained is that $a \cdot b = |a||b| \cos\theta$, where θ is the angle between the two vectors. And we know that cos has magnitude at most 1, so indeed the magnitude of this dot product is less than $|a||b|$. But this isn't a proof, because that's not how we defined the dot product above! So let's do a more rigorous proof: note that the Schwarz inequality actually follows from our **inner product axioms** above, so it doesn't depend on the specific inner product that we're using.

Proof. We use the axiom that $a \cdot a \geq 0$ for any vector a. Consider the **orthogonal projection** from a onto b: that is, split up the vector into components

$$a = a_{\parallel} + a_{\perp},$$

such that $a_{\parallel}$ is along the direction of b and $a_{\perp}$ and $a_{\parallel}$ are perpendicular to each other. So we know that

$$a_{\perp} = a - a_{\parallel},$$

but we also know that (by the **projection formula**) we have

$$a_{\parallel} = \frac{(a \cdot b)b}{b \cdot b} \implies \boxed{a_{\perp} = a - \frac{(a \cdot b)b}{b \cdot b}},$$

because we can think of this as taking the product of a with the unit vector along the b-direction. (Then there is a factor of "length of b" twice in the numerator and also twice in the denominator, so they cancel out.) As a check to make sure this correct, note that

$$a_{\perp} \cdot b = \left(a - \frac{(a \cdot b)b}{b \cdot b}\right) \cdot b$$

(by substitution), which simplifies (by distributivity) to

$$a \cdot b - \frac{(a \cdot b)(b \cdot b)}{b \cdot b} = 0.$$

So indeed $a_{\perp}$ is perpendicular to b, and now we're going to use the fact that $a_{\perp}$ dotted with itself is nonnegative (after all, the equality case of the Schwarz inequality is when a and b are parallel to each other). Thus

$$a_{\perp} \cdot a_{\perp} = \left(a - \frac{(a \cdot b)b}{b \cdot b}\right) \cdot \left(a - \frac{(a \cdot b)b}{b \cdot b}\right) \geq 0,$$

and expanding this out yields

$$a \cdot a - 2\frac{(a \cdot b)^2}{b \cdot b} + \frac{(a \cdot b)^2}{(b \cdot b)} \geq 0.$$

Combining like terms and multiplying through by $(b \cdot b)$, which is nonnegative, yields

$$(a \cdot a)(b \cdot b) - (a \cdot b)^2 \geq 0 \implies |a|^2|b|^2 \geq |a \cdot b|^2,$$

and taking positive square roots yields the result. □

(There will be a version of the Schwarz inequality for complex vector spaces, but we won't prove that one in class.) One interesting question is to ask **where this inequality is saturated** – this means that our inequality is actually an equality. And this only occurs is if $a_\perp$ is the zero vector, which means a and b are **parallel at equality of the Schwarz inequality**.

Again, notice that we never used the formula for the inner product in this proof! So we've abstracted away the important properties, and that will become useful as we transition into complex vector spaces.

Remark 95. *Required content now resumes.*

So now let's take the inner product axioms that we've been discussing in the real vector space case and transfer it to our complex vector space. We'll stop using the dot product notation in favor of a new notation that shows that we start with two vectors and get out a number: our inner product will now look like $\langle \cdot, \cdot \rangle$, where the $\cdot$s are vectors. As before, this inner product will be equal to a number, but now it will be a **complex number**.

This time, the order of our vectors may matter, and for inspiration let's try to imagine how we might define an inner product on $\mathbb{C}^n$. In such a vector space, vectors are of the form $z = (z_1, z_2, \cdots, z_n)$, where the z_is are complex numbers, and we know that we define a complex number's length squared by multiplying it by its complex conjugate. Thus, we'll want to define

$$|z|^2 = z_1^* z_1 + z_2^* z_2 + \cdots + z_n^* z_n.$$

This will be a real number, and it's always nonnegative – in fact, it only vanishes if all of the components are zero. So this is a nice model for the length squared of a vector, and it suggests a possible nice definition for an inner product in general: perhaps we will want

$$\boxed{\langle w, z \rangle = w_1^* z_1 + w_2^* z_2 + \cdots + w_n * z_n}.$$

Notice now that the vectors w and z play different roles – we complex conjugate the ws, but we don't do this for the zs. And we need to do this so that we can actually define a length for our vectors!

But we want to get a set of axioms that tell us all of the interesting and necessary properties of the inner product, and that's what we're going to do now:

Definition 96

An **inner product** on a complex vector space is a number-valued function $\langle \cdot, \cdot \rangle$ which satisfies the following axioms:

1. $\langle v, v \rangle \geq 0$ for all vectors v. (In particular, this quantity is always real.)
2. $\langle v, v \rangle = 0$ if and only if $v = 0$. (This will be useful for proofs of many properties.)
3. $\langle u, v_1 + v_2 \rangle = \langle u, v_1 \rangle + \langle u, v_2 \rangle$.
4. $\langle u, \alpha v \rangle = \alpha \langle u, v \rangle$.
5. $\langle u, v \rangle = \langle v, u \rangle^*$.

Axioms (3) and (4) are particularly noteworthy here: they're not actually identical to the real vector space case! After all, if we switch the order of our vectors, we're conjugating different components.

Proposition 97

For any vector u, we have $\langle u, 0 \rangle = 0$, and similarly $\langle 0, u \rangle = 0$.

Proof. Plug in $v_2 = 0$ into axiom (2) of inner products to find that

$$\langle u, v_1 \rangle = \langle u, v_1 \rangle + \langle u, 0 \rangle,$$

so indeed $\langle u, 0 \rangle = 0$. Take the complex conjugate of both sides to find that $\langle 0, u \rangle = 0$ by axiom (5). □

Axiom (3) shows linearity in the second argument only, and it turns out that we can use this to also figure out what happens with the first argument: suppose we want to compute $\langle u_1 + u_2, v \rangle$. We can use axioms (5) and (3) to say that

$$\langle u_1 + u_2, v \rangle = (\langle v, u_1 + u_2 \rangle)^* = (\langle v, u_1 \rangle + \langle v_1, u_2 \rangle)^* = \langle v, u_1 \rangle^* + \langle v, u_2 \rangle^*.$$

And now use axiom (5) again to reverse the inner products, and we've found linearity in the first entry as well:

$$\boxed{\langle u_1 + u_2, v \rangle = \langle u_1, v \rangle = \langle u_2, v \rangle}.$$

But what's most interesting is axiom (4): if we apply the same logic, we find that

$$\boxed{\langle \alpha u, v \rangle} = (\langle v, \alpha u \rangle)^* = (\alpha \langle v, u \rangle)^* = \boxed{\alpha^* \langle u, v \rangle},$$

and this is a point of potential mistakes: we have **conjugate homogeneity**. A complex number comes out of the left of the bracket with a conjugate, but it comes out of the right of the bracket unaffected! So again, this shows that the role of the first and second entries in our inner product is not identical.

But now that we've defined an inner product, we can do more useful things with it: we can define the length

$$|v|^2 = \langle v, v \rangle,$$

and we can also start relating vectors to each other:

Definition 98

Two vectors u, v are **orthogonal** if $\langle u, v \rangle = 0$ (which also means $\langle v, u \rangle = 0$).

Notice that we've set our inner product to be **non-degenerate** by axiom (2):

Lemma 99

If $\langle x, v \rangle = 0$ for all v, then $x = 0$.

Proof. Set $v = x$: then $\langle x, x \rangle = 0$ if and only if $x = 0$. □

We also have two other nice properties: the Schwarz inequality still holds, so we have

$$\langle u, v \rangle \leq |u||v|.$$

(We'll see the proof in our homework for the complex-valued case.) This is extremely useful – for example, it'll be used to prove the uncertainty principle. And the saturation point of this inequality is where $v = cu$ for a complex number c: this is the equivalent statement to v and u being parallel.

We also have the **triangle inequality**

$$|u + v| \leq |u| + |v|.$$

This is a geometric statement, and it's saturated when v and u point in the same direction: that is, we have $v = cu$ for a **real positive constant** c.

So we've now gotten to a very important point: we can now define a finite dimensional Hilbert space.

Definition 100

A **finite-dimensional Hilbert space** is a finite-dimensional vector space equipped with an inner product satisfying the appropriate axioms.

In the infinite-dimensional Hilbert space case, we actually need to add a more subtle condition: any infinite sequence of vectors with a limit must converge. (This is the mathematical property of being **Cauchy**.) Luckily, for this class, we won't need to worry about this assumption.

With this, it's time for us to go back to our basis and basis vectors. It will be convenient for us to pick nice bases in which computations are simple, and that's what we'll quantify right now:

Definition 101

A set of vectors $(e_1, \cdots, e_n)$ are **orthonormal** if

$$\langle e_i, e_j \rangle = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} = \delta_{ij}.$$

A basis of vectors which are orthonormal is an **orthonormal basis**.

Here, "ortho" comes from "orthogonal," and "normal" comes from "normalized" – any two vectors are orthogonal, and each vector has length 1.

The reason orthonormal bases are nice is that we can do certain computations easily: for example,

$$v = a_1 e_1 + \cdots + a_n e_n \implies |v|^2 = \langle v, v \rangle$$

can be expanded out to

$$= \langle a_1 e_1 + \cdots + a_n e_n, a_1 e_1 + \cdots + a_n e_n \rangle.$$

By homogeneity on the right, we can take out the constants on the right, and similarly we can take out constants (with conjugate factors) from the left. So our terms will look like

$$= \sum_{i,j} a_i^* a_j \langle e_i, e_j \rangle,$$

and the only terms that survive this are where $i = j$, leading us to a final answer of $\boxed{a_1^* a_1 + a_2^* a_2 + \cdots + a_n^* a_n}$: **only the diagonal terms survive**. This is a Pythagorean-like theorem: the length squared is the sum of the squares of the components if we use an orthonormal basis.

Proposition 102

An orthonormal set of vectors is linearly independent.

Proof. Call the vectors in this set $e_1, \cdots, e_n$. Suppose that we know that

$$a_1 e_1 + \cdots + a_n e_n = 0.$$

If this vector is equal to 0, then it must have zero length (by axioms of inner products), and thus the length squared, $a_1^* a_1 + \cdots + a_n^* a_n$, must be zero. So all of the a_i are zero, and indeed the vectors are linearly independent. □

So now if $(e_1, \cdots, e_n)$ is an orthonormal basis, we can write any vector as some linear combination $v = \sum_{i=1}^n a_i e_i$. And then notice that

$$\langle e_j, v\rangle = \sum_{i=1}^n \langle e_j, a_i e_i\rangle$$

by linearity, and then everything disappears except the j terms:

$$= \sum_{i=1}^n a_i \delta_{ij} = a_j.$$

This means that we can write any vector v as

$$\boxed{v = \sum_{i=1}^n \langle e_i, v\rangle e_i}.$$

Near the beginning of our discussion of linear algebra, we mentioned that a basis always exists for a finite-dimensional complex (or real) vector space. And it turns out that **we can always get an orthonormal basis as well!** This procedure is very practical – it's known as the **Gram-Schmidt** procedure, and it goes as follows:

- Assume we're given a list of linearly independent vectors $(v_1, \cdots, v_n)$ that span some subspace of V: we'll construct an orthonormal basis of that same subspace.
- Pick our first vector by normalizing: we let

  $$\boxed{e_1 = \frac{v_1}{|v_1|}}.$$

  (This denominator is not zero, because the zero vector can't be in a linearly independent set.)
- Pick the second vector by starting with v_2 and making it orthogonal to e_1: because v_1 and v_2 are linearly independent, we can use $e_2 = v_2 + \alpha e_1$ for some α. To figure out what α should be, note that we want

  $$\langle e_1, e_2\rangle = \langle e_1, v_2\rangle + \alpha\langle e_1, e_1\rangle = 0 \implies \alpha = -\langle e_1, v_2\rangle.$$

  So we subtract off a bit of e_1 – we won't end up with the zero vector because of linear independence – and then we just need to normalize our vector by dividing by its length:

  $$\boxed{e_2 = \frac{v_2 - \langle e_1, v_2\rangle e_1}{|v_2 - \langle e_1, v_2\rangle e_1|}}.$$

- We can do this inductively as well – we just subtract off a bit of each of e_1 through e_{j-1} when we are creating our jth vector:

  $$\boxed{e_j = \frac{v_j - \langle e_1, v_j\rangle e_1 - \cdots - \langle e_{j-1}, v_j\rangle e_{j-1}}{|v_j - \langle e_1, v_j\rangle e_1 - \cdots - \langle e_{j-1}, v_j\rangle e_{j-1}|}}.$$

  Indeed, we can check that (by construction) this vector is orthogonal to all of the first $j-1$ basis vectors, and it also has length 1.

Again, this is a useful procedure, and we'll get some practice with it soon!

One other thing we can say about the inner product is that it helps us **build subspaces**. The concept of orthogonality is very powerful: for example, **the set of vectors orthogonal to a given vector v is a subspace** (since the sum of two vectors orthogonal to v, as well as a scalar multiple of a vector orthogonal to v, are still orthogonal to v).

Definition 103

Let U be a subset of a vector space V. Then $U^\perp$ is the set of vectors $v \in V$ such that $\langle v, u\rangle = 0$ for all $u \in U$.

With this, a natural case to consider is that where U is a subspace. What's nice is that U and $U^\perp$ then decompose our full vector space nicely:

Theorem 104

Let U be a subspace of a vector space V. Then we can write V as a direct sum

$$V = U \oplus U^\perp.$$

Here, $U^\perp$ is known as the **orthogonal complement** of U. This might be intuitive to us: for example, the xy-plane and the z axis together give a decomposition of three-dimensional space.

Proof. Concretely, $V = U \oplus U^\perp$ means that every vector in V can be uniquely written as the sum of a vector in U and a vector in $U^\perp$.

First, we'll find a way to write V in this way: let $(e_1, \cdots, e_n)$ be a basis for U. We can write any vector v as

$$v = [\langle e_1, v\rangle e_1 + \cdots + \langle e_n, v\rangle e_n] + [v - \langle e_1, v\rangle e_1 - \cdots - \langle e_n, v\rangle e_n]$$

(everything trivially cancels on the right hand side except v), but now we claim that we already have a way of representing v: **the first bracket term is in U, and the second bracket term is in $U^\perp$**. The first term is clearly in U, and it's fairly easy to check that the second term is in $U^\perp$ because it's orthogonal to all of the basis vectors of U!

Finally, we need to show that $U \cap U^\perp$ only contains the zero vector, so that our representation is unique. Suppose that v is in both U and $U^\perp$: then $\langle v, v\rangle$ is the product of something in U and something in $U^\perp$, so it must be 0. And thus $v = 0$ by our inner product axioms. □

So any Hilbert space can be written as a direct sum of a subspace and its orthogonal complement – this result will be very useful in the future. And this brings us to the final idea from this lecture: **orthogonal projectors**. We'll start with a motivating example: in three dimensions, a vector has an x, y, and z-component. Consider a linear operator which just preserves the x-component: this would be a projection into the x-direction, which is a one-dimensional subspace. So we should think of projectors as operators which "forget" some things about our vector.

Let's think about what this projector looks like: it's a linear operator, so we can represent it as a matrix. If a vector has components $v = (v_1, v_2, v_3)$, we have the projector into the x-direction

$$P_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

(Indeed, we can check that $P_x v = (v_1, 0, 0)$, as desired.) Similarly, just having a 1 in the middle will give us P_y, and a 1 in the bottom right entry will give us P_z.

We do want to understand these projectors in more detail, though, beyond what its matrix looks like. This is because we have a **measurement postulate** in quantum mechanics, where our wave function collapses into an eigenstate when we measure it: that's actually a projection operator.

So now we're ready to state things more generally:

Definition 105

Let U be a subspace of a vector space V. The **orthogonal projector** P_U is defined as follows: we can uniquely write any vector $v \in V$ as $u + w$, where $w \in U$ and $w \in U^\perp$, and then we define $P_U(v) = u$.

As we've said already, we keep the part of the vector in U and we throw the rest away. This is a **linear operator** – we can check this by explicitly verifying the conditions – and note that we can also view this operator as saying that

$$P_U(u + w) = P_U(u) + P_U(w) = u + 0.$$

With this more formal definition, we can start thinking about some more properties: it's called the orthogonal projector because it uses the orthogonal decomposition $U \oplus U^\perp$.

Fact 106

The null space of the linear operator P_U is $U^\perp$, because these are the vectors with no component in U.

In particular, if U is not the whole vector space, $U^\perp$ is not just the zero vector, so P_U is **not injective**.

Fact 107

The range of the linear operator P_U is U – we can't get any components outside of U, and any vector $u \in U$ is sent to itself.

Let's restate this last fact in a slightly different way: for any vector $u \in U$, we have $P_U(u) = u$, and for any vector $w \in U^\perp$, we have $P_U(w) = 0$. So we can write a formula for the action of the projection. Letting $(e_1, \cdots, e_n)$ be a basis for U, we have that

$$P_U(v) = \langle e_1, v\rangle e_1 + \cdots + \langle e_n, v\rangle e_n.$$

(Notice that we've **dropped the basis vectors** for $U^\perp$ here, because they are killed by P_U.) Note also that

$$P_U(P_U(v)) = P_U(u) = u \implies P_U P_U = P_U$$

because we don't do anything else to our vector after we project once – we're already in U after one projection.

Fact 108

However, there are linear operators T with $T^2 = T$ that are not orthogonal projectors – this condition is necessary but not sufficient.

Proposition 109

For any orthogonal projection P_U and vector v,

$$|P_U(v)| \leq |v|.$$

This should be intuitively obvious – we're losing perpendicular components, so the total length is smaller.

Proof. More rigorously, note that

$$\langle v, v\rangle = \langle u + w, u + w\rangle,$$

and now we can expand out by linearity. Since u and w are orthogonal by definition, the cross terms disappear, and we have

$$|v|^2 = |u|^2 + |w|^2.$$

This is the Pythagorean theorem, and now $|u| = |P_U(v)|$, so indeed $|v|$ is at least as large as $|u| = |P_U(v)|$, as desired. □

One final way we can describe this projector is in terms of **eigenvalues** here, and this story is particularly simple – we should keep it in mind. Remember that eigenvectors correspond to a specific kind of invariant subspace, and the most obvious invariant subspace of P_U is U itself.

Proposition 110

For an orthogonal projector P_U, any vector in U has eigenvalue 1, and any vector in $U^\perp$ has eigenvalue 0.

In particular, if we want to find a basis of eigenvectors, we can just pick the orthonormal basis vectors of U and $U^\perp$. And notice that we could have predicted this from the start: we know that our operator satisfies the equation $P_U^2 = P_U$, so the eigenvalues must also satisfy that equation: $\lambda^2 = \lambda \implies \lambda \in \{0, 1\}$. And in this case, **the number of ones depends on the dimension of** U, and to understand that better, we can talk again about the matrix representation. If we want the matrix where we have $V = U \oplus U_\perp$, and we have an **orthonormal** basis of V of the form

$$(e_1, \cdots, e_n, f_1, \cdots, f_k),$$

where the es are a basis for U and the fs are a basis for $U^\perp$, we can represent this with the $(n+k) \times (n+k)$ matrix

$$P_U = \begin{bmatrix} 1 & \cdots & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 1 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix},$$

where the top left corner forms an $n \times n$ identity matrix and we have zeros everywhere else. (There are k rows and k columns of all zeros.) This is the representation when our **first** n **vectors** are in U – we can check that this gives us back the components in U.

Of course, this matrix will look different in different bases, but there are a few invariant properties. The **trace** of this matrix will be n, which is the dimension of the space U – in such a case, what we have is called a **rank** n **projector**. And its determinant is 0 (unless the projector is the identity projector), because our projection operator is not injective and therefore not invertible.

We'll only be discussing orthogonal projectors in this class, and the key thing to remember is that these come out of a **decomposition** of a vector space as $U \oplus U^\perp$. And that gives us all of the nice properties that we've been talking about!

10 February 18, 2020

Today, we're continuing with matters of linear algebra – there are about three more lectures on this topic. As a reminder, our second problem set is due on Friday.

We'll start by completing an exercise from last time: as a review, let's look some more at the spin-1/2 model. In about a week, we'll talk about bra and ket vectors formally, but we'll start doing some manipulation of them right now. If we represent our basis states (spin up and down) via $|+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, we can write a general state as

$$|\psi\rangle = c_1 |+\rangle + c_2 |-\rangle = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}.$$

Bra vectors, on the other hand, are the conjugate transpose: we have $\langle +| = \begin{bmatrix} 1 & 0 \end{bmatrix}$ and $\langle -| = \begin{bmatrix} 0 & 1 \end{bmatrix}$, which tells us that

$$\langle \psi| = c_1^* \langle +| + c_2^* \langle -| = \begin{bmatrix} c_1^* & c_2^* \end{bmatrix}.$$

One special state is the one where the spin points along some normal vector $\vec{n}$: we've shown in lectures that

$$|\vec{n}\rangle = \cos\frac{\theta}{2} |+\rangle + \sin\frac{\theta}{2} e^{i\phi} |-\rangle.$$

(This is confirmed via the fact that $|\vec{n}\rangle$ is an eigenvector for our operator $\vec{S}_{\vec{n}} = \vec{n} \cdot \vec{S} = \frac{\hbar}{2} \vec{n} \cdot \vec{\sigma}$.)

So let's say we have some object $|+\rangle \langle +|$: what exactly is this? We should think of this as an **operator**: this object acting on $|+\rangle$ gives us

$$|+\rangle \langle +| |+\rangle = |+\rangle \cdot 1,$$

and acting on $|-\rangle$ gives

$$|+\rangle \langle +| |-\rangle = |+\rangle \cdot 0,$$

because $\{|+\rangle, |-\rangle\}$ form an orthonormal basis. (It takes some getting used to, because $|+\rangle$ and $|-\rangle$ seem to point in opposite directions!) So this tells us the matrix representation: we know how it acts on $|+\rangle$ and $|-\rangle$, and actually one shortcut we can take is to just take the matrix representations of $|+\rangle$ and $\langle +|$ and multiply them together:

$$|+\rangle \langle +| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

A justification for this is that the individual parts $|+\rangle$ and $\langle +|$ are operators of some sort, and writing them next to each other is essentially defined by multiplication.

Example 111

What is the matrix representation of $|\vec{n}\rangle \langle \vec{n}|$? (This should be a 2×2 matrix.)

Much like in the example above, note that

$$|\vec{n}\rangle \langle \vec{n}| |\vec{n}\rangle = |\vec{n}\rangle,$$

while

$$|\vec{n}\rangle \langle \vec{n}| |-\vec{n}\rangle = 0,$$

so this is a projection operator onto the vector in the $\vec{n}$ direction. But we want to use Pauli matrices to represent this more explicitly.

Fact 112

Note that it's good to know the double-angle identities

$$\sin(2x) = 2\sin x \cos x, \cos(2x) = \cos^2 x - \sin^2 x.$$

One way to derive these is to use the formula $e^{2ix} = e^{ix} \cdot e^{ix}$ and equate real and imaginary parts.

Here's the right way to do this problem: note that

$$|\vec{n}\rangle = \begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{bmatrix} \implies \langle \vec{n}| = \begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} e^{-i\phi} \end{bmatrix},$$

So now we do the outer product

$$\begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{bmatrix} \begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} e^{-i\phi} \end{bmatrix} = \begin{bmatrix} \cos^2\frac{\theta}{2} & \cos\frac{\theta}{2}\sin\frac{\theta}{2} e^{-i\phi} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2} e^{i\phi} & \sin^2\frac{\theta}{2} \end{bmatrix}.$$

We want to get to the $\vec{n}$ vector, which contains $\sin\theta$ and $\cos\theta$ (spherical coordinates), so we need to get rid of these $\frac{\theta}{2}$s. Using the double angle formulas, we have

$$\cos\theta = \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} = 2\cos^2\frac{\theta}{2} - 1 \implies \cos^2\frac{\theta}{2} = \frac{1+\cos\theta}{2}.$$

A similar calculation gives us $\sin^2\frac{\theta}{2}$, and we can also use that $\cos\frac{\theta}{2}\sin\frac{\theta}{2} = \frac{\sin\theta}{2}$:

$$|\vec{n}\rangle\langle\vec{n}| = \begin{bmatrix} \frac{1+\cos\theta}{2} & \frac{\sin\theta}{2} e^{-i\phi} \\ \frac{\sin\theta}{2} e^{i\phi} & \frac{1-\cos\theta}{2} \end{bmatrix}.$$

We can now break this up some more into the components of $\vec{n}$, which are $n_x = \sin\theta\cos\phi$, $n_y = \sin\theta\sin\phi$, and $n_z = \cos\theta$:

$$\sin\theta e^{-i\phi} = n_x - i n_y, \quad \sin\theta e^{i\phi} = n_x + i n_y,$$

so our operator is actually equal to

$$\frac{1}{2}\begin{bmatrix} 1+n_z & n_x - i n_y \\ n_x + i n_y & 1-n_z \end{bmatrix} = \frac{1}{2}\left(I + n_z \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} + n_x \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + n_y \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \right),$$

which gives us what we want:

$$|\vec{n}\rangle\langle\vec{n}| = \frac{1}{2}\left(I + \vec{n}\cdot\vec{\sigma}\right),$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ contains the three Pauli matrices. Indeed, we can now check that if $\vec{n}$ points in the z-direction, we recover our matrix $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$.

We'll now move on to another topic: Taylor series for operators. Is this just a notation for physicists, or is this actually an object in mathematics? We have the famous equation

$$e^{i\theta} = \cos\theta + i\sin\theta,$$

which we can derive in many ways, but one is to use a series expansion and equate real and imaginary parts of the Taylor series.

So if we have a matrix M, how can we evaluate the function $e^{iM\theta}$? It probably doesn't make sense to exponentiate

each entry – this wouldn't have nice properties, and it would behave badly. So the best hope we can have is to mimic the power series e^x: **this is a definition**, and that would just tell us that

$$e^{iM\theta} = I + iM\theta - \frac{M^2\theta^2}{2} - \frac{M^3\theta^3 i}{2} + \cdots.$$

Every term here is a matrix, which is why we turn the 1 at the beginning into an identity matrix. And now this sort of makes sense: if M is actually a diagonal matrix, then e^M is just the matrix with the diagonal entries exponentiating.

But one nice thing to notice here: suppose that our matrix M satisfies $M^2 = I$. (For example, this is true for all of our Pauli matrices.) Then $e^{iM\theta}$ will take on a particularly nice form: we derived $e^{i\theta} = \cos\theta + i\sin\theta$ solely from the fact that $i^2 = -1$, and since M also splits up nicely between the odd and even terms, we'll see (on our homework) that this gives something pretty clean as well, because $(iM)^2 = -I$ is the negative identity matrix.

If we're in two dimensions, things are even nicer: specifically, it's nice to look at e^{iM} when M is a Hermitian matrix. Consider an object like

$$e^{i\vec{a}\cdot\vec{\sigma}}.$$

We can rewrite this by factoring out the length of $\vec{a}$:

$$= e^{i(\hat{a}\cdot\vec{\sigma})|\vec{a}|}.$$

and it turns out $(\hat{a}\cdot\vec{\sigma})^2 = I$ (this takes a few lines, but it's not too bad to show), and then we can use the same "Euler's identity" expansion. This yields

$$e^{i\vec{a}\cdot\vec{\sigma}} = \cos|\vec{a}| + i(\hat{a}\cdot\vec{\sigma})\sin|\vec{a}|.$$

Our final topic for today will be that of **inner products**, which are an object that we often have to invent. We usually need to make a definition that satisfies a set of axioms, and here's an example where that definition may not be so obvious.

Example 113

Let $V = M_n(\mathbb{C})$ be the vector space of $N \times N$ complex-valued matrices: how can we define an inner product?

We know that if we multiply any matrix A (which is a vector in our vector space V) by a complex number a, then we just multiply all of the entries by a. So we need to define the quantity $\langle A, B\rangle$ in a way that satisfies all of the axioms: it must be linear on the right entry and antilinear on the left entry, it must be positive definite, and so on.

The most difficult part of this is that $\langle A, A\rangle$ has to be some nonnegative real number, so something silly like $\langle A, B\rangle = A_{13}B_{57}$ isn't going to work. Remember that we have two "machines" that give us numbers out of matrices: the determinant and the trace. Maybe we want something like

$$\langle A, B\rangle = \det(AB),$$

but this is bad – remember that the determinant grows by a^n if we multiply A by a. Luckily, the trace is much better – it scales by the right amount, and if we didn't know anything, we might want to say that we take the squared magnitude of all entries and add them all up. What's great is that if the norm is 0, the matrix has to be 0, so we must be almost correct. So here's the real answer we're going for:

$$\langle A, B\rangle = \mathrm{tr}(A^\dagger B).$$

We can verify that this does give us exactly what we want!

11 Linear Algebra – Vector Spaces and Operators, Part 4

Today, we'll develop the concept of an **adjoint** or **Hermitian conjugate** operator. This is a bit subtle, but we'll work towards its slowly! To get started, we'll need a bit of background first.

Definition 114

A **linear functional** on a vector space V is a linear map ϕ from V to $\mathbb{F}$.

Since this map is linear, we know that

$$\phi(v_1) + \phi(v_2) = \phi(v_1 + v_2), \quad \phi(av) = a\phi(v),$$

where both of these are equalities of numbers in our field.

Example 115

A linear functional on $\mathbb{R}^3$ can take (x_1, x_2, x_3) to the number $3x_1 - x_2 + 7x_3$.

We can also write this in vector notation if we have a (real) inner product:

$$\phi(v) = \phi(v_1, v_2, v_3) = (3, -1, 7) \cdot (v_1, v_2, v_3) = \langle u, v \rangle,$$

where u is the vector $(3, 1, -7)$. So what we've done with the inner product is extract some vector u out of the linear functional which "defines" ϕ, and this turns out to be true in general!

Theorem 116

Any linear functional ϕ on a vector space V can be uniquely represented as $\phi(v) = \langle u, v \rangle$ for some vector $u \in V$ (and we denote the functional ϕ_u).

Proof. We'll assume V is finite-dimensional. Then let $(e_1, \cdots, e_n)$ be an orthonormal basis of V, and we can write any vector v as

$$v = \langle e_1, v \rangle e_1 + \cdots + \langle e_n, v \rangle e_n.$$

Then applying v and using linearity,

$$\phi(v) = \langle e_1, v \rangle \phi(e_1) + \cdots + \langle e_n, v \rangle \phi(e_n)$$

(because the inner products here are just numbers and can come out of the ϕ). But now we can bring $\phi(e_1)$, which is a number, into the inner product:

$$\phi(v) + \langle e_1 \phi(e_1)^*, v \rangle + \cdots + \langle e_n \phi(e_n)^*, v \rangle = \boxed{\langle e_1 \phi(e_1)^* + \cdots + e_n \phi(e_n)^*, v \rangle},$$

where we are plugging the constants into the left term so we need to add conjguates. But now this last term is just an inner product, and we can take $u = e_1 \phi(e_1)^* + \cdots + e_n \phi(e_n)^*$.

Uniqueness is pretty easy: suppose we could write $\phi(v) = \langle u, v \rangle = \langle u', v \rangle$. Then subtracting the two expressions and using linearity, we must have $\langle u - u', v \rangle = 0$ for all v, which means $u - u' = 0$ (for instance by plugging in $v = u - u'$). □

Like with many other proofs, the central idea here is just that we know how the linear map acts on each of the basis vectors, and then we can determine everything directly.

With that, we can now define the adjoint (physicists use "Hermitian conjugate", which is more pictorial). This will be related to the concept of a Hermitian matrix, if we've seen that in linear algebra before.

Definition 117

The **adjoint** or **Hermitian conjugate** of an operator $T \in \mathcal{L}(V)$ is denoted $T^\dagger$, and it is a map satisfying

$$\langle u, Tv\rangle = \langle = \langle T^\dagger u, v\rangle.$$

To show that this is actually well-defined, note that $\langle u, Tv\rangle$ is a linear functional (we can check the linearity axioms because T is a linear map), so there is **some vector** u' such that it is equal to $\langle u', v\rangle$, and here we're defining $T^\dagger u = u'$.

Now we know that $T^\dagger$ is some map from V to V, but we don't really know that it's linear yet!

Proposition 118

$T^\dagger \in \mathcal{L}(V)$ for any linear operator T.

Proof. Notice that

$$\langle u_1 + u_2, Tv\rangle = \boxed{\langle T^\dagger(u_1+u_2), v\rangle}$$

by definition, but we also have

$$\langle u_1+u_2, Tv\rangle = \langle u_1, Tv\rangle + \langle u_2, Tv\rangle = \langle T^\dagger u_1, v\rangle + \langle T^\dagger u_2, v\rangle = \boxed{\langle T^\dagger u_1 + T^\dagger u_2, v\rangle}.$$

Comparing the two boxed statements shows that we do indeed have $T^\dagger(u_1+u_2) + T^\dagger u_1 + T^\dagger u_2$. Similarly,

$$\langle au, Tv\rangle = \langle \boxed{T^\dagger(au), v\rangle},$$

but we also have

$$\langle au, Tv\rangle = a^*\langle u, Tv\rangle = a^*\langle T^\dagger u, v\rangle = \boxed{\langle aT^\dagger u, v\rangle},$$

and thus $T^\dagger(au) = aT^\dagger u$ and we've verified both linearity conditions. □

So $T^\dagger$ is doing all of the right things, but we still don't really know what it's doing. So we'll show some more properties and do some more examples.

Proposition 119

For any two linear operators S, T, we have $(ST)^\dagger = T^\dagger S^\dagger$.

Proof. This is some more symbol pushing:

$$\langle (ST)^\dagger u, v\rangle = \langle u, STv\rangle = \langle S^\dagger u, Tv\rangle = \langle T^\dagger S^\dagger u, v\rangle.$$

□

Proposition 120

For any linear operator S, $(S^\dagger)^\dagger = S$.

Proof. Notice that

$$\langle u, S^\dagger v\rangle = \boxed{\langle S^{\dagger\dagger} u, v\rangle},$$

but we can also flip the order of our arguments:

$$\langle u, S^\dagger v\rangle = \langle S^\dagger v, u\rangle^* = \langle v, Su\rangle^* = \boxed{\langle Su, v\rangle},$$

and equating the boxed statements gives us what we want. □

Example 121

Suppose our vector space is $V = \mathbb{C}^3$, where we represent our vectors as (v_1, v_2, v_3). Suppose we have the linear map

$$T(v_1, v_2, v_3) = (0v_1 + 2v_2 + iv_3, v_1 - iv_2 + 0v_3, 3iv_1 + v_2 + 7v_3).$$

(where we've written out the linear operator in **components**).

Our goal will be to find $T^\dagger$ and to write the matrix representations for both T and $T^\dagger$ in the **standard basis** (that is, with the three basis vectors $\begin{bmatrix}1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\end{bmatrix}$, and $\begin{bmatrix}0\\0\\1\end{bmatrix}$).

We'll find $T^\dagger$ by using the basic property $\langle u, Tv\rangle = \langle T^\dagger u, v\rangle$. We'll first compute the left side: letting $u = (u_1, u_2, u_3)$, and implicitly using the standard inner product $\langle u, v\rangle = u_1^* v_1 + u_2^* v_2 + u_3^* v_3$, we have

$$\langle u, Tv\rangle = u_1^*(2v_2 + iv_3) + u_2^*(v_1 - iv_2) + u_3^*(3iv_1 + v_2 + 7v_3).$$

Since we want to set this equal to the inner product of (something) with v, we can rewrite this so that we **separate the v-components.** Collecting terms, we see that

$$\langle u, Tv\rangle = (u_2^* + 3iu_3^*)v_1 + (2u_1^* - iu_2^* + u_3^*)v_2 + (iu_1^* + 7u_3^*)v_3.$$

Since this is the inner product of the vector $T^\dagger u$ with v, we must have that the components of $T^\dagger u$ are

$$T^\dagger u = (u_2 - 3iu_3, 2u_1 + iu_2 + u_3, -iu_1 + 7u_3),$$

remembering that we need to complex conjugate each entry, so is become $-i$s and we lose all of the conjugates on our u_is!

It's pretty important for us to understand how to get the matrices out of this – we'll do a bit of the work here. First of all, let's do T: we have

$$Te_1 = T(1, 0, 0) = (0, 1, 3i) = e_2 + 3ie_3,$$

and because Te_i is supposed to be $\sum_k T_{ki} e_k$, this means that $T_{11} = 0, T_{21} = 1, T_{31} = 3i$. (In other words, Te_1 gives us the **first column**.) Repeating this argument, we see that

$$T = \begin{bmatrix} 0 & 2 & i \\ 1 & -i & 0 \\ 3i & 1 & 7 \end{bmatrix}.$$

And finding $T^\dagger$ is exactly the same process – we find that

$$T^\dagger = \begin{bmatrix} 0 & 1 & -3i \\ 2 & i & 1 \\ -i & 0 & 7 \end{bmatrix}.$$

And now notice that these two matrices are **Hermitian conjugates** of each other: we get one from the other by taking the transpose and complex conjugate! And this is not an accident – let's try to get that more generally.

We know by definition that we always have

$$\langle T^\dagger u, v\rangle = \langle u, Tv\rangle.$$

Suppose that $u = e_i$ and $v = e_j$ are two elements of our orthonormal basis. This tells us that

$$\langle T^\dagger e_i, e_j\rangle = \langle e_i, Te_j\rangle,$$

and now we can use the matrix action: since $T^\dagger e_i = \sum_k T^\dagger_{ki} e_k$ (this is an equation worth knowing by heart), the left and right hand side will become

$$\left\langle \sum_k T^\dagger_{ki} e_k, e_j \right\rangle = \left\langle e_i, \sum_k T_{kj} e_k \right\rangle.$$

Now we use orthonormality: the matrix terms are just numbers, so

$$\left(T^\dagger_{ki}\right)^* \delta_{kj} = T_{kj}\delta_{ik}$$

where the complex conjugate comes from us taking the number out from the left entry. And now the left side is $(T^\dagger_{ji})^*$, and the right side is T_{ij}, and flipping indices and taking complex conjugates tells us that

$$T^\dagger_{ij} = (T_{ji})^*.$$

And now we've proved it: the (i,j)th entry of the matrix $T^\dagger$ comes from the transposed entry in T after taking a complex conjugate!

Fact 122

Notice that this only worked because we have an orthonormal basis – in other matrix representations, the Hermitian conjugate will not always be orthonormal! Instead of having that δ_{ij} term above on both sides, we'll now get some ugly number $\langle e_i, e_j\rangle = g_{ij}$. And then we have

$$(T^\dagger_{ki})^* g_{kj} = T_{kj} g_{ik},$$

where we're summing over k on both sides, and now we don't have something quite as nice anymore. But if the matrix of g_{ij}s is at least invertible, we can take the inverse matrix on both sides, and then we get a formula for $T^\dagger$ in terms of g and its inverse and matrix multiplication.

The key point here is that the Hermitian conjugate has a **basis-independent** definition: it's not the conjugate transpose in all bases, so it's better to use the definition with the inner product above!

We're now ready for a nice result which is **only true in complex vector spaces**:

Theorem 123

Let V be a complex inner product space. Then if $\langle v, Tv\rangle = 0$ for all vectors v, then $T = 0$.

This is **not true** in real vector spaces: for example, take $V = \mathbb{R}^2$ and let T be the operator that rotates us by 90 degrees. Then indeed v and Tv are always orthogonal, so $\langle v, Tv\rangle = 0$. So this is another reason why complex vector spaces are nice, and we'll be using this result soon!

Proof. It seems at first sight that this will be a difficult proof – we need something that distinguishes real and complex vector spaces. Our strategy will be to prove that $\boxed{\langle u, Tv\rangle = 0}$ for all vectors u, v in V, which is stronger because we have different vectors on the left and right. Then we can set $u = Tv$ for each v, and that means Tv must always be zero by the inner product axioms!

To prove such a thing (which does require a leap of faith), the idea is to rewrite $\langle u, Tv\rangle$ as a combination of $\langle w, w\rangle$s. First, we can try

$$\boxed{\langle u+v, T(u+v)\rangle - \langle u-v, T(u-v)\rangle},$$

and remember that by theorem assumption, both of these must always be zero. Evaluating by expanding cancels the $\langle u, Tu\rangle$ and $\langle v, Tv\rangle$ terms, but we get cross terms of twice each of $\langle u, Tv\rangle$ and $\langle v, Tu\rangle$. So now we introduce the complex numbers: we try adding in

$$\boxed{+\langle u+iv, T(u+iv)\rangle - \langle u-iv, T(u-iv)\rangle}.$$

Again, the terms $\langle u, T(u)\rangle$ and $\langle iv, T(iv)\rangle$ cancel out, but the cross terms this time are twice each of $i\langle u, Tv\rangle$ and $-i\langle v, Tu\rangle$ (the negative sign because of conjugate homogeneity). But now we have a relative negative sign, and now we can put everything together: it turns out that

$$\boxed{\langle u, Tv\rangle = \frac{1}{4}\left(\langle u+v, T(u+v)\rangle - \langle u-v, T(u-v)\rangle + \frac{1}{i}\langle u+iv, T(u+iv)\rangle - \frac{1}{i}\langle u-iv, T(u-iv)\rangle\right)}.$$

Indeed, this gives us four terms of $\langle u, Tv\rangle$ and zero terms of $\langle v, Tu\rangle$ inside the parentheses! But by theorem assumption, the whole right side is always zero, so we've indeed shown $\langle u, Tv\rangle = 0$ and thus $T = 0$, as desired. □

Let's come up with an application for this:

Proposition 124

If $\langle v, Tv\rangle$ is real for all v, then $T^\dagger = T$ (the operator is **Hermitian** or **self-adjoint**).

Proof. Since this quantity $\langle v, Tv\rangle$ is real, we know it's also equal to $\langle v, Tv\rangle^*$, and thus this is equal to $\langle Tv, v\rangle$. But by the definition of the adjoint, $\langle v, Tv\rangle = \langle T^\dagger v, v\rangle$, and thus

$$\langle Tv, v\rangle = \langle T^\dagger v, v\rangle \implies \langle (T^\dagger - T)v, v\rangle = 0$$

for all vectors v. Alternatively, this means $\langle v, (T^\dagger - T)v\rangle = 0$, and now **using the above theorem**, it means $T^\dagger - T = 0$, so $T^\dagger = T$. □

And this theorem actually goes **both ways**: the reverse direction is pretty easy to show. What's important here is that having a Hermitian operator is the same as saying that $\langle v, Tv\rangle$, the **expectation value** of T, is always real. And that is important because we want to eventually get back to physics!

We'll delay a discussion of diagonalization until next lecture – we'll first prove some basic properties of these Hermitian operators.

Proposition 125
Eigenvalues of a Hermitian operator are real.

Proof. Start with $\boxed{\langle v, Tv\rangle}$. Suppose that v is an eigenvector of T with eigenvalue λ: then $Tv = \lambda v$, so

$$\langle v, Tv\rangle = \langle v, \lambda v\rangle = \boxed{\lambda\langle v, v\rangle}.$$

But we can also move the T to the other side:

$$\langle v, Tv\rangle = \langle T^\dagger v, v\rangle = \langle Tv, v\rangle$$

(because T is Hermitian), and then this simplifies to

$$= \langle \lambda v, v\rangle = \boxed{\lambda^*\langle v, v\rangle}.$$

Equating these two expressions, since v is an eigenvector, we can assume it is nonzero, so $\langle v, v\rangle \neq 0$. Dividing that out yields $\lambda = \lambda^*$, and thus λ must be real, as desired. □

Proposition 126
Eigenvectors of a Hermitian operator with different eigenvalues are orthogonal.

Proof. Suppose we have two eigenvectors v_1, v_2 with eigenvalues λ_1, λ_2 respectively. We're assuming $\lambda_1 \neq \lambda_2$; the idea is that we might get degeneracies where higher-dimensional subspaces all have the same eigenvalue. (In that case, every eigenvector in the subspace with some fixed eigenvalue is orthogonal to every eigenvector in another subspace with a different fixed eigenvalue!)

We'll consider the inner product $\langle v_1, Tv_2\rangle$. We can evaluate this in two ways: first of all,

$$\langle v_1, Tv_2\rangle = \langle v_1, \lambda_2 v_2\rangle = \boxed{\lambda_2\langle v_1, v_2\rangle},$$

but we also have that

$$\langle v_1, Tv_2\rangle = \langle Tv_1, v_2\rangle = \langle \lambda_1 v_1, v_2\rangle = \boxed{\lambda_1\langle v_1, v_2\rangle}$$

because our eigenvalues are already real. Since these expressions are equal and λ_1 and λ_2 are different, this means $\langle v_1, v_2\rangle = 0$ as desired. □

Aside from the class of Hermitian operators, there's also another class that are as important: **unitary operators**. Mathematicians say that such operators are an **isometry**: they preserve length, which means that

$$|Su| = |u|$$

for any vector $u \in V$.

Example 127

Consider the operator $T = \lambda I$, which multiplies any vector by λ. If $|\lambda| = 1$, lengths are preserved, and we have an isometry (which is just a rotation in the complex plane). This is because

$$|Tu| = |\lambda Iu| = |\lambda||u| = |u|.$$

Notice that any unitary operator S only sends the zero vector to zero, because lengths are preserved! And this means that the **null space of S is trivial**, and therefore S is actually invertible.

But to make more progress, let's work with the equations a little bit more:

$$|Su| = |u| \implies \langle Su, Su\rangle = \langle u, u\rangle.$$

We can move the S from one side to another and pick up a dagger:

$$\langle u, S^\dagger Su\rangle = \langle u, u\rangle \implies \langle u, (S^\dagger S - I)u\rangle = 0.$$

Since this is true for all u, we can use our favorite theorem above to find that $S^\dagger S = I$. As a nice property, notice that this tells us that

$$\boxed{\langle u, v\rangle} = \langle u, S^\dagger Sv\rangle = \boxed{\langle Su, Sv\rangle}.$$

And now we have a way to define unitary operators formally:

Definition 128

An operator U is **unitary** if $U^{-1} = U^\dagger$.

(We'll assume that being an inverse from the left is the same as being an inverse from the right.) Because of the boxed equation above, this unitary operator **preserves the inner product**, not just the norms of vectors!

It turns out that unitary operators have particular significance for **bases**: suppose we have an orthonormal basis $(e_1, \cdots, e_n)$. Then defining the basis

$$f_i = Ue_i, \quad U \text{ unitary},$$

notice that

$$\langle f_i, f_j\rangle = \langle Ue_i, Ue_j\rangle = \langle e_i, e_j\rangle = \delta_{ij},$$

so our new basis is actually orthonormal as well! And playing a bit more with some indices, we can find that the entries of the unitary matrix

$$U_{ki} = \langle e_k, Ue_i\rangle$$

can also be written in the f basis:

$$U^{(f)}_{ki} = \langle f_k, Uf_i\rangle = \langle Ue_k, Uf_i\rangle = \langle e_k, f_i\rangle = \langle e_k, Ue_i\rangle,$$

which is exactly the same expression! And this means that **a unitary operator looks the same in both orthonormal bases**.

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We'll start by wrapping up our discussion from last time – at the end, we were trying to define an inner product on the space of matrices $M_N(\mathbb{C})$

$$\langle A, B\rangle = \text{tr}(A^\dagger B).$$

To see what this actually is, we can write it out in index notation: we're summing over all diagonal entries

$$= \sum_j (A^\dagger B)_{jj},$$

and then the matrix multiplication is another sum

$$= \sum_j \sum_i (A^+)_{ji} B_{ij}.$$

Fact 129

It's good to know how to write out matrix multiplication in index notation: in general,

$$(A_1 A_2)_{ij} = \sum_k (A_1)_{ik}(A_2)_{kj}.$$

(This is because we're dotting a row with a column, so the first index should be fixed for the first matrix and the second index should be fixed for the second matrix.)

As will be discussed (or was discussed in the lecture videos), we have $(A^+)_{ji} = A^*_{ij}$ if we're using an orthonormal basis (which we'll assume exists – we'll prove this later). And now we have the definition of this inner product in plain English:

$$= \sum_{ij} A^*_{ij} B_{ij}.$$

Basically, we just take the corresponding elements in the two matrices and multiply them component-wise (with a conjugate)! This means that

$$\langle A, A\rangle = \sum_{ij} |A_{ij}|^2$$

is only zero if all the entries are zero, which is what we want.

It may be convenient to add an extra factor in front when we're using $M_2(\mathbb{C})$: if we define $\langle A, B\rangle = \frac{1}{2}\text{tr}(A^\dagger B)$, then

$$\langle \sigma_1, \sigma_1\rangle = |\sigma_1|^2 = \frac{1}{2}\text{tr}(\sigma_1^\dagger \sigma_1) = \frac{1}{2}\text{tr}(\sigma_1^2) = \frac{1}{2}\text{tr}(I) = 1.$$

(We've used here that the Pauli matrices are Hermitian.) And now if we have a general linear combination $A = a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3$, we have that

$$|A|^2 = \langle A, A\rangle = \sum_{1\le i,j\le 3} a_i^* a_j \langle \sigma_i, \sigma_j\rangle.$$

(We don't need to take the Hermitian conjugate of the σ_is, because they are already Hermitian.) Under this basis, we can check that the σ_is form an orthonormal basis – for example, because $\sigma_i\sigma_j = \delta_{ij} I + i\varepsilon_{ijk}\sigma_k$ – and thus we only get nonzero contribution from $i = j$, and we have

$$|A|^2 = |a_1|^2 + |a_2|^2 + |a_3|^2 \implies |A| = \sqrt{|a_1|^2 + |a_2|^2 + |a_3|^2}.$$

Remark 130. *It's okay to put a number like $\frac{1}{2}$ in front in the definition of our inner product, because there isn't any physical interpretation of this "length" that we've defined yet. And it's just useful to give us this particular form of the answer – it's not directly observable! We're basically picking our units here.*

Let's talk a bit more about matrix representations – there's a few different ways they can come up. Suppose that we're working in three dimensions: then we can write any vector in terms of the basis vectors

$$v = v_1 e_1 + v_2 e_2 + v_3 e_3 = (v_1, v_2, v_3).$$

Sometimes, we're told what form a matrix takes based on what it does to the **basis vectors**: for example,

$$\begin{aligned} T e_1 &= a_1 e_1 + b_1 e_2 + c_1 e_3 \\ T e_2 &= a_2 e_1 + b_2 e_2 + c_2 e_3 \\ T e_3 &= a_3 e_1 + b_3 e_2 + c_3 e_3. \end{aligned}$$

Then how does this matrix look? Well, the image of e_1 is the first column of our matrix (we can check this by multiplying our matrix with $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$), so

$$T = \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{bmatrix}.$$

But there's another way that we often might see T represented: perhaps we're told that a vector v has three **components** (v_1, v_2, v_3), and then the new three components are

$$T(v_1, v_2, v_3) = (a_1 v_1 + a_2 v_2 + a_3 v_3, b_1 v_1 + b_2 v_2 + b_3 v_3, c_1 v_1 + c_2 v_2 + c_3 v_3).$$

Then the matrix looks identical, but notice that our coefficients have been relabeled. This means that acting on the components gives us the rows instead of the columns (because we need a_1, a_2, a_3 to be dotted with v_1, v_2, v_3). So we should try not to confuse these two different perspectives!

One last note about unitary operators: the definition of a unitary operator S is that for all vectors v,

$$|Sv| = |v| \implies \langle Sv, Sv \rangle = \langle v, v \rangle.$$

Basically, if we have two S's, we can delete them. And alternatively, we can move one of the S's over to the other side, which shows us that

$$\langle v, S^\dagger S v \rangle = \langle v, v \rangle \implies \langle v, (S^\dagger S - I)v \rangle = 0.$$

One important result for complex vector spaces:

Proposition 131

If a linear operator T satisfies $\langle v, Tv \rangle = 0$ for all vectors v in a **complex** vector space, then $T = 0$.

The result here is particularly interesting because it's not true in real vector spaces! (For example, consider $\mathbb{R}^2$ and the operator T which rotates everything by 90 degrees.)

This means that for any unitary operator,

$$S^\dagger S - I = 0 \implies S^\dagger S = I.$$

We're working with finite-dimensional vector spaces here, so $S^\dagger$ being a left inverse also means that it is also a right inverse. And this is a nice property to have!

Now, we'll turn our attention to some of the exercise problems.

Example 132

Suppose e_1, e_2 form an basis that is **not** orthonormal: for example, say that

$$\langle e_1, e_1\rangle = 1, \langle e_2, e_2\rangle = b, \langle e_1, e_2\rangle = 0.$$

For example, say that we have an operator T which satisfies

$$Te_1 = e_i + ie_2, \quad Te_2 = e_1 - e_2.$$

Then what can we say about the matrix representation of $T^\dagger$, the adjoint operator?

In an orthonormal basis, the adjoint operator $T^\dagger$ has a matrix representation which is just the Hermitian conjugate of the original. But that's not quite true here, and we need to work through things again.

Remember that we define the adjoint operator in a **basis-independent** way: we say that

$$\langle Tu, v\rangle = \langle u, T^\dagger v\rangle.$$

Let's represent our operators in matrix form though: for example,

$$T = \begin{bmatrix} 1 & 1 \\ i & -1 \end{bmatrix}.$$

We can compute things by taking specific values of u and v: for example,

$$\langle Te_2, e_2\rangle = \langle e_1 - e_2, e_2\rangle = -b,$$

but this is also equal to $\langle e_2, T^\dagger e_2\rangle$. So that tells us something about one of the entries of $T^\dagger$: we can work things through, and we'll see that some extra b terms come through.

Finally, let's talk a bit about projectors. Suppose we have a vector space V, and we have a subspace U: define

$$U^\perp = \{u' : \langle u, u'\rangle = 0 \quad \forall u \in U\}.$$

Basically, any vector in U is perpendicular to any vector in $U^\perp$.

Theorem 133

We can write V as the direct sum

$$V = U \oplus U^\perp.$$

To show this, we just need to write down how to break it up into its components in U and $U^\perp$. Assume that $(e_1, \cdots, e_n)$ is a basis in U: first we can rewrite

$$v = \langle e_1, v\rangle + \cdots + \langle e_n, v\rangle e_n + v - \langle e_1, v\rangle - \cdots - \langle e_n, v\rangle e_n.$$

Now the first sum up to $\langle e_n, v\rangle e_n$ belongs to U, but the remaining part $v - \langle e_1, v\rangle - \cdots - \langle e_n, v\rangle e_n$ is orthogonal to all basis vectors $e_1, \cdots, e_n$, so it is in $U^\perp$! And the rest of the theorem follows by showing that this decomposition is unique because U and $U^\perp$ share only the zero vector.

This allows us to define the **projector** onto u

$$P_u(v) = \langle e_1, v\rangle + \cdots + \langle e_n, v\rangle e_n.$$

This says a few things that are actually important:

$$P_u(e_1) = \langle e_1, e_1\rangle e_1 = e_1,$$

and this is true for all basis vectors. So P_u acts as the identity on U (which makes sense, because we're just "projecting down" to it).

On the other hand, say we have a $w \in U^\perp$. Then $P_u(w) = 0$ is the zero vector, because $\langle e_i, w\rangle = 0$ for all i. And with this, we can figure out all of the behavior of P_u! For example,

$$P_u P_u(v) = P_u(v),$$

because the vector $P_u(v)$ is in U and thus it is fixed by the second P_u. And thus the operator $P_u P_u = P_u$, which is an interesting property to have. It's not true that any operator with this property is an orthogonal projector, but we can still say something in general: we know that the eigenvalues must satisfy $\lambda^2 = \lambda \implies \lambda = 1, 0$ – this means there are a lot of repeated eigenvalues! And it's pretty clear what's happening to the eigenvectors in an orthogonal projector, too: the vectors in U have $\lambda = 1$, and the vectors in $U^\perp$ have $\lambda = 0$. The matrix representation in our specific basis is then (in block form)

$$\begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}$$

where I is an identity matrix of size equal to the dimension of U. And that number is also equal to the trace of P_u, as well as its rank.

13 Dirac's Bra and Ket Notation

Dirac bra-kets are a notation that is pretty nice for quantum mechanics – it's very convenient for some physics problems, but it's **just another way of writing mathematics**. We'll need to take two steps: going from inner products to bra-kets, and going from bra-kets to bras and kets.

The first of these steps is just a change of notation: instead of denoting an inner product as $\langle u, v\rangle$, we'll denote it $\langle u|v\rangle$. (Basically, we put a vertical bar instead of a comma.) This is called a **bra-ket**, and recall that these two objects u and v inside the bra-ket are inside our vector space.

So things aren't too complicated here, but we can still try doing some practice:

Example 134

By linearity, we know that $\langle u, c_1 v_1 + c_2 v_2\rangle = c_1\langle u, v_1\rangle + c_2\langle u, v_2\rangle$. This becomes

$$\langle u|c_1 v_1 + c_2 v_2\rangle = c_1 \langle u|v_1\rangle + c_2 \langle u|v_2\rangle .$$

Conjugate homogeneity gives us different constants on the left:

$$\langle c_1 u_1 + c_2 u_2|v\rangle = c_1^* \langle u_1|v\rangle + c_2^* \langle u_2|v\rangle .$$

Example 135

We can write that the norm of a vector is $|v|^2 = \langle v|v\rangle$, and now the Schwarz inequality reads $|\langle u|v\rangle| \leq |u||v|$.

Example 136

In an orthonormal basis (in other words, a basis wehre $\langle e_i|e_j\rangle = \delta_{ij}$), we can write an arbitrary vector v as

$$v = \sum_i e_i \langle e_i|v\rangle .$$

Again, there isn't really much that's new here – we're just getting used to a slightly different notation. So let's move on to the second part: going from bra-kets to kets and bras. The idea this time is that we want to go from an inner product to two separate quantities: we'll spread the object $\langle u|v\rangle$ apart to get two objects $\langle u|$ and $|v\rangle$, called a **bra** and **ket** respectively.

We'll start with the kets: these turn out to just be regular vectors. If we have a vector v in our vector space V, then we'll just say that $|v\rangle$ is also in that same vector space – the meaning isn't changing here. So the ket symbol is kind of like putting an arrow above the letter v: it tells us that we have a vector. And importantly, **sometimes we use different labels** which represent **properties of the vector** instead of the vector itself.

To explain this a bit more, suppose we have a linear operator T acting on a vector $v = |v\rangle$. Then we can say that $T|v\rangle = |Tv\rangle$: everything is consistent here because all of our labels are regular vectors. But in contrast, consider our spin states, which we often label $|+\rangle, |-\rangle, |\vec{n}, +\rangle$, and so on – these labels $+$ and $-$ have nothing to do with the vector space themselves, so we cannot say that $S_x|+\rangle = |S_x+\rangle$: S_x acts on the ket vector represented by the $+$ state, but it can't act on $+$ itself.

Other than that, though, ket vectors are familiar – they are the usual objects in our vector space. So it just remains to understand what bras are – recall that we introduced the concept of a **linear functional** ϕ, which acts on vectors and gives us numbers. We proved that for every ϕ, we could find a unique vector u in our vector space such that $\phi(v) = \langle u, v\rangle$. And we even called these functionals ϕ_u – remember that these form their own vector space, because they can be added or scaled by constants. So these form some vector space V^*, called the **dual vector space** of V. Notice that this space V^* is parameterized by vectors $u \in V$, so it actually has the **same dimension** as V.

But notice that a bra acts in the same way as one of these linear functionals: a bra $\langle u|$ is labeled by a vector, just like a linear functional, and it can act on a vector v as well:

$$\langle u|\, v = \langle u|v\rangle .$$

So let's just make that our definition: **the bra vector $\langle u|$ is the linear functional ϕ_u**.

We can now switch over to a matrix formulation and try to understand bras and kets as **row and column vectors**, respectively. Remember that the inner product between two vectors $a = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}$ and $b = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$ is

$$\langle a|b\rangle = a_1^* b_1 + \cdots + a_n^* b_n .$$

But notice that this also works if we think of $\langle a|$ as the row vector $(a_1^*, \cdots, a_n^*)$: then indeed we have matrix multiplication

$$\begin{bmatrix} a_1^* & \cdots & a_n^* \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix},$$

which gives us a single number equal to the inner product $\langle a|b\rangle$. So it's easy to construct a bra row vector: take the column vector, map it into a row, and take the complex conjugate of all entries.

Note, by the way, that our bra vectors have pretty nice properties (because they are secretly still linear functionals): for example,

$$\langle u|v\rangle = \langle u'|v\rangle \ \ \forall v \in V$$

implies that $u = u'$, so $\langle u| = \langle u'|$. (To prove this, note that the equation can be rewritten as

$$\langle u - u'|v\rangle = 0 \implies \langle u - u'|u - u'\rangle = 0 \implies u - u' = 0.$$

So now it makes sense to **add bra vectors**: since

$$\langle v_1 + v_2|u\rangle = \langle v_1|u\rangle + \langle v_2|u\rangle = (\langle v_1| + \langle v_2|)\,|u\rangle\,,$$

for any vector u, we know that $\langle v_1 + v_2| = \langle v_1| + \langle v_2|$. Similarly, for any $a \in \mathbb{C}$, we know that

$$\langle av|u\rangle = a^*\,\langle v|\,u = (a^*\,\langle v|)u,$$

which means that the bra $\langle av|$ is also just $a^*\,\langle v|$. What we've just derived are properties of linear functionals, and one related idea is that we often want to turn such a bra into a ket. For instance, if we have $v = a_1v_1 + a_2v_2$, we can say that

$$|v\rangle = |a_1v_1 + a_2v_2\rangle\ a_1\,|v_1\rangle + a_2\,|v_2\rangle\,,$$

but the dual space bra is slightly more complicated:

$$\langle v| = \langle a_1v_1 + a_2v_2| = a_1^*\,\langle v_1| + a_2^*\,\langle v_2|\,.$$

So passing from a ket to a bra can be done by complex conjugating every coefficient and turning every ket vector into a bra vector!

And now we can put everything back together: recall from earlier that in an **orthonormal basis**, we can write any vector as $v = \sum_i e_i\,\langle e_i|v\rangle$. We'll **change our notation** a little bit: the ket vector $|e_i\rangle$ will just be written as $|i\rangle$ (so we're using the label instead of the vector itself, and this way we can write less). And now we find (in bra-ket notation) that

$$|v\rangle = \sum_i |i\rangle\,\langle i|v\rangle\,,$$

and we'll soon see the significance of writing our expressions in this way.

Up until now, everything has just been changing notation, but once we introduce **operators** in bra-ket notation, we'll see the properties work out more practically. Recall that in an orthonormal basis, an easy way to get the matrix coefficients is to find

$$T_{ij} = \langle e_i, Te_j\rangle.$$

The indices match easily (so this formula is easy to remember) – if we want to remember how to prove it, note that $Te_j = T_{kj}e_k$ summed over k, and then we use orthonormality. But now we can rewrite this in bra-ket notation:

$$T_{ij} = \langle e_i|Te_j\rangle = \langle e_i|\,T\,|e_j\rangle$$

(remembering that this is the meaning of $|Te_j\rangle$), and now we can just label our bra and ket basis vectors with numbers: we have

$$T_{ij} = \langle i|\,T\,|j\rangle\,.$$

And what's nice about this is that we can now write the **entire operator** as a sum:

Proposition 137

For any operator T, we can write

$$T = \sum_{i,j} |i\rangle T_{ij} \langle j| .$$

Here, the T_{ij} is just a number – we put it in the middle to be convenient, but it doesn't really act on the ket or bra vector here. An important point – **an object of the form** $|u\rangle\langle v|$, where the ket and bra seem to be in the wrong direction, **is an operator**. After all, feeding in any vector $|w\rangle$ will give us

$$|u\rangle \langle v| |w\rangle = \langle v|w\rangle \cdot |u\rangle ,$$

which is another vector. Here's where the Dirac notation is helping us out – we can basically just "move bras and kets close to each other!" And in the proposition above, we're just summing various operators.

Proof. It suffices to calculate $\langle p| T |q\rangle$ for all numbers p, q, and show that this quantity is indeed equal to T_{pq}. Plugging in the operator above, we get (moving the $\langle p|$ inside the sum)

$$\sum_{i,j} \langle p| |i\rangle T_{ij} \langle j| |q\rangle ,$$

and now we can let the outside objects become bra-kets:

$$= \sum_{i,j} \delta_{pi} T_{ij} \delta_{jq},$$

since we have an orthonormal basis. And this is only nonzero if $i = p$ and $j = q$, which indeed gives us T_{pq} as desired. □

Another way to think of this is that each term $|i\rangle T_{ij} \langle j|$ corresponds to the (i,j)**th entry of the matrix.** So each of these terms is an individual entry, and the object $|i\rangle\langle j|$ is the matrix with a 1 in the (i,j)th place and zeros everywhere else. This presentation will be important to keep in mind going forward.

Example 138

Consider the operator $|m\rangle\langle m|$.

Applying this operator to any vector $|v\rangle$ will give us an object proportional to $|m\rangle$, so this **projects down** to the subspace spanned by $|m\rangle$. If we call this operator P_m, notice that we also have the nice property

$$P_m^2 = |m\rangle \langle m| |m\rangle \langle m|$$

and the inner two terms just evaluate to 1 by orthonormality, so this is

$$= |m\rangle\langle m| = P_m.$$

In particular, the matrix representation of this operator is a diagonal matrix with a single 1, so this has trace 1 – it's a **rank one projector**. Similarly, the object

$$P_{mn} = |m\rangle\langle m| + |n\rangle\langle n|$$

is a rank two projector, because it will give something proportional to $|m\rangle$ plus something proportional to $|n\rangle$. (This has two ones in the matrix representation, so the trace is 2.) But if we repeat this logic, eventually we get to the point where we go through all states: the operator

$$|1\rangle\langle 1| + \cdots + |N\rangle\langle N|$$

is just a diagonal matrix with a 1 on every diagonal entry – thus, we've found the identity matrix! So this is an important property:

Proposition 139

If $|i\rangle$ index an orthonormal basis, then

$$\sum_i |i\rangle\langle i| = I.$$

This is a **completeness relation**, and it might actually look familiar: recall that we wrote an arbitrary vector as

$$v = \sum_i |i\rangle\langle i|v\rangle\,.$$

Even though the interpretation of this is that v is the sum of numbers $\langle i|v\rangle$ times basis vectors $|i\rangle$, we can also think of the right hand side as the identity operator acting on v! So ambiguity of notation actually leads to nontrivial mathematical results here.

Fact 140

Often, we'll simplify an expression by introducing this "complete set of states." We should keep this in mind when we're working through problems!

Example 141

Recall the two-dimensional vector space of spin states: since we have $|+\rangle = \begin{bmatrix}1\\0\end{bmatrix}$ and $|-\rangle = \begin{bmatrix}0\\1\end{bmatrix}$, we should have

$$I = |+\rangle\langle +| + |-\rangle\langle -|\,.$$

Indeed, writing things out in vector form, we have

$$\begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}1 & 0\end{bmatrix} + \begin{bmatrix}0\\1\end{bmatrix} + \begin{bmatrix}0 & 1\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + \begin{bmatrix}0 & 0\\0 & 1\end{bmatrix},$$

which is indeed the identity matrix.

The last basic mathematical idea we'll talk about is that of the adjoint operator. Recall that the defining property for an adjoint $T^\dagger$ is that

$$\langle T^\dagger u, v\rangle = \langle u, Tv\rangle \implies \langle T^\dagger u|v\rangle = \langle u|Tv\rangle\,.$$

We can simplify the left hand side by flipping the arguments and taking a complex conjugate: this equation then simplifies to

$$\langle v|T^\dagger u\rangle^* = \langle u|\,T\,|v\rangle \implies \langle v|\,T^\dagger\,|u\rangle^* = \langle u|\,T\,|v\rangle\,,$$

and now taking another complex conjugate tells us the defining bra-ket relation for adjoint operators:

$$\boxed{\langle v|\,T^\dagger\,|u\rangle = \langle u|\,T\,|v\rangle^*}.$$

This is useful, because it tells us what we derived earlier: to find the matrix elements of $T^\dagger$, we take the matrix elements of T, flipping the row and column, and complex conjugate them! Notably, if we look at the right side of this equation, we can rewrite it as

$$\langle u|Tv\rangle^* = \langle Tv|u\rangle\,.$$

And now we can delete the us on both sides to conclude that

$$\boxed{\langle Tv| = \langle v|\,T^\dagger}.$$

This is another property of bra vectors, and in this case notice that the corresponding ket vector Tv is $|Tv\rangle = T\,|v\rangle$.

Fact 142

In other words, to get the associated bra of $T\,|v\rangle$, we flip the whole object around, remembering to take the adjoint of T as well.

In this notation, the Hermitian operators still satisfy $T^\dagger = T$, so we have

$$\langle Tu|v\rangle = \langle u|Tv\rangle\,,$$

which means that we can move a Hermitian operator between bras and kets freely.

Proposition 143

If $T = |u\rangle\,\langle v|$, then $T^\dagger = |v\rangle\,\langle u|$.

(This is an exercise that we can check on our own.)

Now that we understand the flexibility of this notation (we can always go back to the conventional definitions of inner products and linear functions), we're ready to bring in the physics again with **position and momentum states** and the $\hat{x}$ and $\hat{p}$ operators, with the idea of a **non-denumerable basis**. (Everyone likes to use Dirac notation here, because it helps avoid confusion between similar objects.)

The vector space we're talking about here is the **state space**, and we're going to introduce position states that look like $|x\rangle$. Intuitively, this corresponds to **a particle at the position** x, and now we have to be careful. For example,

$$|ax\rangle \neq a\,|x\rangle\,,$$

because the left hand side represents a particle at the coordinate position ax, while the right hand side represents a particle at the coordinate position x, but where the wavefunction has a different amplitude! Similarly, $|-x\rangle \neq -\,|x\rangle$, and $|x_1 + x_2\rangle \neq |x_1\rangle + |x_2\rangle$ – the fundamental reason for the confusion here is that we're labeling with x, but our vectors aren't that directly connected to the x's – they're wavefunctions! As another way to think about this, suppose we have a three-dimensional vector $\vec{x}$. Then we have the ket $|\vec{x}\rangle$, which corresponds to the particle at the position $\vec{x}$. But our vector space isn't the real $\mathbb{R}^3$ that $\vec{x}$ lives in – it's the infinite-dimensional complex vector space of wavefunctions. So we should be very careful about labels when working in this kind of abstraction – hopefully the introduction of the bra vector is helping with this!

So the reason we like this Dirac notation is that we can distinguish the number or coordinate x from the vector $|x\rangle$. The states $|x\rangle$ form a **basis of our state space** (where $x \in \mathbb{R}$, since we're working in a single dimension), and while the xs can be changed by real numbers, our states can be multiplied by complex numbers. So if we want to define our infinite dimensional vector space, we can't just make a list of our basis vectors – it's a **nondenumerable basis**,

because there are uncountably many basis elements. So we'll use a slightly different inner product here: we'll have

$$\langle x|y\rangle = \delta(x-y),$$

and to deal with normalizability issues, we need to manipulate what we did with finite-dimensional vector spaces before: instead of having $I = \sum_i |i\rangle \langle i|$, we now have

$$I = \int dx\, |x\rangle \langle x| .$$

To make sure we have the correct factor in front, let's have this identity operator act on the vector $|y\rangle$: then

$$|y\rangle = I\,|y\rangle = \int dx\, |x\rangle \langle x|y\rangle = \int dx\, |x\rangle\, \delta(x-y) = |y\rangle ,$$

as desired. And the **basis states are position eigenstates**: we can write the equation

$$\hat{x}\,|x\rangle = x\,|x\rangle .$$

So the $\hat{x}$ operator corresponds to the position observable – the eigenvalue for the state $|x\rangle$ is just x.

So now we can make this a bit less abstract: if we have a particle in a state $|\psi\rangle$, we can write the wave function as

$$\psi(x) = \langle x|\psi\rangle .$$

This is the **overlap** between x and ψ, which tells us some complex number dependent on x. And with this knowledge, we can rewrite

$$|\psi\rangle = I\,|\psi\rangle = \int dx\, |x\rangle \langle x|\psi\rangle = \int dx\, |x\rangle\, \psi(x).$$

And we can interpret this equation and saying that our state $|\psi\rangle$ is a superposition of the basis states, and the weight of each basis state $|x\rangle$ in our sum is just the value of our wavefunction at that point x! And this helps us answer a slightly more general question: if we have two states ϕ and ψ, we can calculate their overlap via

$$\boxed{\langle \phi|\psi\rangle} = \langle \psi| \int dx\, |x\rangle \langle x|\psi\rangle$$

(putting a copy of the identity in between), and now we can bring everything inside to find

$$= \int dx\, \langle \phi|x\rangle \langle x|\psi\rangle = \boxed{\int dx \phi^*(x)\psi(x)}.$$

Indeed, this is what we expect – the inner product on the state space comes from integrating the complex conjugate of one function against the other function. A

Now if we try to compute a matrix element of the $\hat{x}$ operator, we'll put in another copy of the identity:

$$\langle \phi|\,\hat{x}\,|\psi\rangle = \int dx\, \langle \phi|\,\hat{x}\,|x\rangle \langle x|\psi\rangle = \int dx\, x\, \langle \phi|x\rangle \langle x|\psi\rangle .$$

In other words, we're just putting an extra x into the integral here, which is again what we expect.

To make this interesting, we'll introduce **momentum states** as well: these behave exactly the same way, so we'll just list some properties. The basis states are labeled by $|p\rangle$, where $p \in \mathbb{R}$, and we have the familiar equations

$$\langle p'|p\rangle = \delta(p-p'), \quad I = \int dp\, |p\rangle \langle p| , \quad \hat{p}\,|p\rangle = p\,|p\rangle .$$

So completeness and normalization work the same way: the only difference is that we now have to establish a **relation** between the x-basis and p-basis. The **physical assumption** here is that a particle with momentum p has the wave

function

$$\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

(Remember that the first equality here is established by the idea of an "overlap" itself.) So now if we want to compute something like $\langle p|\psi\rangle$ in terms of x-wavefunctions, we introduce another complete set of states:

$$\langle p|\psi\rangle = \int dx \langle p|x\rangle \langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ipx/\hbar}\psi(x),$$

which is the **Fourier transform** of the wave function! To distinguish it from the usual wave function, we'll call it $\tilde{\psi}(p)$ (it lives in the momentum space instead of the coordinate space). In other words, this is the wave function in our p basis.

Example 144

Now we're ready for a classic computation, where we have momentum operator states with a coordinate bra: how can we compute

$$\langle x|\,\hat{p}\,|\psi\rangle?$$

This looks like the momentum operator acting on the wave function (that's $\hat{p}\,|\psi\rangle$)in the x-basis (that's the $\langle x|$ part). So we expect that it'll be $\frac{\hbar}{i}\frac{d}{dx}\psi(x)$, but we can check this directly! To manipulate this expression, we need to figure out what to do with $\hat{p}$. All we know about this operator is that it has momentum eigenstates, so we'll introduce a complete set of states:

$$\langle x|\,\hat{p}\,|\psi\rangle = \int dp \langle x|\,\hat{p}\,|p\rangle \langle p|\psi\rangle\,.$$

And now we can evaluate this a bit: $\hat{p}\,|p\rangle$ is just $p\,|p\rangle$, so this gives us

$$= \int dp (p\langle x|p\rangle)\langle p|\psi\rangle\,.$$

So we don't need to work too hard from here – the idea is that we can get a p to multiply the $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$ by applying $\frac{\hbar}{i}\frac{d}{dx}$ to it. So this is just equal to

$$= \int dp \frac{\hbar}{i}\frac{d}{dx}\langle x|p\rangle\langle p|\psi\rangle\,,$$

and now we can take the $\frac{\hbar}{i}\frac{d}{dx}$ out of the integral because it's a p-integral and there's only a single factor that depends on x – ψ itself doesn't have an x dependence explicitly! So now our expression is just

$$\frac{\hbar}{i}\frac{d}{dx}\int dp \langle x|p\rangle\langle p|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\langle x|\psi\rangle$$

(last step by getting rid of the complete set of states), which is exactly what we claimed. But once we've seen this once, we don't need to repeat it again: the operator $\hat{p}$ is indeed what we expect. And if we want to do some more practice, we can derive the opposite relation

$$\langle p|\,\hat{x}\,|\psi\rangle = i\hbar\frac{d}{dp}\tilde{\psi}(p).$$

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We're starting to talk about bra-kets now – let's focus on projectors, and specifically the punchline we should keep in mind is that in a general projector, we project down onto a subspace U (so every vector is sent to U). But in an

orthogonal projector, we have an **orthogonal subspace** $U^\perp$ which is sent to zero under the projection.

Example 145

Pick a line in the plane through the origin: this gives us a one-dimensional subspace U. Then the orthogonal subspace $U^\perp$ is the perpendicular line to U, and $U \oplus U^\perp$ is the whole space.

This means that any vector v in the plane, can be written as the sum of a vector in U and a vector in $U^\perp$. What's nice about orthogonal projectors in particular is that the component in $U^\perp$ will disappear when wwe project!

Example 146

Pick a plane U through the origin, which is a two-dimensional subspace of our three-dimensional space. One way to specify this plane is to specify a **unit vector** $\vec{n}$ orthogonal to the plane. Then we can define the plane via

$$\vec{n} \cdot \vec{x} = 0 \implies n_1 x_1 + n_2 x_2 + n_3 x_3 = 0.$$

It's interesting that we're defining U, instead of $U^\perp$, to be the set of vectors that are "perpendicular" in some sense instead of $U^\perp$, but hopefully this shows us some of this symmetry here.

Remark 147. *A few notes about this: subspaces have to go through the origin because every subspace has the zero vector. Also, the orthogonal subspace $U^\perp$ is the scalar multiples of $\vec{n}$.*

Problem 148

So now here's a challenge: how can we find the projector P_{U_n} and **describe it as a** 3×3 **matrix?**

One strategy is that assuming $(n_1, n_2) \neq (0, 0)$ (the other case is easy because it's just the projector onto the xy-plane), we can construct an orthonormal basis $\vec{x} = \frac{1}{\sqrt{n_1^2+n_2^2}}(-n_2, n_1, 0)$ and $\vec{y} = \vec{n} \times \vec{x}$ (the cross product). And then

$$Pv = \langle \vec{x}, v \rangle \vec{x} + \langle \vec{y}, v \rangle \vec{y},$$

so the matrix P takes the form $D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ in this orthonormal basis, and then we can do a change of basis $B^{-1}DB$, where B has columns $\vec{n}, \vec{x}, \vec{y}$, to get the matrix in the standard basis.

But there's a simpler way: note that

$$P_{U_n} v = v - P_{\vec{n}} v \implies \boxed{P_{U_n} = I - |\vec{n}\rangle \langle \vec{n}|},$$

because we take the vector and subtract off the component projected onto the orthogonal subspace. (Another way to write this in more standard math notation is that $P\vec{v} = \vec{v} - (\vec{v} \cdot \vec{n})\vec{n}$.) And this is just

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix} \begin{bmatrix} n_1 & n_2 & n_3 \end{bmatrix} = \boxed{\begin{bmatrix} 1-n_1^2 & -n_1 n_2 & -n_1 n_3 \\ -n_1 n_2 & 1-n_2^2 & -n_2 n_3 \\ -n_1 n_3 & -n_2 n_3 & 1-n_3^2 \end{bmatrix}}.$$

(an alternative way to arrive at this answer is to write out $(\vec{v} \cdot \vec{n})\vec{n}$ in terms of $v_1, v_2, v_3, n_1, n_2, n_3$, or to use index notation to show that $P_{ij} = \delta_{ij} - n_i n_j$.) We can check that this has some of the properties we expect: for example, the trace is $3 - n_1^2 - n_2^2 - n_3^2 = 2$, which is indeed the trace of a two-dimensional projector (the rank of the space).

Remark 149. *The main idea here is that if we know that Pv_1 is some specific linear combination $a_1v_1 + a_2v_2 + a_3v_3$, then a_1, a_2, a_3 are specific elements we can write down in our matrix. But alternatively, we can just use some nice properties of projectors and calculate easily with bra-ket notation.*

Remember that we can write down projectors more generally in bra-ket notation: for example, if $\hat{e}_1$ and $\hat{e}_2$ form an orthonormal basis for U_n, then

$$P_{u_n} = |\hat{e}_1\rangle \langle \hat{e}_1| + |\hat{e}_2\rangle \langle \hat{e}_2| .$$

One important property to check is that our projector is Hermitian: indeed, because bras and kets flip, but we also look at a list of operators in reverse, projectors are indeed equal to their adjoint.

And finally, we can think a bit more about **completeness** to bring everything together:

$$|\hat{e}_1\rangle \langle \hat{e}_1| + |\hat{e}_2\rangle \langle \hat{e}_2| + |\vec{n}\rangle \langle \vec{n}| = I.$$

And so indeed this is another way we could have arrived at the fact that the projector is just $I - |\vec{n}\rangle \langle \vec{n}|$.

15 Uncertainty Principle and Compatible Observables, Part 1

Today, we're going to start talking about the **uncertainty** associated to a Hermitian operator. An important idea is that **uncertainty is always measured relative to a state** (mathematically, a deviation is always measured relative to some center point). So we'll always have some Hermitian operator A and some state ψ when we're making our arguments.

Definition 150

The **expectation value** of an operator A in a state ψ is

$$\langle A\rangle_\psi = \langle \psi | A\psi\rangle = \langle \psi, A\psi\rangle.$$

The important point here is that this is always real, because the expectation value of a Hermitian operator is real (since $\langle \psi, A\psi\rangle = \langle A\psi, \psi\rangle = \langle \psi, A\psi\rangle^*$).

From this, how can we define an uncertainty? We need to make sure this quantity is **zero at an eigenstate** and nonzero otherwise.

Definition 151

The **uncertainty** of an operator A relative to a **normalized** state ψ is

$$\Delta A(\psi) = |(A - \langle A\rangle I)\psi|.$$

The idea is that this uncertainty should always be a nonnegative number, and the norm is a natural object that behaves in that way. In fact, the norm of a vector is only zero if we have the zero vector. So let's check that we have what we want: **if the uncertainty were zero**, then we must have $(A - \langle A\rangle I)\psi = 0$, which means that

$$A\psi - \langle A\rangle I\psi = 0 \implies A\psi = \langle A\rangle \psi.$$

And this is an eigenvector equation with the eigenvalue $\langle A\rangle$, so we are indeed in an **eigenstate** when the uncertainty is zero. In fact, in such a state,

$$\langle \psi, A\psi\rangle = \langle \psi, \langle A\rangle \psi\rangle = \langle A\rangle$$

because ψ is normalized, and thus the expectation value of A is indeed $\langle A \rangle$, the eigenvalue of this particular eigenstate. (So everything is nice and consistent!)

Going back to our argument, if we're in an eigenstate, we indeed have the eigenvalue equation, so the vector $(A - \langle A \rangle I)\psi$ is zero, and thus the uncertainty is zero. So we do have an if and only if statement – this second fact, where the only vector with zero norm is the zero vector, is quite powerful.

Squaring the definition, we'll find a formula that is more familiar and better for computations. Note that

$$(\Delta A(\psi))^2 = \langle (A - \langle A \rangle I)\psi, (A - \langle A \rangle I)\psi \rangle$$

(the norm squared is the inner product of the vector with itself), and now we want to move $(A - \langle A \rangle)$ from one argument to the other. We should then take the adjoint of our operator, but A is Hermitian and $\langle A \rangle$ is a real number, so the Hermitian operator is equal to itself! This means that

$$(\Delta A(\psi))^2 = \langle \psi, (A - \langle A \rangle I)(A - \langle A \rangle I)\psi \rangle.$$

And now we can simplify the operator in the right argument: expanding out gives us

$$= \langle \psi, (A^2 - A\langle A \rangle - \langle A \rangle A + \langle A \rangle^2)\psi \rangle$$

(where we've dropped the identity operator for convenience of notation), and now we can expand out the terms one by one. The first term is $\langle \psi, A^2\psi \rangle = \langle A^2 \rangle$, and the second term gives us (pulling out the number inside) $-\langle A \rangle \langle \psi, A\psi \rangle = -\langle A \rangle^2$. Similarly, the last two terms evaluate to $-\langle A \rangle^2$ and $+\langle A \rangle^2$ respectively, and putting this all together gives us the important formula:

Proposition 152

The uncertainty of an operator A can be expressed via the equation

$$(\Delta A(\psi))^2 = \langle A^2 \rangle - \langle A \rangle^2.$$

(This obviously has connections with standard deviation if we use the probabilistic interpretation!) And in particular, this tells us that

$$\langle A^2 \rangle \geq \langle A \rangle^2,$$

because $(\Delta A(\psi))^2$ is always nonnegative.

We'll take a moment to give a **geometrical interpretation** of the uncertainty here – this isn't quite as well known as the rest of the discussion. We can imagine having a vector ψ and an operator A – if ψ is not an eigenstate of A, $A\psi$ will point in a different direction to ψ. If we think of the vector space U_ψ as being the one-dimensional vector space spanned by ψ, we can make two claims when we do an **orthogonal projection** of $A\psi$ down to U_ψ:

- The result of the orthogonal projector is $\langle A \rangle \psi$.
- The orthogonal component $\psi_\perp$ has length equal to the uncertainty of A in the state ψ.

In other words, the amount we've moved away from our U_ψ tells us about the uncertainty! To prove this, we can write our orthogonal projector as

$$P_\psi = |\psi\rangle \langle\psi|,$$

and then when we project our state $A\psi$, we have

$$P_\psi(A\psi) = |\psi\rangle \langle\psi| A |\psi\rangle = |\psi\rangle \langle A \rangle,$$

which is the first claim that we made. And the rest is pretty simple: the vector $A|\psi\rangle - |\psi|\langle A\rangle$ is **orthogonal** to ψ, because we can put a $\langle\psi|$ on the left to get $\langle A\rangle - \langle A\rangle = 0$, so this vector is indeed $\psi_\perp$. And now the norm of this perpendicular vector is the definition of our uncertainty! So the main point here is that our ideas from orthogonal projectors help us to understand uncertainty more pictorally.

So now let's do a computation as an example:

Example 153

Suppose we have a state $|\psi\rangle = |+\rangle$ which is an eigenstate of S_z. What is the uncertainty ΔS_x in the state ψ?

We know that if we're in an eigenstate of z, we're not in an eigenstate of x – in fact, we're in a superposition of two eigenstates of x. So there should be some amount of uncertainty – let's try to figure out the quickest way to do the problem.

Many times, we'll just want to use the formula

$$(\Delta A(\psi))^2 = \langle A^2\rangle_\psi - \langle A\rangle_\psi^2.$$

The expectation of S_x in this state is

$$\langle S_x\rangle = \langle +|\, S_x\, |+\rangle\,,$$

and we should expect this expectation to be zero (because there's an equal chance to be $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$). But if we didn't know that, the best way to do this is to use the matrix representation of S_x (which we don't need to know by heart): writing out $S_x = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$ and $|+\rangle = \begin{bmatrix}1\\0\end{bmatrix}$, and now

$$S_x\,|+\rangle = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \frac{\hbar}{2}\,|-\rangle\,.$$

Since we're taking the inner product of this by multiplying it with $\langle +|$ on the left, we'll indeed get zero (by orthogonality).

Remember, though, that this does not mean the actual uncertainty is zero – we have an $\langle S_x\rangle^2$ term, which does have some uncertainty value. Remember that S_x is a funny matrix: $S_x^2 = \left(\frac{\hbar}{2}\right)^2 I$, which means that the expectation value of S_x^2 is just $\left(\frac{\hbar}{2}\right)^2$ (because the identity always has expectation value 1 on any normalized state). So plugging everything back in,

$$(\Delta S_x)^2 = \left(\frac{\hbar}{2}\right)^2 - 0 \implies \Delta S_x = \frac{\hbar}{2}.$$

Now we're ready to state something more powerful:

Theorem 154 (Uncertainty principle)

For two Hermitian operators A, B and a normalized state ψ,

$$(\Delta A)^2(\Delta B)^2 \geq \left(\left\langle \psi \left| \frac{1}{2i}[A,B] \right| \psi \right\rangle\right)^2$$

(where the uncertainties are taken relative to ψ).

First of all, we have an inequality, so we need to first make sure that this number on the right side is **real**. (Otherwise, it doesn't make sense to compare the two sides.) And it's particularly confusing because there seems to be an i here. But the right idea is to focus on the operator $\frac{1}{2i}[A,B] = \frac{1}{2i}(AB - BA)$. We know that the commutator $[A,B]$ on its own is not going to give you a real number – for instance, $[x,p] = i\hbar$. So that gives us a hint as to why

the i is important: the real idea is that the Hermitian conjugate

$$\left(\frac{1}{i}[A,B]\right)^\dagger = -\frac{1}{i}(AB-BA)^\dagger = -\frac{1}{i}(B^\dagger A^\dagger - A^\dagger B^\dagger),$$

and now because A and B are Hermitian, this is equal to

$$= -\frac{1}{i}(BA-AB) = \frac{1}{i}[A,B].$$

So indeed this operator is equal to its adjoint, so the operator $\frac{1}{2i}[A,B]$ is **Hermitian** and thus has **real expectation values**! And now we don't need to worry: the right side of the uncertainty equality is indeed a nonnegative real number, so everything makes sense.

Remark 155. *We can also take the square root of both sides above and write*

$$\Delta A \Delta B \geq \left|\left\langle \psi \left| \frac{1}{2i}[A,B] \right| \psi \right\rangle\right|,$$

where the outer bars are just the ordinary absolute value.

Either way, the uncertainty principle is nice because we've now defined uncertainties of an observable precisely: we don't need to make an approximate order-of-magnitude statement. And this is an important result, so we need to prove it – not just because it's mathematically better, but also because many interesting questions are based on the concept of **reducing uncertainty**. For example, if the two operators A and B both commute, the uncertainty principle tell us that the product is at least 0, but it doesn't actually tell us outright whether we can get equality: we care when the uncertainty relation is **saturated** (that is, when we get the equality case), and we'll figure that out through our proof.

First, though, we should mention the classic case:

Example 156

Consider the two operators $A = \hat{x}$ and $B = \hat{p}$.

Then $[A,B] = i\hbar$, so the uncertainty principle tells us that

$$(\Delta x)^2(\Delta p)^2 \geq \left(\left\langle \psi \left| \frac{1}{2i} i\hbar I \right| \psi \right\rangle\right)^2.$$

Simplifying, the is cancel and ψ is normalized, so we get

$$(\Delta x)^2(\Delta p)^2 = \left(\frac{\hbar}{2}\right)^2,$$

which is the classic result. The wave functions that **saturate** this (yielding equality) are the strange functions where ψ is actually an eigenstate of x (a totally localized particle) or of p (a totally delocalized particle).

Proof of the uncertainty principle. The central idea of this proof is using the Schwarz inequality. We'll use two auxiliary variables here:

$$|f\rangle = (A - \langle A\rangle I)|\psi\rangle, \quad |g\rangle = (B - \langle B\rangle I)|\psi\rangle.$$

By definition, we know that $(\Delta A)^2 = \langle f|f\rangle$, and $(\Delta B)^2 = \langle g|g\rangle$. Then Schwarz's inequality tells us that

$$(\Delta A)^2(\Delta B)^2 = \langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2,$$

where saturation comes when the vectors f and g are **parallel** to each other. And now we can write this as

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq \text{Re}(\langle f|g\rangle)^2 + \text{Im}(\langle f|g\rangle)^2},$$

since $\langle f|g\rangle^2$ is just some number with a real and imaginary part. Now we can compute

$$\langle f|g\rangle = \langle\psi|\,(A-\langle A\rangle)(B-\langle B\rangle)\,|\psi\rangle\,,$$

and we can find the inner operator by directly expanding:

$$(A-\langle A\rangle)(B-\langle B\rangle) = AB - \langle A\rangle B - A\rangle B\rangle + \langle A\rangle\langle B\rangle,$$

and the expectation of each of these terms is $\langle AB\rangle$, $-\langle A\rangle\langle B\rangle$, $-\langle A\rangle\langle B\rangle$, and $\langle A\rangle\langle B\rangle$, respectively (with the middle two terms, we pull out the constants first). And thus we end up with

$$\langle f|g\rangle = \langle AB\rangle - \langle A\rangle\langle B\rangle,$$

and similarly (so that we can find the real and imaginary parts)

$$\langle g|f\rangle = \langle BA\rangle - \langle A\rangle\langle B\rangle,$$

just by interchanging the roles of A and B. So now we plug back into the boxed equation above: we have that

$$\text{Im}\,\langle f|g\rangle = \frac{1}{2i}\left(\langle f|g\rangle - \langle g|f\rangle\right),$$

and now this simplifies very nicely: the product of expectations cancels, and we just end up with the commutator $\frac{1}{2i}\langle\psi|\,[A,B]\,|\psi\rangle$. And notice that this is exactly what we want – we can even toss the first term on the right side of the boxed equation above, because it's always nonnegative. But let's compute this for completeness: we have

$$Re\,\langle f|g\rangle = \frac{1}{2}\left(\langle f|g\rangle + \langle g|f\rangle\right),$$

and this is $\frac{1}{2}$ of the **anticommutator** of the two operators $\check{A} = A - \langle A\rangle$ and $\check{B} = B - \langle B\rangle$. So at the end of the day, the Schwarz inequality gives us

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq \left(\left\langle\psi\left|\frac{1}{2i}[A,B]\right|\psi\right\rangle\right)^2 + \left(\left\langle\psi\left|\frac{1}{2i}\{\check{A},\check{B}\}\right|\psi\right\rangle\right)^2},$$

which is often called the **generalized uncertainty principle**. But to finish the proof, the second term on the right side is a nonnegative real number, so tossing it keeps the inequality, and we've arrived at our final result. (And in almost all physical examples, the second example is not useful.) □

So let's return now to the question of **saturation**. In order for the uncertainty inequality to actually be an equality, we need two conditions. First of all, we need the Schwarz inequality to be satured, so f and g must be states that are proportional to each other: $|g\rangle = \beta\,|f\rangle$ for some complex number β. But we also need the second term $\left(\left\langle\psi\left|\frac{1}{2i}\{\check{A},\check{B}\}\right|\psi\right\rangle\right)^2$ to be zero – that is, the real part of $\langle f|g\rangle$ is zero. In other words, we need

$$\langle f|g\rangle + \langle g|f\rangle = 0 \implies \langle f|\beta f\rangle + \langle\beta f|f\rangle = (\beta+\beta^*)\,\langle f|f\rangle = 0.$$

Since f does not have zero norm – there is some uncertainty in all of this – $\beta + \beta^* = 0$, which means β is a **pure imaginary number**. So the equality condition is actually nice: f and g are parallel with a purely imaginary constant,

and rewriting this out, our **condition for saturation** is that

$$(B - \langle B \rangle)|\psi\rangle = i\lambda(A - \langle A \rangle)|\psi\rangle$$

for some real number λ. This is a somewhat weird equation to work with, but we'll often have, for instance, a **differential equation** between our two variables (such as in $\hat{x}$ and $\hat{p}$) if we use the same coordinate representation for both operators. Solving for ψ, we can then find $\langle B \rangle$ and $\langle A \rangle$ and see whether that ansatz allows for a value λ. But before we try too hard, let's take the norm of the equation above: we find that

$$\Delta B = |\lambda| \Delta A,$$

and thus $\lambda = \pm \frac{\Delta B}{\Delta A}$.

In the remainder of this lecture, we'll talk about some related notions of uncertainty. We'll start with a handwavy motivation for **energy-time uncertainty**, just to get a picture of what's going on here.

Example 157
Suppose we detect a fluctuation of a waveform in time which suddenly turns on some waves and dies off after a while: the whole process lasts for a time T.

In such a situation, we can try to count the number of full waves that we see: this will be

$$N = \frac{\omega T}{2\pi},$$

where $\frac{2\pi}{\omega}$ is the period of the wave. The problem is that the waves begin and end, so we can't really see the beginning or end: there's an **uncertainty of order** 1 in ΔN. And if there's no uncertainty in T, there's, in some sense, the uncertainty in ω of

$$\frac{T}{2\pi}\Delta\omega = 1 \implies \Delta\omega = \frac{2\pi}{T}.$$

And now we can associate this with a quantum mechanical object: for a **photon**, for example, the uncertainty

$$\Delta E = \hbar \Delta\omega \implies \Delta E = \frac{2\pi\hbar}{T}.$$

So now T is the amount of time it took for the photon to go through our detector: we saw the wave for some time T, and this is now related in some way to the uncertainty of our photon. And now there's some kind of relationship between time and energy!

But there's a delicate issue here: what exactly is "time uncertainty?" We can't really do this precisely, because there's no Hermitian operator for which the eigenstates are times. Instead, we'll need to do something different – we'll use the current uncertainty principle with the Hamiltonian operator $A = H$, along with some operator $B = Q$ which has **no explicit time dependence**. What we find, then, is that

$$(\Delta H)^2 (\Delta Q)^2 \geq \left(\left\langle \psi \left| \frac{1}{2i}[H, Q] \right| \psi \right\rangle \right)^2.$$

And from here, we'll need an auxiliary result: this commutator actually has to do with the **time derivative**! (Even though Q has no explicit time-dependence, $\frac{dQ}{dt}$ will still be nonzero.) Basically, we can write

$$\langle Q \rangle = \langle \psi, Q\psi \rangle$$

and take the time-derivative of this expectation. Even though Q has no explicit dependence on t, it might depends on

x and p, which can change as the wavefunction evolves. So

$$\frac{d\langle Q\rangle}{dt} = \langle \tfrac{\partial\psi}{\partial t}, Q\psi\rangle + \langle \psi, Q\tfrac{\partial\psi}{\partial t}\rangle$$

by the product rule, where we've used that Q has no explicit time-dependence, and here's where the Schrodinger equation comes in:

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi,$$

and plugging this in yields

$$\frac{d\langle Q\rangle Q}{dt} = \langle \tfrac{1}{i\hbar}H\psi, Q\psi\rangle + \langle \psi, Q\tfrac{1}{i\hbar}H\psi\rangle.$$

The constants come out – one as its complex conjugate and one as normal – and we can send H to the other side because H is Hermitian. Thus, this is

$$= \frac{1}{-i\hbar}\langle\psi, HQ\psi\rangle + \frac{1}{i\hbar}\langle\psi, QH\psi\rangle = \frac{i}{\hbar}\langle\psi, (HQ - QH)\psi\rangle.$$

And now we've arrived at our result:

Proposition 158

For any operator Q with no explicit time-dependence,

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle\psi|\,[H,Q]\,|\psi\rangle\,.$$

We'll see in a few lectures how to write this in the **Heisenberg way** as well. But the point is that we can plug this back into our uncertainty relation betwen H and Q: now we have

$$(\Delta H)^2(\Delta Q)^2 = \left(\left\langle\psi\left|\frac{1}{2i}\frac{\hbar}{i}\frac{d}{dt}\langle Q\rangle\right|\psi\right\rangle\right)^2,$$

and since we're taking norms of everything, we find that

$$(\Delta H)^2(\Delta Q)^2 \geq \left(\frac{\hbar}{2}\right)^2\left(\frac{d\langle Q\rangle}{dt}\right)^2 \implies \boxed{\Delta H\Delta Q \geq \frac{\hbar}{2}\left|\frac{dQ}{dt}\right|}.$$

This isn't quite a time uncertainty relation yet, but now we just need to figure out some definitions: we can consider the quantity

$$\Delta t = \frac{\Delta Q}{|d\langle Q\rangle/dt|},$$

which has the units of time and can be physically interpreted as the amount of time it takes for $\langle Q\rangle$ to change by some amount ΔQ – that is, it's a measure of how much time is required for a significant change. If ΔQ is significant and comparable to Q, this is the time needed for significant change, and now we have that

$$\Delta H\Delta t \geq \frac{\hbar}{2}.$$

And this is the best kind of "time" we can get with our current uncertainty principle. We can make some complaints about this equation we've just written down – for example, Δt depends on which operator Q we're using, but we can try different Q's and get more precise results. And there's a version of the uncertainty principle which gives an alternative picture of all of this: if we have a state ψ which is an eigenstate, then nothing changes (it's stationary). Indeed, in such a state, ΔH is zero, and there is an "infinite" time Δt for things to change. But if we have a state that is not an eigenstate of energy, perhaps a superposition of two eigenstates at different energies, we can time-evolve our

state, and we can measure the changes of this state by seeing **how long it takes for the state to become orthogonal to itself.** It turns out that we can get another uncertainty principle out of that:

Proposition 159

Suppose Δt is the **quickest possible time** it takes for $\psi(x,t)$ to become orthogonal to $\psi(x,0)$. Then

$$\Delta t \Delta E \geq \frac{h}{4}.$$

The next statement we'll make is a further comment on this "uncertainty of energy:"

Proposition 160

In an isolated system (that is, one where the Hamiltonian is time-independent), ΔE is constant.

Proof. Take $Q = H$ in Proposition 158 to find that

$$\frac{d}{dt}\langle H \rangle = \frac{i}{\hbar}\langle \psi | [H,H] | \psi \rangle,$$

and now $[H,H] = 0$ (any operator commutes with itself), so the right hand side is zero. So $\langle E \rangle$ is constant, and similarly if we take $Q = H^2$,

$$\frac{d}{dt}\langle H^2 \rangle = \frac{i}{\hbar}\langle \psi | [H,H^2] | \psi \rangle,$$

and again H and H^2 commute with each other, so this is also zero. Thus

$$\frac{d}{dt}(\Delta H)^2 = \frac{d}{dt}\left(\langle H^2 \rangle - \langle H \rangle^2\right) = 0,$$

because both terms on the right side are zero. Thus ΔH must be constant. □

This is useful for thinking about **time-independent processes**:

Example 161

Consider a decay (transition in an atom) which leads to photon radiation. Basically, an atom decays from an excited state to a ground state, and it shoots out a photon.

The concept of energy uncertainty helps us organize our thoughts here: there is a typical lifetime τ, corresponding to the amount of time we need to wait for the excited state to decay. As this lifetime goes through, some observable Q changes a lot – for example, the position of the electron in our orbit, or its squared momentum, or some other quantity. So it is indeed reasonable to define a time uncertainty here relative to that Q, and we'll also have an energy uncertainty: we're in some combination of different states in this atom's excited state, or else we'd be in a stationary state! So the dynamics are such that the interactions (for example) between the electron and nucleus, or with a radiation field, makes this state unstable and associates an uncertainty ΔE. So we get

$$\Delta E \tau \sim \frac{\hbar}{2},$$

where ΔE is the "width" of our set of excited states. But later on, the particle goes to the ground state, so the particle no longer has any uncertainty: conservation of uncertainty means that our **photon** now has an uncertainty $\Delta E = \hbar \Delta \omega$.

This is related to the **hyperfine transition of hydrogen** – this is a situation where physicists get very lucky. We'll study later in this class that because of proton and electron spins in the hydrogen atom, energies actually split (due

to the magnetic dipole interaction), and we get a **hyperfine splitting**. Between the top and bottom states here, we get a photon with a wavelength of about 21 centimeters, which corresponds to a 1420 MHz frequency and an energy difference of 5.9×10^{-6} eV.

But we shouldn't apply this energy difference for our uncertainty principle – the uncertainty in energy comes from how broad the "energy width" of the top state looks, due to interactions. And it turns out that the lifetime τ is about 10 million years, and this corresponds to an energy uncertainty ΔE which is extremely small:

$$\frac{\Delta\lambda}{\lambda} = 10^{-8}.$$

So the nice thing is that the 21 centimeter wavelength is easy to measure – energy-time uncertainty shows us that the gap between the bottom and top states will be pretty much exactly constant!

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We're starting to talk about properties of our (state) vectors and the uncertainty principle. Remember that if we have a Hermitian operator $\hat{A}$ (corresponding to an observable), we can define the uncertainty relative to a state as

$$\boxed{\Delta\hat{A}(\Psi) = |(A - \langle A\rangle)\psi|}.$$

The idea here is that we will measure our operator $\hat{A}$ a bunch of times, and this will give us some statistics (such as the mean and standard deviation). It's important that the uncertainty is **dependent** on our state: for example, the uncertainty in the position depends on how "wide" our wavefunction is; it doesn't make sense to just say "uncertainty in position."

Recall that if Ψ is an eigenstate of $\hat{A}$, we will always measure the same value – the eigenvalue of $\hat{A}$ corresponding to Ψ. Here, $\langle A\rangle$ is the expectation value of our measurement of A, and thus if $\hat{A}\Psi_1 = \lambda\Psi_1$ for some eigenvector Ψ, then

$$\hat{A}(\Psi) = \lambda\Psi \implies \langle\Psi, \hat{A}\Psi\rangle = \langle\Psi, \lambda\Psi\rangle \implies \langle A\rangle = \lambda.$$

So the eigenvalue will also be the expectation value for our operator in an eigenstate! This may explain the notation $\hat{A}\Psi = \langle A\rangle_\Psi\Psi$. And remember that the expectation is only zero if the vector inside the norm on the right side is zero: this means $(A - \langle A\rangle)\Psi = 0$, which only occurs for an eigenstate. This gives us a nice characterization:

Corollary 162
The uncertainty of an operator at a state Ψ vanishes if and only if Ψ is an eigenstate for the operator.

A geometric interpretation of this is to think of our states again as vectors. Let Ψ be some state, and let U_Ψ be the span of Ψ (all scalar multiples of our original state). Then $A\Psi$ will be some other vector – it may not have unit length, so it need not be normalized. And then one interpretation of our result is that **the orthogonal projection of $A\Psi$ into U_Ψ is $\langle A\rangle\Psi$, while the orthogonal part $(A\Psi)_\perp$ has length ΔA.**

Remark 163. *Note that the collapse of the wavefunction doesn't have to do with this projection onto Ψ unless Ψ itself is an eigenstate (because the collapse of the wavefunction is probabilistic).*

There are some operators which are time-dependent, but generally we can "forget about time." At any fixed time, we have a Hermitian operator, and we have a state, which allows us to calculate the uncertainty that time. But later in time, the state may have changed, which means the uncertainty also may change. Usually our operators $\hat{A}$ are time-independent, which makes our calculations easier, and that's what we'll be doing for a while.

What do we do about degenerate eigenstates? It turns out that it doesn't really matter: if e_1, e_2 are two eigenstates with the same eigenvalue, any linear combination of those states is going to be an eigenstate, too. Remember that uncertainty is measured with respect to a given state, so the uncertainty can still be zero in a whole plane of eigenvectors!

Example 164

Let $\hat{A}$ be a Hermitian operator with two eigenstates:

$$\hat{A}\left|\psi_1\right\rangle = \lambda_1\left|\psi_1\right\rangle, \quad \hat{A}\left|\psi_2\right\rangle = \lambda_2\left|\psi_2\right\rangle.$$

Take an arbitrary superposition $\left|\psi\right\rangle = \alpha_1\left|\psi_1\right\rangle + \alpha_2\left|\psi_2\right\rangle$, and assume that it is normalized. What is the uncertainty of $\hat{A}$ with respect to ψ?

We can use the formula (derived by squaring the definition of $\Delta\hat{A}$ and then writing out the norm squared on the right hand side as an inner product)

$$(\Delta\hat{A}(\psi))^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2.$$

Remark 165. *Before we get too lost in the algebra, note that if $\alpha_1 = 0$ or $\alpha_2 = 0$, we have an eigenstate. This means $\Delta\hat{A}(\Psi)$ should be zero if α_1 or α_2 vanish. Also, if the λs are the same, the uncertainty should also be zero (because we always measure the same value).*

Remember that $\hat{A}$ takes on value λ_1 with probability $|\alpha_1|^2$ and λ_2 with probability $|\alpha_2|^2$ (where $|\alpha_1|^2 + |\alpha_2|^2 = 1$), so

$$\langle\hat{A}\rangle = |\alpha_1|^2\lambda_1 + |\alpha_2|^2\lambda_2.$$

(One way to do this is to think of ψ_1 and ψ_2 as basis vectors $\begin{bmatrix}1\\0\end{bmatrix}$ and $\begin{bmatrix}0\\1\end{bmatrix}$, so we know that $\hat{A} = \begin{bmatrix}\lambda_1 & 0\\0 & \lambda_2\end{bmatrix}$ in this basis. Then we can find the expectation of ψ via $\psi^*\hat{A}\psi$.) Similarly, we find that

$$\langle\hat{A^2}\rangle = |\alpha_1|^2\lambda_1^2 + |\alpha_2|^2\lambda_2^2.$$

So now we can calculate the uncertainty directly, but we can do some thinking first: we know that the uncertainty should vanish when $\alpha_1, \alpha_2, \lambda_1 - \lambda_2$ are zero. But we also need to make sure the quantity is always nonnegative and real, so a good guess is

$$\Delta\hat{A}(\psi) \stackrel{?}{=} |\alpha_1||\alpha_2||\lambda_1 - \lambda_2|.$$

(Remember that the uncertainty should have units of λ.) At this point, we might just be off by a constant factor, but of course this is just a guess. Anyway, we can calculate now:

$$(\Delta A)^2 = \lambda_1^2|\alpha_1|^2 + \lambda_2^2|\alpha_2|^2 - \left(\lambda_1^2|\alpha_1|^4 + \lambda_2^2|\alpha_2|^4 + 2\lambda_1\lambda_2|\alpha_1|^2|\alpha_2^2|\right).$$

Collecting terms, noting that $|\alpha_1|^2 - |\alpha_1|^4 = |\alpha_1|^2(1 - |\alpha_1|^2) = |\alpha_1|^2|\alpha_2|^2$,

$$(\Delta A)^2 = \lambda_1^2|\alpha_1|^2|\alpha_2|^2 + \lambda_2^2|\alpha_2|^2|\alpha_1|^2 - 2\lambda_1\lambda_2|\alpha_1|^2|\alpha_2|^2$$

simplifies nicely to

$$(\Delta A)^2 = (\lambda_1 - \lambda_2)^2|\alpha_1|^2|\alpha_2|^2,$$

and indeed our earlier guess is accurate!

17 Uncertainty Principle and Compatible Observables, Part 2

Last time, we talked about the **energy-time uncertainty relations**, which tell us something about how fast the state can change. One interesting way to analyze this is to look at the inner product

$$\langle\psi(0)|\psi(t)\rangle = \int d\vec{x}\psi^*(t=0,\vec{x})\psi(t,\vec{x}).$$

In a sense, this tells us how quickly a state can change: at $t = 0$, this overlap is 1, and perhaps after some time the overlap is 0. (At that point, we can say that the state has changed a lot.) To make this quantity a bit easier to work with, we might as well take its squared norm $|\langle\psi(0)|\psi(t)\rangle|^2$. If we assume that the system is governed by a **time-independent Hamiltonian** (which will help us prove the time-energy uncertainty relationship we established at the end of last lecture), we can consider the case in which ψ is some energy eigenstate. Such states evolve with a phase $e^{-iHt/\hbar}$, so **the overlap would remain equal to** 1 **for all times** t.

And in general, we can evaluate $\psi(t)$ as a Taylor series in t – if we go to quadratic order, we'd find that this overlap only depends on things like ΔH and Δt. This kind of analysis has to do with quantum computation – in a quantum computer, we want to change states quickly, and these inequalities limit the speed of a quantum computer!

Now that we've discussed a lot of properties of uncertainty, we'll do an example:

Example 166

Consider the Hamiltonian (for a one-dimensional particle)

$$H = \frac{p^2}{2m} + \alpha x^4,$$

where $\alpha > 0$.

We know the expectation value of the energy in the ground state, and we used the **variational principle** to find an upper bound on the ground state energy. We're going to use the uncertainty principle now to get a **lower bound**, so we have a window for the energy of the ground state. First of all, we know that

$$\langle H^2\rangle_{\text{gs}} = \frac{\langle p^2\rangle_{\text{gs}}}{2m} + \alpha\langle x^4\rangle_{\text{gs}},$$

and now we know that $\langle x\rangle_{\text{gs}} = 0$, because symmetric potentials have either symmetric or antisymmetric wavefunctions – it's not antisymmetric because it's a ground state. Similarly, the expectation of the momentum $\langle p\rangle_{\text{gs}} = 0$ as well, because we can imagine computing it:

$$\int \psi \frac{\hbar}{i}\frac{\partial}{\partial x}\psi,$$

and this integrand is a total derivative (it's $\frac{d}{dx}$ of a constant times ψ^2), so it evaluates to zero for a bound state where the value is zero at both ends. So now we can control the $\langle p^2\rangle_{\text{gs}}$ term: we know that

$$(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2,$$

so in the ground state, we know that $(\Delta p)^2_{\text{gs}} = \langle p^2\rangle_{\text{gs}}$, and now we can get a Δp into our expression. The main problem is that we need to deal with $\langle x^4\rangle$, and now we're going to use the fact that $\langle x^4\rangle \geq \langle x^2\rangle^2$ (using the fact that $\langle A^2\rangle \geq \langle A\rangle^2$ for the operator $A = x^2$), and thus we can get a Δx into our expression as well! So now

$$\langle x^4\rangle_{\text{gs}} \geq (\Delta x)^4_{\text{gs}},$$

where we've used that $\langle x^2 \rangle = (\Delta x)^2$ in the ground state, and thus

$$\langle H \rangle_{\text{gs}} = \frac{(\Delta p)^2_{\text{gs}}}{2m} + \alpha \langle x^4 \rangle_{\text{gs}} \geq \frac{(\Delta p)^2_{\text{gs}}}{2m} + \alpha (\Delta x)^4_{\text{gs}}.$$

And this is all good – we're on track to get a lower bound for $\langle H \rangle$ – and now we're ready to use the uncertainty principle! Since $\Delta p \Delta x \geq \frac{\hbar}{2}$ in any state, this holds for the ground state, and thus $\Delta p \geq \frac{\hbar}{2\Delta x}$. Plugging this in, we find that

$$\langle H \rangle_{\text{gs}} \geq \frac{\hbar^2}{8m(\Delta x)^2_{\text{gs}}} + \alpha (\Delta x)^4_{\text{gs}}.$$

And now we have an inequality, but we don't know the actual value of Δx. Fortunately, if we **minimize the right hand side** over all Δx, we'll get a bound that's true regardless of what Δx actually is! So

$$\langle H \rangle_{\text{gs}} \geq \min_{\Delta x} \left(\frac{\hbar^2}{8m(\Delta x)^2_{\text{gs}}} + \alpha (\Delta x)^4_{\text{gs}} \right),$$

and this is now just a calculus problem – we can take the derivative with respect to Δx and set it equal to 0. It turns out that $\frac{A}{x^2} + Bx^4$ is minimized at $x^2 = \frac{1}{2^{1/3}} \left(\frac{A}{B}\right)^{1/3}$, and the value of the function is $2^{1/3} \frac{3}{2} A^{2/3} B^{1/3}$. So plugging in the coefficients, we find our final answer:

$$\langle H \rangle_{\text{gs}} \geq 2^{1/3} \frac{3}{8} \left(\frac{\hbar^2 \sqrt{\alpha}}{m} \right)^{2/3} \approx 0.4724 \left(\frac{\hbar^2 \sqrt{\alpha}}{m} \right)^{2/3}.$$

This turns out to be an okay bound – the actual answer has a constant of 0.668, and the variational principle gave something like 0.69. But this gave us something, and the point is that this is **completely rigorous**! Sometimes the uncertainty principle is used to make a handwavy argument which is basically just dimensional analysis, but every inequality we've established here is exact.

This concludes our initial discussion of uncertainty, and we're going to move on to a new topic now: **diagonalization of operators**. Essentially, suppose we have some operator which is important to us. To understand it better, we want to **find an ideal basis** so that the operator is as simple as possible in this basis.

Definition 167

An operator T is **diagonalizable** if there is a basis in which the matrix representation of T is diagonal (only the diagonal entries are allowed to be nonzero).

Conceptually, suppose we have a diagonal matrix for T in some basis $(u_1, \cdots, u_n)$: then the matrix action on our basis looks like

$$T u_i = T_{ki} u_k,$$

but the only nonzero term here is the one where $i = k$, so this is actually just equal to $T_{ii} u_i$. This is some number times u_i – call it λ_i – and now we know that $T u_1 = \lambda_1 u_1$, $T u_2 = \lambda_2 u_2$, and so on, which means that **the basis vectors are eigenvectors of our operator**. But the logic goes both ways here – if we have a set of eigenvectors spanning the space, we can just pick that to be our basis. That gives us the following result:

Proposition 168

An operator is diagonalizable if and only if it has a set of eigenvectors that span the vector space.

Example 169

We know that $\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$ is not diagonalizable.

This is because the characteristic equation is $\lambda^2 = 0$, so the only eigenvalue is $\lambda = 0$. But the only eigenvectors there are of the form

$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

which means we're forced to have $b = 0$. Thus there is only one dimension of eigenvectors (along $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$), but we have a two-dimensional vector space. So it's impossible to diagonalize this linear operator!

So now we'll be a bit more concrete: say we have a vector space with some basis $(v_1, \cdots, v_n)$, and we have some linear operator T. Its matrix representation $T_{ij}(\{v\})$ has no particular reason to be diagonal, and we want to figure out a concrete condition to understand whether we can **change bases** to make the matrix diagonal. Recall that we use an invertible linear operator A to change the vectors such that our new basis is $u_k = Av_k$ (for all $1 \leq k \leq n$). We proved that there is a relationship between the matrix elements in the two bases: we have

$$T(\{u\}) = A^{-1}T(\{v\})A,$$

or more explicitly, the element

$$T_{ij}(\{u\}) = A^{-1}_{ik}T_{kp}(\{v\})A_{pj},$$

where we're summing over p and k. So we want to find a matrix A where this works out, and an important idea at this point is that there are **two different ways** to think about diagonalization: one is that we're **changing bases** to make our operator diagonal in the **new basis**, and the other is that we're finding a **new operator** such that $A^{-1}TA$ is diagonal in our **original basis**. We can write this out more explicitly: suppose that $Tu_i = \lambda_i u_i$, where the u_i are our eigenvectors for T. (We're not summing over i here – this is a problem with notation.) Then to show that $A^{-1}TA$ is diagonal in our v_i basis, we know that

$$Tu_i = \lambda u_i \implies TAv_i = \lambda_i Av_i \implies A^{-1}TAv_i = \lambda_i v_i.$$

And now, indeed $A^{-1}TA$ has eigenvectors equal to our basis elements, so $A^{-1}TA$ is diagonal in our v basis.

Fact 170

Notice that the columns of A are the eigenvectors of T. This is because $u_k = Av_k$, and A acting on v_k gives us $\sum_i A_{ik}v_i$. And indeed, this tells us that the kth column of A should be u_k, as long as we think of v_k as a column vector with a 1 in the kth entry and a 0 everywhere else.

Beyond the idea of diagonalization, though, we want to talk about a more relevant term for our Hermitian operators:

Definition 171

A matrix is **unitarily diagonalizable** if there exists an orthonormal basis of eigenvectors.

This is a stronger condition than just being diagonalizable, and being able to achieve this is very good – this is because we've then broken down our vector space into basis spaces that are all orthonormal! Concretely, imagine that

we start with some orthonormal basis $\{v\}$: we can then pass to some other orthonormal basis $\{u\}$ with some operator (analogous to the A above), and remember that we achieve this with a **unitary operator**. So a matrix that is unitarily diagonalizable must be of the form

$$T(\{u\}) = U^{-1}T(\{v\})U$$

for a unitary operator U – in words, this means **there is a unitary operator which takes us to the "privileged basis" in which our operator is diagonalizable**.

And the main theorem of this subject is one of the most important theorems of linear algebra – we can characterize the set of operators for which we can have an orthonormal basis of eigenvectors. It turns out that Hermitian operators are indeed unitarily diagonalizable, but that's not actually the complete result. Here's the class of operators we care about:

Definition 172

An operator M is **normal** if $[M^\dagger, M] = 0$.

So Hermitian operators are normal, because $M^\dagger$ and M are the same matrix. Similarly, anti-Hermitian operators are also normal, because $M^\dagger$ is $-M$, and unitary operators are normal because $U^\dagger U$ and $UU^\dagger$ are both the identity matrix. So many of the nice classes of operators we've been talking about are all normal!

Proposition 173

If M is a normal operator, and $|w\rangle$ is an eigenvector of M with eigenvalue $\lambda \in \mathbb{C}$, then $M^\dagger w$ is an eigenvalue of $M^\dagger$ with eigenvalue λ^*.

The usual strategy for proving something like this is to show that $(M^\dagger - \lambda^*)w$ is the zero vector, because it has zero norm. And with this, we're ready to get to the result that we've been working towards:

Theorem 174 (Spectral theorem)

Let M be an operator in a complex vector space V. Then V has an orthonormal basis of eigenvectors if and only if M is normal.

To prove this, we need to prove that any unitary diagonalizable operator is normal, and also that any normal operator can be unitarily diagonalized.

Proof sketch. Suppose M is unitarily diagonalizable. Then there is a unitary operator U such that $U^\dagger M U = D_M$ for some diagonal matrix D_M, which means that

$$M = U D_M U^\dagger.$$

Therefore,

$$M^\dagger = (U D_M U^\dagger)^\dagger = U D_M^\dagger U.$$

Now to check that the matrix is normal, we need to check that the computator is zero:

$$M^\dagger M = U D_M^\dagger D_M U^\dagger,$$

where we've used that the middle $U^\dagger U$ are just the identity matrix, and

$$M M^\dagger = U D_M D_M^\dagger U^\dagger.$$

But these are the same, because any two diagonal matrices commute – we multiply elements along the diagonal! So indeed M is normal.

The other part of the proof – showing that a normal operator is unitarily diagonalizable – is done by induction, and the idea is that any matrix in a complex vector space has at least one eigenvalue with a corresponding eigenvector. Use that eigenvector as our first basis vector, and show that we can reduce the matrix so that there are zeros in the first row and column – now do this again step by step with the remaining smaller matrix. The point is that normality allows us to show that we can indeed get zeros in the off-diagonal entries, and eventually we'll have a diagonal matrix as desired. (It's good for us to read through the proof, because it will make a lot of what's going on more clear!) □

Our final topic of this lecture is **simultaneous diagonalization**, and we're going to focus on Hermitian operators from here on out. This is one of the most important ideas in quantum mechanics, because it's what allows us to label and understand a state system! For example, if we have a set of energy eigenstates, but there is a degeneracy in the eigenvalues, we might have a lot of states with the same energy. And we need to be able to distinguish these states – they are different, or else they'd be the same state – so there is likely some other physical property corresponding to some other operator, and we'll want to **simultaneously diagonalize** these two operators so that we can characterize with the two properties at the same time.

Definition 175

Two linear operators S and T are **simultaneously diagonalizable** if there is a basis in which every basis vector is an eigenstate of both S and T.

Proposition 176

If S and T are simultaneously diagonalizable, S and T must commute.

Proof. The fact that two operators commute (or don't) is a **basis-independent** statement. If S and T are simultaneously diagonalizable, there is a basis in which both S and T have diagonal matrices – since diagonal matrices always commute, S and T must commute in any basis. □

This is **not** a sufficient statement, though – not every matrix is diagonalizable. But we do know that normal operators are diagonalizable, and now we can make a plausible claim:

Theorem 177

If S and T are **commuting Hermitian** operators, then they can be simultaneously diagonalized.

This result is easy to prove in the case where there are **no degeneracies**. Remember that a **degenerate spectrum** is a situation where an eigenvalue is repeated – then we have three different cases. Either (1) both are non-degenerate, (2) one is non-degenerate, or (3) both are degenerate. We can prove cases (1) and (2) together, and we'll do that first: suppose that the operator with a non-degenerate spectrum is T.

Proof when T's spectrum is non-degenerate. In this case, there exists an orthonormal basis $(u_1, \cdots, u_n)$ by the spectral theorem, such that

$$T u_i = \lambda_i u_i$$

for all i, and $\lambda_i \neq \lambda_j$ for all $i \neq j$. So now each of the u_i eigenvectors generate one-dimensional **invariant subspaces**: we now want to know what happens to these u_is under S. Note that

$$ST u_i = \boxed{\lambda_i S u_i},$$

but S and T commute, so we also have

$$ST u_i = \boxed{TS u_i}.$$

So the vector Su_i must belong to the invariant subspace for u_i, because it's an eigenvector of T with eigenvalue λ_i (and there's only one dimension of eigenvalues for which this is true)! So $Su_i = w_i u_i$ for some w_i, and indeed we've shown that u_i is also an eigenvector of S (possibly with a different eigenvalue). So **eigenstates of T are also eigenstates of S**, and we've indeed shown that S and T have a common set of eigenvectors, as desired. □

The other case is a bit more interesting:

Proof when operators have degeneracies. If S has degeneracies, we will have eigenstates that generate subspaces with dimension larger than 1. Let U_k denote the set of all vectors such that $Su = \lambda_k u$, and say that this space U_k has dimension d_k. In other words, the kth eigenvalue has a corresponding space U_k such that the entire space is getting scaled by **the same amount** λ_k. And our vector space can be decomposed as

$$V = U_1 \oplus U_2 \oplus \cdots \oplus U_m,$$

where all of these subspaces U_i have different dimensions – some might have no degeneracy, while others have degeneracy three.

Regardless, we can denote the basis of eigenvectors for U_k as $(u_1^{(k)}, u_2^{(k)}, \cdots, u_{d_k}^{(k)})$ – by the spectral theorem, this is an orthonormal basis. So we have a basis for V by putting all of these basis elements together: we can thus say that

$$(u_1^{(1)}, u_2^{(1)}, \cdots, u_{d_1}^{(1)}, \cdots, u_1^{(m)}, u_2^{(m)}, \cdots, u_{d_m}^{(m)})$$

is a basis for V. And we know that S is indeed diagonal in this basis, because every vector is an eigenvector of S by construction – the first d_1 diagonal entries are λ_1, the next d_2 are λ_2, and so on.

So this is a good basis, but there's another basis that also works well: we can consider the basis

$$(V_1 u_1^{(1)}, V_1 u_2^{(1)}, \cdots, V_1 u_{d_1}^{(1)}, \cdots, V_m u_1^{(m)}, V_m u_2^{(m)}, \cdots, V_m u_{d_m}^{(m)}),$$

where $V_1, \cdots, V_m$ are some **arbitrary unitary operators** acting on the spaces $U_1, \cdots, U_m$. Basically, we take the subspace U_1 and act with a unitary operator V_1 on it, take the subspace U_2 and act with a unitary operator V_2 on it, and so on. Because our operators are **unitary**, we still have an **orthonormal basis** for each U_i, and thus we still have an orthonormal basis of V here (because the different spaces with different eigenvalues are already orthogonal)!

So now here's the catch: the spaces U_k are S-invariant subspaces, and we want to show that they are also T-invariant! Suppose that $u \in U_k$: then

$$S(Tu) = T(Su) = \lambda_k (Tu),$$

so the vector Tu also has eigenvalue λ_k. Since we defined U_k to be the space of eigenvectors with eigenvalue λ_k, $Tu \in U_k$ as well! So the idea now is that T keeps the invariant subspaces: it's in the block form $\begin{bmatrix} D_1 & 0 & \cdots & 0 \\ 0 & D_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D_m \end{bmatrix}$, where D_i is a d_i by d_i block matrix. Right now, we haven't simultaneously diagonalized T yet, but now we can take those **arbitrary unitary operators** V_i that we defined above. Since T is Hermitian, it's also Hermitian on each diagonal block matrix, so we can diagonalize each block: those are the V_is that we use! So once we do this for each block matrix, we can diagonalize T without destroying the diagonalization of S, as desired. □

This argument also extends to an arbitrary number of operators: if $S_1, \cdots, S_n$ are all mutually commuting Hermitian operators, then we can simultaneously diagonalize them.

18 March 2, 2020

There's a test next week, Wednesday night at 7:30 (in our regular recitation room). MIT regulations require lecture/recitations to be canceled on the day of an exam, so we will **not have class on Wednesday, March 11**. It should take about an hour and a half long, but the room is booked for two hours.

We'll get a formula sheet with main results – a good way to start studying is to read over the formulas and make sure we understand everything there. The exam itself will have some wave mechanics, spin 1/2, uncertainty, and some (about a third) linear algebra.

Today, we'll discuss operators, bras and kets, and other related topics. We'll start a real treatment of time evolution soon – next lecture, we'll see an argument why having a unitary operator that evolves states implies the Schrodinger equation.

Example 178

Consider a **time-independent** Hamiltonian H: that means that there is no explicit t. Then how can we solve the Schrodinger equation $i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$? (Note that Ψ denotes "full" wavefunctions in terms of both x and t.)

The idea is that we can write the **energy eigenstates** in the separable form

$$\Psi(x,t) = \psi(\hat{x})e^{-iEt/\hbar}$$

as long as $H\psi = E\psi$. The time-independent phase $e^{-iEt/\hbar}$ only comes up in the final form of the solution: it does not directly affect the $\psi(x)$ component! And now this means that if we can write our initial wavefunction as a linear combination of **energy eigenstates**

$$\Psi(x,0) = \sum_n \alpha_n\psi_n(x), \quad H\psi_n(x) = E\psi_n(x),$$

then we can just evolve the "basic solutions" individually:

$$\Psi(x,t) = \sum_n \alpha_n\psi_n(x)e^{-iE_nt/\hbar}.$$

Another way to say this is that we have a **unitary operator** $U(t) = e^{-iHt/\hbar}$ which does the time evolution for us. This operator has the property that

$$\Psi(t) = U(t)\Psi(t=0).$$

Specifically, what's happening is that when we have $e^{-iHt/\hbar}$ acting on our eigenstate $\psi_n(x)$, H always gives E_n. So the exponential of H hitting ψ_n just gives the exponential of E_n instead!

Remark 179. *Things will get a bit more sophisticated starting next lecture, where we'll consider the time-evolution operator in general. If H depends on time, this can look much more complicated. But if H depends on time, but H commutes at different times, we have a simple generalized formula. (And if H rotates from one component of spin to another or does something else crazy, the formula is just messy.)*

Let's discuss a little now about some of the diagonalization arguments we've been making. There's a few points to pay attention to for the Spectral Theorem:

- The theorem is usually stated for Hermitian operators, but it's more generally true for **normal operators**: that is, operators M such that $[M^\dagger, M] = 0$.
- The result says that **there is an orthonormal basis of eigenvectors**, which actually tells us a lot: it gives as many eigenvectors as the dimension of our vector space. In addition, this basis has very nice properties, because all of the eigenvectors are perpendicular. (Note that there isn't a **unique** orthonormal basis, because of degeneracies in eigenvalues. For example, if we have a plane of eigenvectors with the same eigenvalue, then we can pick any two orthonormal vectors in that plane.)

We've probably heard the phrase **unitarily diagonalizable**: what this really means is that if we start with a normal (but not diagonal) operator M on an orthonormal basis $(e_1, \cdots, e_n)$, we can apply a unitary transformation to turn our basis into $(\tilde{e}_1, \cdots, \tilde{e}_n)$, **in which** M is diagonal:

$$U^\dagger M U = D_M.$$

And it makes sense that we want a unitary operator U: such operators are those that preserve the inner product.

Fact 180

By the way, we know that any operator has at least one eigenvector: this is because the eigenvalues λ of an operator satisfy

$$\det |M - \lambda I| = 0.$$

This gives a degree n polynomial equation in λ, and the Fundamental Theorem of Algebra says that this always has a solution.

This is particularly important, because we show the Spectral Theorem by induction, extracting one eigenvalue at a time and showing that we can diagonalize the resulting matrix.

Problem 181

Is the matrix $M = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$ diagonalizable?

Because the determinant of $M - \lambda I$ is just $(1-\lambda)^3$, the only eigenvalue of this matrix is 1. But then if we try to solve the equation $v = Mv$,

$$v = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \begin{bmatrix} v_1 + v_2 + v_3 \\ v_2 + v_3 \\ v_3 \end{bmatrix} = Mv$$

only has solutions where $v_2 = v_3 = 0$, so we only have one (set of) eigenvector(s). Basically, what's going on is that we have a "shear matrix," so things aren't being scaled in the same way as they would in (for example) a Hermitian operator.

Another way to think of this is that if we had three eigenvalues of 1, we would want to diagonalize our matrix into $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, the identity matrix. But this is definitely not going to happen, because for any unitary operator, $U^\dagger I U = U^\dagger U = U^{-1} U = I$ is just the identity matrix, so it can't turn into M.

We'll finish with some exercises involving bra-ket notation:

Problem 182

Consider the operator $T = |u\rangle\langle v|$. What is the operator $T^\dagger$, and what is the trace of T?

We know that T applied to any vector will give a $c|u\rangle$ for some complex number c. (Specifically, we have $T|w\rangle = |u\rangle\langle v|w\rangle$). Thus, this is a projection onto the space spanned by $|u\rangle$: the only nonzero eigenvalue is

$$T|u\rangle = |u\rangle\langle v|u\rangle \implies \lambda = \boxed{\langle v, u\rangle},$$

so that is also the trace (sum of the eigenvalues) of T. Another way is to write

$$\text{tr}(T) = \sum T_{ii} = \sum \langle i|T|i\rangle = \sum_i \langle i|u\rangle\langle v|i\rangle,$$

which we then rewrite as

$$\sum_i \langle v|i\rangle\langle i|u\rangle = \langle v|\sum_i |i\rangle\langle i|u\rangle = \langle v|u\rangle = \langle v, u\rangle.$$

Bra-ket notation helps us find the adjoint as well:

$$T|w\rangle = |u\rangle\langle v|w\rangle \implies \langle w|T^\dagger = \langle u|\langle w|v\rangle$$

(because $\langle v|w\rangle$ is just a complex number, so the adjoint turns it into its conjugate). And now we can just move things around:

$$\langle w|T^\dagger = \langle w|v\rangle\langle u|,$$

so we have a simple form $\boxed{T^\dagger = |v\rangle\langle u|}$.

19 Quantum Dynamics

In a lot of our study so far, we're working with a vector space of states, and our states are wavefunctions. But there's been no **time** in this vector space, but we do care about time in physics because we have clocks! So we can wait some time, and we will see that our vector has moved to some other vector in our state space. So this is the concept of **dynamics** in quantum mechanics: we need a picture to describe time evolution.

A picture to keep in mind is that we have a vector space H (for Hilbert space), and we'll have some state $|\psi, t_0\rangle$ at time t_0. Then $|\psi, t\rangle$ is some other state in our Hilbert space, but it should definitely have **unit length** if we normalize our states. So we can think of having a unit sphere on which all our vector tips live, and then our vector moves in time and traces out a trajectory, all while **preserving the norm of the vector**. (And if we don't use a normalized vector, we'll still preserve the norm – it'll just be a different value from 1.) We proved earlier on that an operator which preserves the length of all vectors is a **unitary operator**, and now we're going to make a physical postulate:

Proposition 183

The state $|\psi, t\rangle$ is obtained by the **action of a unitary operator** from the state $|\psi, t_0\rangle$:

$$|\psi, t\rangle = U(t, t_0)|\psi, t_0\rangle.$$

Here, $|\psi, t_0\rangle$ is some arbitrary state, so if we use some other arbitrary starting state $|\psi', t_0\rangle$, it also evolves with this formula, and the unitary operator U **is the same for all states**! If we give this unitary operator U any state, it'll tell us how it evolves in time.

This is actually a very big assumption – it turns out that this postulate already gives us the Schrodinger equation! We'll see that shortly.

Proposition 184
The unitary operator $U(t, t_0)$ is unique (if it exists).

Proof. If two operators do the same thing to all vectors in our vector space, then they are the same operator. □

We also know that if $U(t, t_0)$ is a unitary operator, we have

$$(U(t, t_0))^\dagger (U(t, t_0)) = I.$$

This notation is a bit cumbersome, so we'll just write $(U(t, t_0))^\dagger$ as $U^\dagger(t, t_0)$: it means the same thing.

We can now establish a few important properties of this operator U:

- $U(t_0, t_0) = I$: just plug in $t = t_0$ in our defining equation, and the only operator that leaves all states the same is the identity operator.
- Since we have
$$|\psi, t_2\rangle = U(t_2, t_1)\,|\psi, t_1\rangle = U(t_2, t_1)U(t_1, t_0)\,|\psi, t_0\rangle$$
but also
$$|\psi, t_2\rangle = U(t_2, t_0)\,|\psi, t_0\rangle\,,$$
we must have $\boxed{U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)}$. In other words, time composition works like matrix multiplication: we go from t_0 to t_1, then from t_1 to t_2.
- If we take $t_2 = t_0$ in the above equation, we find that
$$I = U(t_0, t_0) = U(t_0, t_1)U(t_1, t_0).$$
Thus $U(t_0, t)$ and $U(t, t_0)$ are inverses for all t, and we can also write this as
$$U^{-1}(t, t_0) = U(t_0, t) = U^\dagger(t, t_0)$$
(because U is unitary). This means that we can delete the "inverse" or "dagger" from our operator by just flipping the order of the arguments.

With this, we're now ready to find the Schrodinger equation. Since the Schrodinger equation is a differential equation, we'll try to use time evolution. We have that

$$\frac{\partial}{\partial t}\,|\psi, t\rangle = \left(\frac{\partial}{\partial t}U(t, t_0)\right)|\psi, t_0\rangle\,,$$

where we only differentiate the operator because $|\psi, t_0\rangle$ is a fixed state independent of t. We want to get an equation for $|\psi, t\rangle$ out of this, and we have $|\psi, t_0\rangle$ on the right side of the equation, so we can rewrite this as

$$= \frac{\partial U(t, t_0)}{\partial t}U(t_0, t)\,|\psi, t\rangle\,.$$

So we now have a complicated operator acting on $|\psi, t\rangle$, but we can rewrite this as

$$= \frac{\partial U(t, t_0)}{\partial t}U^\dagger(t, t_0)\,|\psi, t\rangle$$

(so that we have t and t_0 in the same order), and we'll call this operator $\Lambda(t, t_0)$. So now we have

$$\frac{\partial}{\partial t} |\psi, t\rangle = \Lambda(t, t_0) |\psi, t\rangle .$$

We want to learn some important properties of Λ at this point, so that we can turn this more into the Schrodinger equation:

Lemma 185
The operator Λ is anti-Hermitian.

Proof. Note that (to apply a dagger, we reverse all the operators in a product and put daggers on them)

$$\Lambda^\dagger = U(t, t_0) \frac{\partial U^\dagger}{\partial t}(t - t_0).$$

because **the time-derivative doesn't interfere with daggers**. To justify this last point, we're taking an operator at two slightly different times and subtracting them – since $A^\dagger - B^\dagger = (A - B)^\dagger$, the dagger indeed goes through the derivative. And now this is $-\Lambda$, and we can show that by noting that

$$U(t, t_0) U^\dagger(t, t_0) = I,$$

and now differentiating this with respect to time: the product rule tells us that

$$\frac{\partial U}{\partial t}(t, t_0) U^\dagger(t, t_0) + U(t, t_0) \frac{\partial U^\dagger}{\partial t}(t, t_0) = 0 \implies \Lambda + \Lambda^\dagger = 0,$$

as desired. □

The next point of business is to get rid of the t_0 in Λ:

Proposition 186
The operator Λ is independent of t_0: that is, $\Lambda(t, t_0) = \lambda(t, t_1)$ for any t_0, t_1.

What this allows us to do is to take $t_1 = t_0 + \varepsilon$ and take the limit as $\varepsilon \to 0$, which means the derivative is zero everywhere – that means that Λ is indeed absolutely independent of the second argument.

Proof. We know that

$$\Lambda(t, t_0) = \frac{\partial U(t, t_0)}{\partial t} U^\dagger(t, t_0) = \frac{\partial U(t, t_0)}{\partial t} U(t_0, t_1) U^\dagger(t_0, t_1) U^\dagger(t, t_0),$$

where we've introduced an identity operator between the two terms. But now we can group the first two terms together: even though the derivative only acts on the first term, it's also okay for it to act on the first two terms (because there's no time dependence anyway). And similarly, we can rewrite the last two terms:

$$= \frac{\partial}{\partial t}(U(t, t_0) U(t_0, t_1)) U(t_1, t_0) U(t_0, t).$$

Now by composition, this is equal to

$$= \frac{\partial}{\partial t} U(t, t_1) U(t_1, t) = \frac{\partial}{\partial t} U(t, t_1) U^\dagger(t, t_1) = \Lambda(t, t_1)$$

as desired. □

So now we have an operator Λ which is anti-Hermitian and only depends on t: we'll multiply it by i to make this into a **Hermitian** operator. Also, since Λ of units of $\frac{1}{\text{time}}$ (because unitary operators U have no units and we take a single time derivative), we can actually replace Λ by $i\hbar\Lambda$ to get a Hermitian operator with units of **energy**. And now there isn't much more we have to do: if we define $H = i\hbar\Lambda$

$$\frac{\partial}{\partial t}|\psi, t\rangle = \Lambda(t)|\psi, t\rangle \implies \boxed{i\hbar\frac{\partial}{\partial t}|\psi\rangle = H(t)|\psi, t\rangle},$$

and we've derived the Schrodinger equation! **This is basically most of the information in the Schrodinger equation: it's just unitary time evolution**.

Fact 187

There's a clear correspondence between the operator Λ and the **Poisson brackets** from classical mechanics, which we should read about if we're curious.

When we want to invent a quantum system, we don't really know how to find the operator U, but we do know how to find the Hamiltonian H from U: it's just $i\hbar\frac{\partial U}{\partial t}(t, t_0)U^\dagger(t, t_0)$. And the Hamiltonians are nice – we know energy functionals of systems, so often we can write down an explicit H.

But we should also think about the opposite problem: how can we get U from H? It's easier to invent a quantum system with H, but we do care about how the unitary evolution operator looks.

To do that, first multiply both sides of the defining equation of H by U: we have

$$i\hbar\frac{\partial U}{\partial t}(t, t_0) = H(t)U(t, t_0)$$

(where the $U^\dagger$ and U terms cancel on the right hand side above, and then we've switched around the two sides). There's no confusion with derivatives between partial and total derivatives, so we have

$$i\hbar\frac{d}{dt}U(t, t_0) = H(t)U(t, t_0).$$

And we should be able to see the Schrodinger equation in here: if we put in a $|\psi, t_0\rangle$, the right side becomes $H(t)$ acting on $|\psi(t)\rangle$, and the left hand side becomes $i\hbar\frac{d}{dt}|\psi(t)\rangle$ (because we can bring $|\psi, t_0\rangle$ into the derivative). To solve further, there are three cases here:

- In our first case, H is time-independent, so $H(t) = H$ for some operator H. Then

$$\boxed{i\hbar\frac{dU}{dt} = HU},$$

and we'll try to write down a solution of the form $U = e^{-iHt/\hbar}U_0$. Plugging this in, we find that

$$i\hbar\frac{dU}{dt} = i\hbar\left(-\frac{iH}{\hbar}\right)e^{-iHt/\hbar}U_0.$$

Here, we've used the fact that H doesn't depend on time – H acts like a number, so the derivative just lets us take the H out of the exponential (for example, we can imagine taking the power series expansion). So canceling constant terms, we find that the left side of our boxed equation above is

$$i\hbar\frac{dU}{dt} = He^{-iHt/\hbar}U_0,$$

which is exactly HU as desired! So we know that our unitary operator

$$U(t, t_0) = e^{-iHt/\hbar} U_0$$

for some constant matrix U_0. Plugging in $t = t_0$, the operator should be the unit matrix, so $1 = e^{-iHt_0/\hbar} U_0$, and thus $U_0 = e^{iHt_0/\hbar}$. Substituting everything back, we get our final answer:

$$\boxed{U(t, t_0) = e^{-\frac{iH}{\hbar}(t-t_0)}},$$

as long as H is time-independent. And if we have U act on any energy eigenstate (which is an eigenstate of H), we can just substitute in the eigenvalue E: that is,

$$e^{\alpha H} |\psi_n\rangle = e^{\alpha E_n} |\psi_n\rangle$$

as long as $H|\psi_n\rangle = E_n |\psi_n\rangle$.

- In our second case, H has a little bit of time-dependence: we design this case so that it's still possible to solve the equation. We'll assume that

$$[\hat{H}(t_1), \hat{H}(t_2)] = 0$$

for all t_1, t_2 (that is, the Hamiltonians at different times always commute). For example, a particle in a magnetic spin has $H = -\gamma \hat{B}(t) \cdot \hat{s}$, and it's possible to have a time-dependent magnetic field $B(t)$. But if the direction is fixed, so we have something like $H = -\gamma B_z(t) S_z$, then the Hamiltonians at different times will commute because S_z commutes with itself. (But later in the class, we'll do things like nuclear magnetic resonance, and then the system is more complicated than this.)

Well, the claim we have in this case is that $U(t, t_0)$ ends up being something generalized from the above case. We want to put $e^{-iHt/\hbar}$ like before, but the time derivative $\frac{dU}{dt}$ isn't quite so simple now because H does depend on time. So we can fix this by trying an ansatz of

$$\boxed{U(t, t_0) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'\right]}.$$

(Notice that if H is time-independent, this reduces to the boxed equation for $U(t, t_0)$ in the first case.) To verify this, we'll call the expression inside the exponential $R(t)$. We have

$$\dot{R}(t) = -\frac{i}{\hbar} H(t)$$

by the fundamental theorem of calculus, and now we want to differentiate

$$U = e^R \implies \frac{dU}{dt} = (1 + R + \frac{1}{2!}RR + \frac{1}{3!}RRR + \cdots),$$

and this simplifies to

$$\frac{dU}{dt} = \dot{R} + \frac{1}{2!}(\dot{R}R + R\dot{R}) + \frac{1}{3!}(\dot{R}RR + R\dot{R}R + RR\dot{R}) + \cdots,$$

but now $\dot{R}$ **commutes with** R, because $\dot{R}$ depends on H, while R is an integral of H's – we're assuming that the Hs at different times commute. So the expression simplifies by moving all of the $\dot{R}$s to the left, and we just end up with

$$\frac{dU}{dt} = \dot{R} e^R = -\frac{i}{\hbar} H(t) U,$$

which means the unitary operator U that we've established is the correct one for time-evolution, **as long as the Hs commute at different times**.

- In the general case, the idea is that $\dot{R}$ and R may not commute with each other. There's not very much we can do, but there is one way to get something that makes sense.

  Our answer will look like

$$\boxed{U(t,t_0) = T\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')\right]},$$

  where T is defined to be the **time-ordered exponential**. Basically, we expand the exponential term by term: we start with the usual expansion, but then we change the limits of integration:

$$= 1 + \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t} dt_1 H(t_1) + \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 H(t_1)\int_{t_0}^{t_1} dt_2 H(t_2) + \cdots,$$

  where the idea is that the second integral in the "squared" term always has $t_1 > t_2$. The next term will be similar: it'll look like

$$+\frac{1}{3!}\left(-\frac{i}{\hbar}\right)^3 \int_{t_0}^{t} dt_1 H(t_1)\int_{t_0}^{t_1} dt_2 H(t_2)\int_{t_0}^{t_2} dt_3 H(t_3),$$

  and we can check on our own that the time-derivative works exactly as it should: specifically, if this time-ordered exponential is our U, then $i\hbar\frac{dU}{dt}$ will end up being equal to HU.

  So it's reassuring that a solution exists, but this isn't a very practical way to find a solution U. And when we do the rotating magnetic field problem for magnetic resonance, this isn't what we'll be doing! But we'll see a bit more of this in 8.06.

And now we're ready for an **alternate formulation** of all of this, known as the **Heisenberg picture** of quantum mechanics. This isn't something that we formulate on its own – the idea is to start with a Schrodinger picture in which we've already defined all of our operators $\hat{x}, \hat{P}, \hat{S}_x, \hat{H}$ and wave functions ψ, and we'll **think about them in a new way**.

To get started, we first consider a Schrodinger operator $\hat{A}_S$ (S stands for Schrodinger here). The motivation for the Heisenberg picture is that we have two independent time-dependent states $|\alpha, t\rangle$ and $|\beta, t\rangle$, and we might want to understand the quantity

$$\langle \alpha, t | \hat{A}_S | \beta, t\rangle .$$

We know, though, that we can represent the bra and ket vectors here by using unitary operators:

$$= \langle \alpha, 0 | U^\dagger(t,0)\hat{A}_s U(t,0) | \beta, 0\rangle .$$

So instead of having time-dependence in α and β, we can use the unitary operators to say that we have a time-dependent operator $U^\dagger(t,0)\hat{A}_s U(t,0)$ between the initial states. And this object is very important:

Definition 188

The **Heisenberg version** of the Schrodinger operator $\hat{A}_S$ is

$$\hat{A}_H(t) = U^\dagger(t,0)\hat{A}_S U(t,0).$$

So any Schrodinger operator corresponds to a Heisenberg operator – we just act with U from both the left and the right (which is the natural way for operators to act on operators). There's a lot of things we can say about this new operator that we've established:

- At $t = 0$, $\hat{A}_H(t = 0) = \hat{A}_S$. This is because $U(t, 0)$ is the unitary time-evolution operator, and when $t = 0$, this is just the identity – nothing is changing. So our two operators (Schrodinger and Heisenberg) start off being exactly the same.

- The unit operator in the Heisenberg picture is

$$U^\dagger(t, 0) I U(t, 0),$$

but I doesn't do anything and $U^\dagger$ and U multiply to the identity, and indeed **the unit operator doesn't change** in the Heisenberg picture.

- Suppose $\hat{C}_S = \hat{A}_S \hat{B}_S$. Then we can find the Heisenberg operator for $\hat{C}$:

$$\boxed{\hat{C}_H} = U^\dagger \hat{C}_S U = U^\dagger \hat{A}_S \hat{B}_S U = U^\dagger \hat{A}_S U U^\dagger \hat{B}_S U,$$

and now this is just the product of the Heisenberg operators $\boxed{\hat{A}_H \hat{B}_H}$! Similarly, this tells us that commutators also behave nicely:

$$\hat{C}_S = [\hat{A}_S, \hat{B}_S] \implies \hat{C}_H = [\hat{A}_H, \hat{B}_H].$$

The key thing to keep in mind is that

$$[x, p] = i\hbar I \implies [x_H(t), p_H(t)] = i\hbar I$$

(because $i\hbar$ is just a constant, and the unit operator stays the same in the Heisenberg picture). So any commutation relation in Schrodinger is also a commutation relation in Heisenberg.

- Let's now look at Hamiltonians: by definition, we have

$$\hat{H}_H(t) = U^\dagger(t, 0) \hat{H}_S U(t, 0).$$

If the Schrodinger Hamiltonian commutes at all times, meaning that $[H_s(t_1), H_s(t_2)] = 0$ for all t_1, t_2, then the unitary operator is built by an exponential in terms of H. But then we can move the $U^\dagger(t, 0)$ past the $\hat{H}_S$, and we find that

$$\hat{H}_H(t) = \hat{H}_S U^\dagger(t, 0) U(t, 0) = \hat{H}_S(t);$$

that is, the Schrodinger and Heisenberg Hamiltonians are equal **if the Hamiltonians commute at all times**. (We'll be able to check this in a nice example as well!)

Note that whenever $H_S(t)$ is a function of x, p, and t (for example), we can turn it into a Heisenberg operator by putting a $U^\dagger$ on the left and a U on the right. But then the Us will work its way inside – x's become Heisenberg x's, and so on. So what we're claiming is that

$$\hat{H}_H(t) = U^\dagger \hat{H}_S(\hat{x}_S, \hat{p}_S, t) U = \hat{H}_S(\hat{x}_H, \hat{p}_H, t),$$

which means that **we get the Heisenberg Hamiltonian by replacing the Schrodinger variables with their Heisenberg versions.** So **if we're in the case** above where the Hamiltonians commute at all times, then

$$\hat{H}_S(\hat{x}_H, \hat{p}_H, t) = \hat{H}_S(\hat{x}_S, \hat{p}_S, t) :$$

somehow putting in Heisenberg operators into the Schrodinger Hamiltonian gives us exactly the same thing. This will be a useful identity, and we'll use it later on!

- Our last point is about expectation values: remember that we started this discussion with two arbitrary states $|\alpha, t\rangle$ and $|\beta, t\rangle$. If we set those states equal to ψ, we find that

$$\boxed{\langle \psi, t | \hat{A}_S | \psi, t \rangle = \langle \psi, 0 | \hat{A}_H(t) | \psi, 0 \rangle}.$$

  This is an equation which tells us that the Schrodinger operator's expectation value at a time t is just the Heisenberg operator's expectation value at time 0, and we can write this **schematically** as

$$\langle A_S \rangle = \langle A_H \rangle.$$

  We just have to be careful to understand how to interpret this equation: in the left side, we're using time-independent states, but in the right side, we're using the $t = 0$ states.

So far, these Heisenberg operators are a little bit difficult to work with – they're hard to calculate, so we want to find an equation satisfied by the Heisenberg operator. The reason for this is that we seldom know U, and even when we know it, it's a bit difficult to do the simplification $U^\dagger \hat{A}_S U$.

The idea is to calculate the quantity

$$i\hbar \frac{d}{dt} \hat{A}_H,$$

which is also equal to $i\hbar \frac{d}{dt} \left(U^\dagger \hat{A}_S U \right)$. We should remember that the Schrodinger operator can have some explicit time dependence, so we should apply the product rule to all three terms: this is equal to

$$i\hbar \frac{\partial U^\dagger}{\partial t} \hat{A}_S U + i\hbar U^\dagger \hat{A}_S \frac{\partial U}{\partial t} + i\hbar U^\dagger \frac{\partial \hat{A}_S}{\partial t} U,$$

where U is always $U(t, t_0)$.

Remark 189. *It may be confusing why we have partial derivatives in one expression and total derivatives in the other – the important thing to keep in mind is whether we're fixing the Heisenberg or the Schrodinger variables. For the first two terms in the product rule, it doesn't matter whether we use a partial or total derivative – in both cases it's the same – but we need to use the partial derivative for the last term so that we're fixing Schrodinger observables, while we need to take the total derivative for the initial expression because $\hat{A}_H$ is written in terms of Heisenberg variables, which can have some additional time dependence (and we want to fix Schrodinger variables throughout everything).*

But we also know how to find the derivatives of U and $U^\dagger$: since $i\hbar \frac{\partial U}{\partial t} = HU$, we also know that (taking the dagger of that equation and moving the negative sign over) $i\hbar \frac{\partial U^\dagger}{\partial t} = -U^\dagger H_S$. So plugging those in, we find that

$$i\hbar \frac{d}{dt} \hat{A}_H = -U^\dagger \hat{H}_S \hat{A}_S U + U^\dagger \hat{A}_S \hat{H}_S U + i\hbar \frac{\partial \hat{A}_H}{\partial t}.$$

(The last term will be 0 if $\hat{A}_S$ doesn't have any explicit time dependence, so we'll just leave it as it is and rewrite it as its Heisenberg version.) And now we can turn the first two terms into their Heisenberg versions as well:

$$\boxed{i\hbar \frac{d}{dt} \hat{A}_H(t) = [\hat{A}_H, \hat{H}_H] + i\hbar \frac{\partial \hat{A}_H}{\partial t}}.$$

This is the **Heisenberg equation of motion**, and solving this differential equation is often the simplest way we can calculate $\hat{A}_H$! Again, we'll consider some particular cases:

- If $\hat{A}_S$ has **no explicit time dependence**, then the second term disappears because $\frac{\partial \hat{A}_S}{\partial t} = 0$, and the equation simplifies to

$$i\hbar \frac{d}{dt} \hat{A}_H(t) = [\hat{A}_H, \hat{H}_H].$$

And the Heisenberg operator is simple – if the Schrodinger operator is time-independent (or commutes at different times), then $\hat{H}_H = \hat{H}_S$. But we'll leave it as is so that we have an equation in terms of $\hat{A}_H$ itself.

Now suppose we want to compute how the expectation value of a Schrodinger operator depends on time: we can calculate

$$i\hbar \frac{d}{dt} \langle \psi, t | \hat{A}_S | \psi, t \rangle = i\hbar \frac{d}{dt} \langle \psi, 0 | \hat{A}_H | \psi, 0 \rangle .$$

Now putting the derivative between the bra and ket, we get

$$\langle \psi, 0 | i\hbar \frac{d}{dt} \hat{A}_H | \psi, 0 \rangle ,$$

and assuming still that $\hat{A}$ has no time-dependence, this is equal to

$$\langle \psi, 0 | [\hat{A}_H, \hat{H}_H] | \psi, 0 \rangle .$$

So the time derivative of the expectation value satisfies

$$\boxed{i\hbar \frac{d}{dt} \langle \hat{A}_H(t) \rangle = \langle [\hat{A}_H, \hat{H}_H] \rangle}.$$

We say that Heisenberg expectation values are the same as Schrodinger expectation values – this can also be written as

$$\boxed{i\hbar \frac{d}{dt} \langle \hat{A}_S \rangle = \langle [\hat{A}_S, \hat{H}_S] \rangle},$$

which we derived a few classes ago. So this means that the expectation values of Schrodinger operators are the same as the expectation values of Heisenberg operators, except that we take the states at $t = 0$ in the latter case.

- Now consider the case where $\hat{A}_S$ is time-independent and **conserved** (meaning that it commutes with the Schrodinger Hamiltonian). Then $[\hat{A}_S, \hat{H}_S] = 0$, which also means that $[\hat{A}_H, \hat{H}_H] = 0$, which means that

$$\frac{d\hat{A}_H}{dt} = 0.$$

So the Heisenberg operator is also time-independent – if the Schrodinger operator has no t's and is conserved, the Heisenberg operator doesn't actually have any t's either.

We'll finish this class with a nice example:

Example 190

Consider the harmonic oscillator with the Schrodinger Hamiltonian

$$\hat{H}_S = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2,$$

where $\hat{x}$ and $\hat{p}$ are the usual Schrodinger operators.

Now the Heisenberg Hamiltonian should be identical, because we have a time-independent Hamiltonian. But we'll write it in general first, where we have $U^\dagger$ and U coming in from the left and right: we get that

$$\hat{H}_H = \frac{\hat{p}_H^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}_H^2.$$

We'll check that this is time-independent, but first we need to evaluate the operators $\hat{x}_H$ and $\hat{p}_H$. The most straight-

forward way is to plug in the $e^{-iHt/\hbar}$ operators and multiply everything through, but this is a little bit complicated: we'll use the Heisenberg equation of motion instead! Since $\hat{x}$ and $\hat{p}$ are time-independent Schrodinger operators,

$$i\hbar\frac{d\hat{x}_H}{dt} = [\hat{x}_H, \hat{H}_H] = \left[\hat{x}_H, \frac{\hat{p}_H^2}{2m}\right].$$

And now this commutator gives us $\frac{1}{2m}\hat{p}_H[\hat{x}_H, \hat{x}_P]\cdot 2 = \frac{i\hbar}{m}\hat{p}_H$, and plugging this in yields

$$\boxed{\frac{d\hat{x}_H}{dt} = \frac{1}{m}\hat{p}_H}.$$

So this looks like an equation in classical mechanics – we have $\frac{dx}{dt} = \frac{p}{m}$, and that's another good point of Heisenberg equations of motion – they look like ordinary dynamical variable equations! Similarly, we find that

$$i\hbar\frac{d\hat{p}_H}{dt} = [\hat{p}_H, \hat{H}_H] = \frac{1}{2}m\omega^2[\hat{p}_H, \hat{x}_H^2] = m\omega^2\hat{x}_H\cdot(-i\hbar),$$

and thus we have

$$\boxed{\frac{d\hat{p}_H}{dt} = -m\omega^2\hat{x}_H}.$$

We can now solve for these in the same way that we classically: taking a second derivative of the first boxed equation, we have that

$$\frac{d^2\hat{x}_H}{dt^2} = \frac{1}{m}\frac{d\hat{p}_H}{dt} = \frac{1}{m}(-m\omega^2\hat{x}_H),$$

so we just get the simple harmonic oscillator equation of motion

$$\frac{d^2\hat{x}_H}{dt^2} = -\omega^2\hat{x}_H.$$

Here, what we should notice about the Heisenberg picture is that we're solving for the Heisenberg operators, which tells us about the time evolution of all states at the same time! So we know that we have

$$\hat{x}_H = \hat{A}\cos(\omega t) + \hat{B}\sin(\omega t),$$

and then similarly the momentum

$$\hat{p}_H = m\frac{d\hat{x}_H}{dt} = -m\omega\sin(\omega t)\hat{A} + m\omega\cos(\omega t)\hat{B}.$$

But we can figure out what these operators $\hat{A}$ and $\hat{B}$ are: at time $t = 0$, the Heisenberg operators should be identical to the Schrodinger operators, so $\hat{x}_H(t) = \hat{A} = \hat{x}$ (the Schrodinger operator), and $\hat{p}_H(t) = m\omega\hat{B} = \hat{p}$. So we know that $\hat{B} = \frac{\hat{p}}{m\omega}$, and now we get our equations:

$$\boxed{\hat{x}_H(t) = \hat{x}\cos(\omega t) + \frac{\hat{p}}{m\omega}\sin(\omega t)}, \quad \boxed{\hat{p}_H(t) = \hat{p}\cos(\omega t) - m\omega\hat{x}\sin(\omega t)}.$$

So now any expectation of a combination of $\hat{x}$ and $\hat{p}$ can be found by plugging things in at time $t = 0$! So now we can find the Heisenberg Hamiltonian:

$$\hat{H}_H = \frac{\hat{p}_H^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_H^2 = \frac{1}{2m}\left(\hat{p}\cos(\omega t) - m\omega\hat{x}\sin(\omega t)\right)^2 + \frac{1}{2}m\omega^2\left(\hat{x}\cos(\omega t) + \frac{\hat{p}}{m\omega}\sin(\omega t)\right)^2,$$

and expanding out yields

$$= \left[\frac{1}{2m}\cos^2\omega t\,\hat{p}^2 + \frac{1}{2m}m^2\omega^2\sin^2\omega t\,\hat{x}^2 - \frac{1}{2m}(m\omega\sin\omega t\cos\omega t(\hat{p}\hat{x} + \hat{x}\hat{p}))\right]$$

$$+\left[\frac{1}{2}\frac{m\omega^2}{m^2\omega^2}\sin^2\omega t\,\hat{p}^2+\frac{1}{2}m\omega^2\cos^2\omega t\,\hat{x}^2+\frac{1}{2}\frac{m\omega^2}{m\omega}(\cos\omega t\sin\omega t t(\hat{x}\hat{p}+\hat{p}\hat{x}))\right].$$

And now everything cancels very nicely: the $\hat{p}^2$ coefficients evaluate to $\frac{1}{2m}(\cos^2\omega t+\sin^2\omega t)=\frac{1}{2m}$, and the $\hat{x}^2$ coefficients evaluate to $\frac{1}{2}m\omega^2\hat{x}^2$ similarly. The cross-terms cancel, and we get a final expression which is **identical to the Schrodinger Hamiltonian!** So what this means is that the when we substitute in the expression for the Heisenberg operators into the Heisenberg Hamiltonian, we get an expression which is exactly equal to the Schrodinger Hamiltonian.

20 March 4, 2020

(Two) practice tests for the exam next week will be posted, so that we can get an idea of what it will be like. Solving problems from previous tests is a good way to study; another one is to review past homework and recitation material! And it is good to read the lecture notes as well if we've only been using the videos. (By the way, the material for today's lecture on the Heisenberg picture will not be on the exam – we just need to understand concepts up to problem set 4.)

Problem 191

Suppose $\hat{A}$ and $\hat{B}$ are Hermitian operators. How can we check if they are simultaneously diagonalizable?

We know that Hermitian operators are **normal**, and all normal operators are diagonalizable. (In fact, they are unitarily diagonalizable, so we can get an orthonormal basis.) So we just need to know whether the eigenvectors line up.

Well, the most important thing is to check the commutator $[\hat{A},\hat{B}]=\hat{A}\hat{B}-\hat{B}\hat{A}$. If this is equal to zero, it will be equal to zero under any linear transformation:

$$\hat{A}'=P^{-1}\hat{A}P\implies\hat{A}'\hat{B}'=P^{-1}\hat{A}PP^{-1}\hat{B}P=P^{-1}\hat{A}\hat{B}P.$$

So $[\hat{A}',\hat{B}']=P^{-1}[\hat{A},\hat{B}]P$, and thus one commutator is zero if and only if the other is zero. Because diagonal matrices commute, this means that if $\hat{A}$ and $\hat{B}$ must be diagonalizable in the original basis as well.

On the other hand, if $\hat{A}$ and $\hat{B}$ do not commute, then we cannot end up with a zero commutator. Thus the two operators are not simultaneously diagonalizable.

Remark 192. *Using this same idea, note that an operator proportional to the identity looks the same in all bases, because*

$$P^{-1}(cI)P=cP^{-1}P=cI.$$

So if we're given two operators that commute, how should we proceed? The idea is that we should check the eigenvalues of **each matrix**, and try to work with the one with **less degeneracies** (ideally none)! (This is because having no degeneracy in eigenvalues makes it more clear what the (simultaneous) eigenvectors are.) Remember that if an eigenvalue shows up twice for our operator $\hat{A}$, there is a whole plane of eigenvectors that would all work – however, it takes some work to see which of those actually diagonalize the other operator $\hat{B}$. Specifically, if we didn't pick the right ones, we'd have some invariant subspace of dimension 2 for $\hat{B}$, which we'd have to diagonalize separately in $\hat{B}$ to give us the final answer.

Remark 193. *Remember that a lot of quantities and properties for our operators are basis-independent: for example, the eigenvalues of $\hat{A}$ or whether $\hat{A}$ is Hermitian do not depend on our choice of basis.*

We'll continue on with some practice for a different topic:

Problem 194

We have the uncertainty inequality

$$\Delta A \Delta B \geq \left| \left\langle \Psi \left| \frac{1}{2i}[\hat{A}, \hat{B}] \right| \Psi \right\rangle \right|$$

(we can put the hats above the operators if we want, but it's not that important). **When is this inequality saturated**, meaning we have an equality case?

This was analyzed in the lecture videos: it requires

$$(\hat{B} - \langle \hat{B} \rangle) |\Psi\rangle = i\gamma (\hat{A} - \langle A \rangle) |\Psi\rangle .$$

At the end of the day, we care about the state $|\Psi\rangle$ where the identity is indeed saturated. And we need to also find γ as well – it's some **real number**. But there's more we don't know here – the expectation values $\langle A \rangle$ and $\langle B \rangle$ are also taken with respect to a state Ψ!

So if we expand out the equation in terms of Ψ, we have cubic terms:

$$B\Psi - \langle \Psi | B | \Psi \rangle \Psi = i\gamma \left(\hat{A}\Psi - \langle \Psi | A | \Psi \rangle \Psi \right) .$$

But we can be a bit clever. If we want to solve the equation $A\Psi = \langle A \rangle \Psi$, this looks ugly to expand out. But we can instead first find the eigenvalues of $\hat{A}$ and $\hat{B}$, and we can just think of $\langle A \rangle$ and $\langle B \rangle$ as numbers a, b. (It's not true that Ψ is an eigenvector of $\hat{A}$ and $\hat{B}$, but this is showing us a general method.) And now our equation just becomes

$$(\hat{B} - b) |\Psi\rangle = i\gamma (\hat{A} - a) |\Psi\rangle .$$

And now we can rearrange some terms:

$$\boxed{(\hat{B} - i\gamma \hat{A}) |\Psi\rangle = (b - i\gamma a) |\Psi\rangle}.$$

And now we have something that looks like an eigenvector equation! The operator $\hat{B} - i\gamma\hat{A}$ is not Hermitian, so eigenvalues can be complex (not just real). But now let's add $\langle \Psi |$ to the left hand side: this now gives us

$$\langle B \rangle - i\gamma \langle A \rangle = b - i\gamma a.$$

And now equating real and imaginary parts (A, B are hermitian), we find that we indeed have $b = \langle \hat{B} \rangle, a = \langle \hat{A} \rangle$. So it's okay to replace the expectation values with a, b, because they will turn out to be equal to the expectation values!

We have likely seen the concept of **coherent states** in the harmonic oscillator:

$$\hat{a} |\alpha\rangle = \alpha |\alpha\rangle , \quad \hat{a} = \hat{x} - \frac{i\hat{p}}{\hbar\omega}.$$

Here, $\hat{a}$ (and $\hat{a}^\dagger$) are non-Hermitian operators, so when we solve for coherent states, we're solving this kind of boxed equation above.

Remark 195. *By the way, if we take the norms of our uncertainty saturation relation, we find that*

$$\Delta B = |\gamma| \Delta A.$$

This is something we solve for later on – we shouldn't write it in terms of $\frac{\Delta B}{\Delta A}$ in our equation.

In the homework, we do this with the operators $\hat{A} = \hat{x}, \hat{B} = \hat{p}$. Then we have

$$(\hat{p} - i\gamma\hat{x})\Psi = (p_0 - i\gamma x_0)\Psi,$$

so in coordinate space,

$$\frac{\hbar}{i}\frac{d\Psi}{dx} - i\gamma(x)\Psi(x) = (p_0 - i\ )\Psi,$$

so

$$\frac{d\Psi}{dx} = \frac{i}{\hbar}(i\gamma x + p_0 - i\gamma x_0)\Psi.$$

We can now write this in a separable form

$$\frac{d\Psi}{\Psi} = \left(\frac{ip_0}{\hbar} - \frac{\gamma}{\hbar}(x - x_0)\right)dx,$$

and then integrating both sides will give us

$$\log\Psi = \frac{ip_0x}{\hbar} - \frac{\gamma}{2\hbar}(x - x_0)^2.$$

And thus Ψ is a Gaussian – these are exactly the states that saturate the uncertainty! They take the form

$$\Psi(x) = c'e^{ip_0x/\hbar}e^{-\gamma(x-x_0)^2/(2\hbar)}.$$

21 Coherent States

First of all, we'll do a little bit of review. We learned how to calculate the Heisenberg operators, where we subject a Schrodinger operator to the transformation $U^\dagger(t,0)A_sU(t,0)$. The resulting operator A_H has a few important properties: if the Hamiltonian H is time-independent, we just have $A_H = e^{iHt/\hbar}A_se^{-iHt/\hbar}$, and in general we have the **Heisenberg equations of motion** to help us solve for A_H. Our main achievement of last time was developing a formula for the time-development of $\hat{x}_H$ and $\hat{p}_H$ for the harmonic oscillator, and we'll see today that these Heisenberg operators contain all of the information about the dynamics of this whole system.

Remark 196. *We should read up on creation and annihilation operators: the idea is that $\hat{a}$ and $\hat{a}^\dagger$ are linear combinations of $\hat{x}$ and $\hat{p}$, so they also have no time dependence, and in the Heisenberg picture they are also time-independent operators: we have $\hat{a}_H(t) = e^{-i\omega t}\hat{a}$ and $\hat{a}_H^\dagger(t) = e^{i\omega t}\hat{a}^\dagger$.*

The important thing is that we can write $\hat{x}$ and $\hat{p}$ as linear combinations of $\hat{a}$ and $\hat{a}^\dagger$ as well:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a}).$$

And indeed, if we take the Heisenberg version of this operator (making every $\hat{x}$ into a $\hat{x}_H$ and so on), the equation still holds, and then we can substitute in our new creation and annihilation operators and we'll recover the familiar

$$\hat{x}_H(t) = \hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t, \quad \hat{p}_H(t) = \hat{p}\cos\omega t - m\omega\hat{x}\sin\omega t.$$

Today, we'll use these concepts to understand the **coherent states** of the harmonic oscillator. The motivation here is that in any energy eigenstate of the harmonic oscillator, operators have constant expectation values! So if we ask about the position or momentum or other property of our particle, it will look the same at all times. This is still an interesting state, but we want to **construct quantum mechanical states that behave somewhat classically**. And this will have applications to light and photons soon!

The first step we'll take is to understand **translation operators**. We'll start with the unitary translation operator

$$T_{x_0} = e^{-i\hat{p}x_0/\hbar} :$$

we've seen these operators a lot in the homework. This is unitary, because x_0 is a real number, $\hat{p}$ is a Hermitian operator, so the exponent $-i\hat{p}x_0/\hbar$ is anti-Hermitian. And then the exponential of any anti-Hermitian operator is unitary.

The reason these operators are particularly nice is that the multiplication of two such operators

$$T_{x_0}T_{y_0} = e^{-i\hat{p}x_0/\hbar}e^{-i\hat{p}y_0/\hbar},$$

and now the two operators in the exponents are just multiples of each other, so they commute – thus this is just

$$= e^{-i\hat{p}(x_0+y_0)/\hbar} = T_{x_0+y_0}.$$

So we don't need Campbell–Baker–Hausdorff here! We can also get a simple expression for the inverse: plugging in $y_0 = -x_0$), we find that

$$T_{x_0}T_{-x_0} = T_0 = I,$$

so the operators T_{x_0} and T_{-x_0} are inverses. But to get more intuition, we need to do a bit more computation by having our operator **act on** $\hat{x}$ and $\hat{p}$ – that is, we want to compute the two quantities

$$T_{x_0}^\dagger \hat{x} T_{x_0}, \quad T_{x_0}^\dagger \hat{p} T_{x_0}.$$

We've already shown in our own work that these are actually $\hat{x} + x_0 I$ and $\hat{p}$, respectively (the second expression is simple because everything commutes). So if we have a state ψ, we can ask for the expectation value $\langle\hat{x}\rangle_\psi$, and if this is a particle that is somewhat localized, the expectation will be roughly where the particle is. But then we can also compute $\langle\hat{x}\rangle_{T_{x_0}\psi}$ – that is, what T_{x_0} is really doing – and this expectation is

$$\langle\psi| T_{x_0}^\dagger \hat{x} T_{x_0} |\psi\rangle = \langle\psi| (\hat{x} + x_0) |\psi\rangle = \langle\hat{x}\rangle_\psi + x_0.$$

In other words, the expectation value in the new state $T_{x_0}\psi$ is the expectation value in ψ, except we've **translated everything by a displacement of** x_0. (And that explains the name "translation operator!) We should re-verify that we have

$$T_{x_0}|x\rangle = |x + x_0\rangle, \quad T_{x_0}|\psi\rangle = \psi(x - x_0),$$

because $\psi(x - x_0)$ is the wave function translated to the **right** by x_0 units (by function transformation rules).

So now we can use this translation operator to get our **coherent states**. We'll start by taking the ground state of the harmonic oscillator, and we'll displace it by some x_0: the resulting state looks like

$$|\tilde{x_0}\rangle = T_{x_0}|0\rangle = e^{-i\hat{p}x_0/\hbar}|0\rangle.$$

Intuitively, we should imagine the ground state wave function in the harmonic oscillator potential, except we translate it so that its center is at some position x_0 instead of 0. We have no time dependence so far – we'll first understand a few more properties of this state, and then we'll time-evolve it.

Example 197

What is the value of $\langle\tilde{x_0}|\tilde{x_0}\rangle$?

We should be careful to note that **this is not a position eigenstate**, so we can't use the formula $\langle x|y\rangle = \delta(x-y)$. But we do know that $\tilde{x_0}$ is the result of a unitary operator acting on $|0\rangle$, which preserves length. Thus,

$$\langle \tilde{x_0}|\tilde{x_0}\rangle = \langle 0|0\rangle = 1.$$

The ψ associated to this state is then $\psi_0(x-x_0)$, where $\langle x|0\rangle = \psi_0(x)$ is the ground state wave function.

We can now proceed with a few other calculations: if we want to compute the expectation value of **any operator** A on our coherent state, we want to calculate it in a vacuum, so

$$\langle \tilde{x_0}| A |\tilde{x_0}\rangle = \langle 0| T_{x_0}^\dagger A T_{x_0} |0\rangle .$$

Basically, we're tracing the problem back to what the regular ground state (vacuum) is doing. For example, if $A = \hat{x}$, we have that

$$\langle \tilde{x_0}| \hat{x} |\tilde{x_0}\rangle = \langle 0| T_{x_0}^\dagger \hat{x} T_{x_0} |0\rangle = \langle 0| (\hat{x} + x_0) |0\rangle = x_0,$$

as we expect, and similarly

$$\langle \tilde{x_0}| \hat{p} |\tilde{x_0}\rangle = \langle 0| T_{x_0}^\dagger \hat{p} T_{x_0} |0\rangle = \langle 0| (\hat{p}) |0\rangle = 0.$$

Putting these together, we can find the expectation value of the Hamiltonian: because the $\hat{p}$ is unchanged while the $\hat{x}$ becomes $(\hat{x}+x_0)$, we have

$$\langle \tilde{x_0}| H |\tilde{x_0}\rangle = \left\langle 0 \left| \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 (\hat{x}+x_0)^2 \right| 0 \right\rangle .$$

To avoid computing too hard, we can take the original Hamiltonian and separate it from the other terms here: this evaluates to

$$= \langle 0| H |0\rangle + \left\langle 0 \left| \frac{1}{2} m\omega^2 (2\hat{x}x_0) + \frac{1}{2} m\omega^2 x_0^2 \right| 0 \right\rangle .$$

The first term here is a constant times an expectation of $\hat{x}$, so it is just zero, and then the last term is just some constant. Putting everything together and using that the expectation of the Hamiltonian in the vacuum (ground state) is $\frac{\hbar\omega}{2}$, we have that

$$\boxed{\langle \tilde{x_0}| H |\tilde{x_0}\rangle = \frac{1}{2}\hbar\omega + \frac{1}{2} m\omega^2 x_0^2}.$$

But this is now looking very classical: the expectation value of the energy is a small quantum term, plus the cost of stretching everything out to x_0, which is $\frac{1}{2}kx_0^2$. In other words, for large enough x_0, we can think of the second term as being the "cost" of having the particle being off to the side in a potential!

Remark 198. *As small exercises, it's worth calculating that*

$$\langle \tilde{x_0}| \hat{x}^2 |\tilde{x_0}\rangle = x_0^2 + \frac{\hbar}{2m\omega}, \quad \langle \tilde{x_0}| \hat{p}^2 |\tilde{x_0}\rangle = \frac{m\hbar\omega}{2}, \quad \langle \tilde{x_0}| \hat{x}\hat{p} + \hat{p}\hat{x} |\tilde{x_0}\rangle = 0.$$

The idea we're approaching now is that of **time-evolution**: it's going to turn out that even though this coherent state is not an energy eigenstate, the wavefunction will not actually change shape – it'll just move back and forth! This is surprising – usually superimposing only two energy eigenstates will change the shape, but this is an exceptional case. Let's use the notation that a state $|\tilde{x_0}\rangle$ looks like $|\tilde{x_0}, t\rangle$ at some time t: to explore what this looks like, we'll take some expectation values with the Heisenberg operator:

$$\langle A\rangle_t = \langle \tilde{x_0}, t| A |\tilde{x_0}, t\rangle = \langle \tilde{x_0}| A_H |\tilde{x_0}\rangle ,$$

and if we wanted, we could also write this as $\langle 0| T_{x_0}^\dagger A_H T_{x_0} |0\rangle$, so everything can be computed from expectation values on the vacuum.

Example 199

What is the expectation value of $\hat{x}$ as a function of time on this x_0 coherent state?

We plug in the Heisenberg operator $\hat{x}_H$ to find that

$$\langle \hat{x} \rangle_{\tilde{x}_0}(t) = \left\langle \tilde{x_0} \middle| \left(\hat{x} \cos \omega t + \frac{\hat{p}}{m\omega} \sin \omega t \right) \middle| \tilde{x_0} \right\rangle$$

(remember that the key idea is to evolve the **operators**, not the states), and now we know the expectation values of $\hat{x}$ and $\hat{p}$ in the coherent state: they're x_0 and 0 respectively, so this just evaluates to

$$\boxed{\langle \hat{x} \rangle_{\tilde{x}_0}(t) = x_0 \cos \omega t}.$$

In other words, this object oscillates classically – we again have classical behavior of a quantum state!

Example 200

What is the expectation value of $\hat{p}$ as a function of time?

This expectation should not just be zero for all time, since an object that is oscillating must move and therefore must have some momentum. We plug in the Heisenberg operator $\hat{p}_H$ to find that

$$\langle \hat{p} \rangle_{\tilde{x}_0}(t) = \langle \tilde{x_0} | (\hat{p} \cos \omega t - m\omega \hat{x} \sin \omega t) | \tilde{x_0} \rangle = \boxed{-m\omega x_0 \sin \omega t}.$$

Indeed, we now find that

$$\langle \hat{p} \rangle_{\tilde{x}_0}(t) = m \frac{d}{dt} \langle \hat{x} \rangle_{\tilde{x}_0}(t),$$

so we get classical behavior in the momentum as well.

But now here's the key calculation: we want to show that we have coherent evolution. In the harmonic oscillator ground state, we have a **minimum uncertainty** packet – the ground state has some Δx and Δp, where their product saturates the uncertainty principle. But to make sure we have coherency, we just need to make sure that the uncertainties remain the same and that they're saturated. That would imply that the shape is always Gaussian, so we do have the same shape moving around in this classical manner.

Example 201

What are the uncertainties Δx and Δp as a function of time?

This is an example now where the calculation becomes a nightmare if we don't have the Heisenberg picture. We know that (using the ususla formula for uncertainty)

$$(\Delta x)^2(t) = \left\langle \tilde{x_0}, t \middle| \hat{x}^2 \middle| \tilde{x_0}, t \right\rangle - \langle \tilde{x_0}, t | \hat{x} | \tilde{x_0}, t \rangle^2,$$

and we've calculated the second term already: we have

$$(\Delta x)^2(t) = \left\langle \tilde{x_0} \middle| x_H^2(t) \middle| \tilde{x_0} \right\rangle - x_0^2 \cos^2 \omega t.$$

And now we focus on the first term: expanding out the expression for x_H, we have

$$\left\langle \tilde{x_0} \middle| x_H^2(t) \middle| \tilde{x_0} \right\rangle = \left\langle \tilde{x_0} \middle| \hat{x}^2 \cos^2 \omega t + \frac{\hat{p}^2}{m^2\omega^2} \sin^2 \omega t + \frac{1}{m\omega} \cos \omega t \sin \omega t (\hat{x}\hat{p} + \hat{p}\hat{x}) \middle| \tilde{x_0} \right\rangle,$$

and now we can calculate each of these terms by referring to the "small exercises" above: all of this simplifies to

$$= \left(x_0^2 + \frac{\hbar}{2m\omega} \right) \cos^2 \omega t + \frac{m\hbar\omega}{2m^2\omega^2} \sin^2 \omega t + 0,$$

so plugging this into our uncertainty, the x_0^2 terms cancel and we just have

$$(\Delta x)^2(t) = \frac{\hbar}{2m\omega}(\cos^2 \omega t + \sin^2 \omega t) = \boxed{\frac{\hbar}{2m\omega}}.$$

So the time dependence disappears – the uncertainty Δx remains the same throughout the process! As an exercise, we can verify that we indeed have

$$(\Delta p)^2(t) = \frac{m\hbar\omega}{2},$$

and now $\Delta p \Delta x = \frac{\hbar}{2}$ is a **saturation of the uncertainty principle**, so our state maintains its shape through time-evolution.

So we'll now turn our attention to looking at this coherent state in the energy basis. Somehow, we've created a superposition of different energy states that move nicely together – if we can understand where this comes from, we'll be able to generalize our coherent states completely.

If we write

$$|\tilde{x_0}\rangle = \exp\left(-\frac{i\hat{p}x_0}{\hbar} \right) |0\rangle ,$$

there is a famous length scale in the harmonic oscillator

$$d_0^2 = \frac{\hbar}{m\omega}.$$

This is basically the uncertainty of the position in the ground state up to a factor of $\sqrt{2}$, and this is the only way we can really construct a length by dimensional analysis. So let's plug in the expression for $\hat{p}$ into our coherent state: we have that

$$|\tilde{x_0}\rangle = \exp\left(\frac{x_0}{\sqrt{2}d_0}(\hat{a}^\dagger - \hat{a}) \right) |0\rangle .$$

So now this is nicer because $\frac{x_0}{d_0}$ has no units, and the operators $\hat{a}$ and $\hat{a}^\dagger$ have no units either. (And remember that because $\hat{a}^\dagger - \hat{a}$ is anti-Hermitian, so it makes sense that we have no i in the exponent.) We're going to **reorder** this exponential, which is a job for our Baker–Campbell–Hausdorff formula:

$$e^{X+Y} = e^X e^Y e^{-\frac{1}{2}[X,Y]}$$

as long as $[X, Y]$ commutes with both X and Y. The idea here is that we want to split up the creation and annihiliation operators – we want them in separate exponentials – because we don't want to have to expand powers of $\hat{a}^\dagger - \hat{a}$. But if we use the formula, we have that (letting $X = \frac{x_0}{\sqrt{2}d_0}\hat{a}^\dagger$ and $Y = -\frac{x_0}{\sqrt{2}d_0}\hat{a}$)

$$e^{\frac{x_0}{\sqrt{2}d_0}\hat{a}^\dagger - \frac{x_0}{\sqrt{2}d_0}\hat{a}}$$

(**note that we choose things in this order so that the** $\hat{a}$ **annihiliators act on** $|0\rangle$ **first**, because instead of creating states, we can kill the vacuum!) can be rewritten as

$$e^{\frac{x_0}{\sqrt{2}d_0}\hat{a}^\dagger} e^{-\frac{x_0}{\sqrt{2}d_0}\hat{a}} e^{-\frac{1}{2}[X,Y]},$$

and $[X, Y]$ is now a number (which is good, because it now commutes with X and Y) equal to $\frac{x_0^2}{2d_0^2}$, where we've used

that $[\hat{a}^\dagger, \hat{a}] = -1$. This gives us a final coherent state of the form

$$|\tilde{x_0}\rangle = e^{\frac{x_0}{\sqrt{2}d_0}\hat{a}^\dagger} e^{-\frac{x_0}{\sqrt{2}d_0}\hat{a}} e^{-\frac{1}{4}\frac{x_0^2}{d_0^2}} |0\rangle .$$

Now the $e^{-\frac{1}{4}\frac{x_0^2}{d_0^2}}$ is just some number, and then the exponential of the annihilator operator is 1 plus some annihiliator terms – **everything except the** 1 **kills the vacuum**! So the annihilator exponential acts as the **identity** on $|0\rangle$, and now we can write that

$$\boxed{|\tilde{x_0}\rangle = e^{-\frac{1}{4}\frac{x_0^2}{d_0^2}} e^{\frac{x_0}{\sqrt{2}d_0}\hat{a}^\dagger} |0\rangle}.$$

To talk about our energy eigenstates, we can now expand our exponential:

$$|\tilde{x_0}\rangle = e^{-\frac{1}{4}\frac{x_0^2}{d_0^2}} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{x_0}{2d_0}\right)^n \hat{a}^\dagger |0\rangle ,$$

and now we plug in our nth energy eigenstates:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle ,$$

so we now have an expression for our coherent state in terms of the energy eigenstates:

$$\boxed{|\tilde{x_0}\rangle = e^{-\frac{1}{4}\frac{x_0^2}{d_0^2}} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \left(\frac{x_0}{2d_0}\right)^n |n\rangle}.$$

If we think of this as a sum $\sum_{n=0}^{\infty} c_n |n\rangle$, we have a precise combination of energy eigenstates, and we can calculate $|c_n|^2$, which tells us the **probability to find the coherent state in the** n**th eigenstate**. We find that

$$|c_n|^2 = \exp\left(-\frac{1}{2}\frac{x_0^2}{d_0^2}\right) \frac{1}{n!} \left(\frac{x_0^2}{2d_0^2}\right)^n .$$

And now we have the same expression inside the exponential and the power: if we define $\lambda = \frac{x_0^2}{2d_0^2}$, we now have that

$$\boxed{|c_n|^2 = e^{-\lambda} \frac{\lambda^n}{n!}}.$$

This is called the **Poisson distribution**! In other words, the energy is (in some sense) Poisson distributed in a coherent state.

Remark 202. *Poisson distributions come up when we, for example, have a radioactive material of a certain lifetime. Then the number of events that happen in a week is Poisson distributed.*

We'll first check that we do have a probability distribution:

$$\sum_{n=0}^{\infty} |c_n|^2 = e^{-\lambda} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!},$$

and now the infinite sum is the power series for e^λ, so this does evaluate to 1. One relevant property of any probability distribution is its expectation value – this isn't necessarily the most **probable** n, but we can still find it:

$$\sum_{n=0}^{\infty} n|c_n|^2 = e^{-\lambda} \sum_{n=0}^{\infty} n\frac{\lambda^n}{n!},$$

and we can get this by applying a λ-derivative:

$$= e^{-\lambda}\lambda\frac{d}{d\lambda}\sum_{n=0}^{\infty}\frac{\lambda^n}{n!} = e^{-\lambda}\lambda\frac{d}{d\lambda}e^{\lambda} = \lambda.$$

Example 203

Remembering that $\lambda = \frac{x_0^2}{2d_0^2}$, this tells us that if we have $x_0 = 1000d_0$ (that is, we've moved the particle 1000 times the quantum uncertainty), the most strongly occupied levels are on the order of 1 million.

And we can think of our occupation number by using the expectation value of the **number operator**:

$$\langle\tilde{x_0}|\hat{N}|\tilde{x_0}\rangle = \sum_{m,n} c_m^* \langle m|\hat{N}|n\rangle c_n,$$

where we've substituted in the values of $|\tilde{x_0}\rangle$ and its corresponding bra. Since $|n\rangle$ is an eigenvector of $\hat{N}$ with eigenvalue n, and $c_m^* = c_m$, this all just reduces to

$$= \sum_{n,m} c_m c_n n\delta_{mn} = \sum_n c_n^2,$$

which is again the λ we were just talking about. From here, we can do some more calculations: we've found the **expectation value** of the energy, and it's worth also thinking about the **uncertainty** as well – is the set of energies sharply peaked or more spread out? This is left as an exercise for us – it turns out that

$$(\Delta E)_{\tilde{x_0}} = \hbar\omega\frac{x_0}{\sqrt{2}d} \implies \frac{\Delta E}{\hbar\omega} = \frac{x_0}{d}.$$

So the energy uncertainty for a classical-looking coherent state – that is, where $x_0 \gg d$ – has ΔE large compared to the spacing of the harmonic oscillator. So lots of different energy levels will be excited, but we also know that

$$\frac{\langle E\rangle}{\Delta E} \approx \frac{\frac{1}{2}m\omega^2 x_0^2}{\hbar\omega\frac{x_0}{2}} = \frac{x_0}{\sqrt{2}d}.$$

So this state has an interesting property: the energy uncertainty corresponds to many different levels of energy eigenstates, but this uncertainty is still much smaller (in fact by the same factor) compared to the actual average energy. In other words, we have a **state with an almost definite energy, containing many levels in the oscillator**.

And now we're ready to generalize our coherent states in a way that makes them more flexible:

Definition 204

The **α coherent state** for $\alpha \in \mathbb{C}$ is defined to be

$$|\alpha\rangle = D(\alpha)|0\rangle = \exp\left(\alpha\hat{\alpha}^\dagger - \alpha^*\hat{\alpha}\right)|0\rangle.$$

The operator $D(\alpha)$ is unitary: its exponent is

$$\alpha\hat{a}^\dagger - \alpha^*\hat{a},$$

which is equal to its own dagger, so the exponent is anti-Hermitian and therefore the exponential is unitary. And we can check that when α is real, this will reduce to the previous case.

First of all, let's calculate

$$\hat{a}|\alpha\rangle = \hat{a}\exp\left(\alpha\hat{\alpha}^\dagger - \alpha^*\hat{\alpha}\right)|0\rangle.$$

We know that $\hat{a}$ kills the vacuum, so we would want to switch around the two terms: we can replace the product with a commutator

$$= \left[\hat{a}, \exp\left(\alpha\hat{\alpha}^\dagger - \alpha^*\hat{\alpha}\right)|0\rangle\right].$$

This is again in the formula sheet Campbell–Baker–Hausdroff says that

$$[A, e^B] = [A, B]e^B$$

as long as $[A, B]$ commutes with B. So taking $A = \hat{a}$ and $B = \alpha\hat{a}^\dagger - \alpha^*\hat{a}$, their commutator is just a number, and we find that

$$\boxed{\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle}.$$

So we've now **diagonalized a non-Hermitian operator** – we found its eigenvalues! Unfortunately, we don't get any of the nice theorems about Hermitian operators – states of different eigenvalues aren't orthogonal, and we don't have completeness, so nothing works quite as nicely as we want. But this is still pretty remarkable – **coherent states are eigenstates of the annihiliator operator**.

The physical interpretation of such a state is that $|\alpha\rangle$ is a coherent state with some **initial momentum** (in the real case where our position is $x_0\cos\omega t$, the particle starts off with zero momentum). Indeed, we can check that

$$\langle\alpha|\hat{x}|\alpha\rangle = \frac{d}{\sqrt{2}}\left\langle\alpha\middle|\hat{a} + \hat{a}^\dagger\middle|\alpha\right\rangle.$$

We can now apply $\hat{a}$ on the $|\alpha\rangle$ ket and $\hat{a}^\dagger$ on the $\langle\alpha|$ bra, and we find that this is equal to

$$= \frac{d}{\sqrt{2}}(\alpha + \alpha^*) = d\sqrt{2}\,\mathrm{Re}(\alpha).$$

Similarly, we can calculate the expectation value of the momentum: we find that

$$\langle\alpha|\hat{p}|\alpha\rangle = \frac{\sqrt{2}\hbar}{d}\,\mathrm{Im}(\alpha).$$

The formulas are a bit messy, but the main point is that the **real part** of α corresponds to the **position** of the coherent state, while the **imaginary part** of α tells us the **initial momentum**. And we can describe this geometrically by considering the complex α-plane: this α vector will then evolve in time in a nice way, because

$$|\alpha, t\rangle = e^{-iHt/\hbar}e^{\alpha a^\dagger - \alpha^* a}e^{iHt/\hbar}e^{-iHt/\hbar}|0\rangle$$

(where we've added the blue terms to make computation nicer), and now the last two terms evaluate to $e^{-i\omega t/2}|0\rangle$ (we have an energy eigenstate for H of the ground state energy $\frac{\hbar\omega}{2}$), while the first three terms are basically the Heisenberg operator, except that we have opposite signs for the t. Thus, we have the Heisenberg operator at time $-t$:

$$|\alpha, t\rangle = e^{\alpha\hat{a}_H^\dagger(-t) - \alpha^*\hat{a}_H(-t)}e^{-i\omega t/2}|0\rangle.$$

But we have the formula for the Heisenberg operators $\hat{a}_H$ and $\hat{a}_H^\dagger$: plugging those in (which just gives us an additional phase) yields

$$|\alpha, t\rangle = e^{\alpha e^{-i\omega t}\hat{a}^\dagger - \alpha^* e^{i\omega t}\hat{a}}e^{-i\omega t/2}|0\rangle.$$

So α has now become $\alpha e^{i\omega t}$! In other words,

$$|\alpha, t\rangle = e^{-i\omega t/2}\left|e^{-i\omega t}\alpha\right\rangle.$$

The $e^{-i\omega t/2}$ in the front is an irrelevant phase for the whole state: all that's happening is that α is rotating in a circle

with frequency ω in our complex plane, and at any time, the real part is proportional to the expectation value of the position, while the imaginary part is proportional to the expectation value of the momentum.

Fact 205

We do need to choose appropriate units on our real and imaginary axes: the length scale for the real axis is $\frac{\langle x\rangle}{\sqrt{2}d_0}$, and the length scale for the imaginary axis is $\frac{\langle p\rangle d_0}{\sqrt{2}\hbar}$. This way, we do indeed rotate in a **circle**, rather than just an ellipse.

So **in summary** of everything we've been discussing: coherent states came out of taking the ground states of our harmonic oscillator and displacing them with some translation operator. But ultimately, the reason this all works out is that this operator is actually that we have an exponential of something depending on our creation and annihiliation operators, which allowed us to define a more general α coherent state. Because our operator $D(\alpha)$ is unitary, our state $|\alpha\rangle$ is indeed well-normalized, and in fact this state remains a coherent state with a value of α rotating with some angular velocity ω in the complex plane.

We'll finish by developing one more idea here. α coherent states are not position, momentum, or energy eigenstates, so there are measures of **uncertainty** in each of these observables. So we should really draw α as a kind of Gaussian blob: while we know the exact value of the expectation value of $\hat{x}$ and $\hat{p}$, that's not necessarily going to be the exact value that we measure.

And we'll relate that to the concept of an **electromagnetic wave**. Suppose this EM wave has energy E, and its electric field is described by a function $A\cos\omega t$. Earlier, we discussed briefly the idea of energy-time uncertainty – let's do a handwavy argument first. The phase of this wave $\phi = \omega t$ has some error

$$\frac{\Delta\phi}{\omega} = \Delta t,$$

and now this wave has an energy

$$E = N\hbar\omega \implies \Delta E = \Delta N\hbar\omega,$$

where N is the number of photons. Then

$$\Delta E\Delta t \sim \frac{\hbar}{2} \implies \Delta N\hbar\omega\frac{\Delta\phi}{\omega} \sim \frac{\hbar}{2} \implies \boxed{\Delta N\Delta\phi \sim 1}.$$

This last relation is actually taken somewhat seriously: comparing the uncertainty in the number of photons and the phase in a wave in quantum optics does yield a result that looks like this. Of course, our derivation is bad – we haven't really explained what Δt means, but this gives us a bit of intuition.

So let's do a more explicit calculation: in our coherent state, we know that

$$\langle\hat{N}\rangle_\alpha = \left\langle\alpha\middle|\hat{a}^\dagger\hat{a}\middle|\alpha\right\rangle,$$

and now we can have $\hat{a}^\dagger$ act on the left and $\hat{a}$ act on the right to get

$$\langle\alpha|\alpha^*\alpha|\alpha\rangle = |\alpha|^2\langle\alpha|\alpha\rangle = |\alpha|^2.$$

So in a harmonic oscillator, the expectation of the number operator is the squared length of α. Similarly, we can find that

$$\langle\hat{N}\rangle_\alpha = \left\langle\alpha\middle|\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\middle|\alpha\right\rangle = |\alpha|^2\left\langle\alpha\middle|\hat{a}\hat{a}^\dagger\middle|\alpha\right\rangle.$$

Now $\hat{a}$ and $\hat{a}^\dagger$ are kind of in the wrong order – we want $\hat{a}$ to act on a ket, but it's acting on a bra – so we replace this

object by the commutator plus its reverse order: this yields

$$= |\alpha|^2(1 + \langle\alpha|\hat{a}^\dagger\hat{a}|\alpha\rangle) = \boxed{|\alpha|^2(1 + |\alpha|^2)}.$$

And this allows us to calculate the **uncertainty in** N:

$$\Delta N = \sqrt{|\alpha|^4 + |\alpha|^2 - |\alpha|^4} = |\alpha|.$$

In other words, the uncertainty in N is the square root of the expected value of N – thus the "length" of α in our complex plane is actually ΔN, not $\langle N\rangle$.

And now we can be more precise with our uncertainty relation. α is rotating in our complex plane, and the uncertainty of the position, and also the momentum, in a coherent state are just the uncertainty in the ground state:

$$\Delta x = \frac{d_0}{\sqrt{2}}, \quad \Delta p = \frac{\hbar}{\sqrt{2}d_0}.$$

Remembering how we chose the units on our real and imaginary axis, we find that our Gaussian "blob" of α spans an uncertainty on the order of $\frac{1}{2}$ in the real axis, as well as in the imaginary axis. So we can say that the diameter of the Gaussian blob is on the order of 1, so the **phase of α in the complex plane has some amount of uncertainty as well!** Since the length of α is ΔN, and the blob covers a length of 1 along the circumference of the circle, this tells us that the uncertainty in the angle is $\frac{1}{\Delta N}$. So this at least gives us a picture of where the equation

$$\Delta N \Delta\phi \sim 1,$$

the **phase uncertainty relation**, originates from.

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We've now started talking about Heisenberg operators and coherent states – questions on this material were postponed last lecture, but we can talk about them now. And we'll do some practice problems to help prepare for the exam. (There will be a formula sheet, but the test is closed book, closed notes. If we have a request for a particular equation, we should let the 8.051 instructors know.)

As a general rule, we should not rely too much on trying to memorize equations and principles, but we should know by heart things like the harmonic oscillator Hamiltonian or Schrodinger equation because we've worked with them repeatedly. For example, if we know that we can write

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = h\omega\left(\hat{N} + \frac{1}{2}\right),$$

where the number operator $\hat{N} = \hat{a}^\dagger\hat{a}$, we can know that $\hat{x}$ and $\hat{p}$ are some constants times $\hat{a} + \hat{a}^\dagger$ and $\hat{a} - \hat{a}^\dagger$. We know that $\frac{\hbar}{m\omega}$ is a helpful length scale, because $\hat{p}$ has units of $\frac{\hbar}{L}$, which means H has units of $\frac{\hbar^2}{mL^2} = m\omega^2L^2$ (by comparing it to the kinetic energy term). And this tells us that

$$L^4 = \left(\frac{h}{m\omega}\right)^2 \implies L^2 = \frac{\hbar}{m\omega},$$

which tells us that the $\hat{x}$ operator should have a $\sqrt{\frac{\hbar}{m\omega}}$ term, plus some additional constants. And if we're not sure, we can always check them by using $[\hat{a}, \hat{a}^\dagger] = 1$. And this means that we can find out what the explicit formulas for $\hat{a}$ and $\hat{a}^\dagger$ look like by taking linear combinations of $\hat{x}$ and $\hat{p}$.

So in this example, knowing that we should write the Hamiltonian as $\hbar\omega\left(\hat{N}+\frac{1}{2}\right)$ is important on an intuitive level to help us find the direction of how to proceed. But then the rest can be deduced step by step!

Similarly, if we've been practicing, we should know the Pauli matrices pretty well (maybe knowing σ_z and σ_x). But also important is knowing their properties: they're Hermitian, traceless, and so on.

Example 206

Consider an infinite square well with

$$V(x)=\begin{cases}0 & -\frac{L}{2}\le x\le\frac{L}{2}\\ \infty & \text{otherwise.}\end{cases}$$

Show that $\Delta x\le\frac{L}{2}$. Can this be saturated?

Note that

$$\boxed{(\Delta x)^2}=\langle x^2\rangle-\langle x\rangle^2\le\langle x^2\rangle,$$

and since $|x|\le\frac{L}{2}$ everywhere, $\langle x^2\rangle\le\boxed{\left(\frac{L}{2}\right)^2}$. Taking square roots on both sides yields the desired result. But equality would occur if the particle is only found at $-\frac{L}{2}$ or $\frac{L}{2}$ (with equal probability of each so that $\langle x\rangle=0$), and this would give us a discontinuous wavefunction. So it is not possible to saturate the inequality.

By the way, a state with zero position uncertainty is a delta function, which is not normalizable (because we have to square it)! So that's a kind of degenerate state on the other end.

Example 207

Consider position eigenstates in the simple harmonic oscillator: we wish to construct a state

$$\hat{x}\,|x\rangle=x\,|x\rangle\,.$$

As a hint, $\hat{x}=\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^{+})$, and we should use the ansatz

$$|x\rangle=N(x)\exp\left(\beta\hat{a^\dagger}-\frac{1}{2}\gamma\hat{a^\dagger}\hat{a^\dagger}\right)|0\rangle$$

where β,γ are constants to be determined with the eigenstate condition and $N(x)$ is determined with the overlap $\langle 0|\,|x\rangle$.

First, we use the eigenstate condition: this tells us (plugging in the definition of $\hat{x}$) that

$$\hat{x}|x\rangle\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^{+})N(x)\exp\left(\beta\hat{a^\dagger}-\frac{1}{2}\gamma\hat{a^\dagger}\hat{a^\dagger}\right)|0\rangle=xN(x)\exp\left(\beta\hat{a^\dagger}-\frac{1}{2}\gamma\hat{a^\dagger}\hat{a^\dagger}\right)|0\rangle\,.$$

We wish to move that $(\hat{a})$ past the exponential term, but this makes us pick up a commutator term for the $\hat{a}$: since $[A,e^B]=[A,B]e^B$ if $[A,B]$ is a constant (more generally, when $[[A,B],B]=0$), we start this problem by doing the side calculation

$$\hat{a}e^{\beta\hat{a^\dagger}-\frac{1}{2}\gamma\hat{a^\dagger}\hat{a^\dagger}}=e^{\beta\hat{a^\dagger}-\frac{1}{2}\gamma\hat{a^\dagger}\hat{a^\dagger}}\hat{a}+\left[\hat{a},beta\hat{a^\dagger}-\frac{1}{2}\gamma\hat{a^\dagger}\hat{a^\dagger}\right]e^{beta\hat{a^\dagger}-\frac{1}{2}\gamma\hat{a^\dagger}\hat{a^\dagger}}.$$

The whole point is that plugging everything back in, we require

$$\beta-\gamma a^\dagger+a^\dagger,$$

so $\gamma = 1$ and $\beta\sqrt{\frac{\hbar}{2m\omega}} = x$. We can see the rest of the solutions online.

Here's one more problem we can think about:

Example 208

Consider the uncertainty relation

$$\Delta S_x \Delta S_y \geq C.$$

Find C, and rewrite it as $\Delta\sigma_x \Delta\sigma_y \geq C'$. Find the states that saturate this inequality (with $|\gamma| \leq 1$)

$$(\hat{A} - \langle\hat{A}\rangle)\,|\psi\rangle = -i\gamma(\hat{B} - \langle\hat{B}\rangle)\,|\psi\rangle\,.$$

23 Photon States and Two State Systems, Part 1

Today, we're going to talk about a new kind of system – **quantum states of the electromagnetic field**. A photon is a discrete quantum of that field, so in some sense, this is a first introduction to quantum field theory! It turns out that the harmonic oscillator plays a pretty important role here, and a key idea will be the set of coherent states that we defined last time:

$$|\alpha\rangle = D(\alpha)\,|0\rangle\,, \quad D(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}.$$

(These states have the property that $\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle$.) So photon states have to do with the electric and magnetic field, and we're going to try to do a quantum description of this by starting with a description of its energy. Recall that the energy E can be evaluated by an integral of the form

$$E = \frac{1}{2}\int d^3x\varepsilon_0\left[\vec{E}^2(\vec{r},t) + c^2\vec{B}^2(\vec{r},t)\right].$$

We'll focus on a **particular mode** of this that we've seen from 8.02, where we have a finite volume cavity and a single plane wave with some wavelength and some frequency. Suppose this wave is along the z-direction – then we can write our field as

$$E_x(z,t) = \sqrt{\frac{2}{\varepsilon_0 V}}\omega q(t)\sin(kz),$$

where V is the volume of the cavity (we can think of it as a large box, or we can imagine it being almost infinite), and ω and $k = \frac{\omega}{c}$ are the frequency and wavenumber of our electromagnetic wave, respectively. (The factor in the front is just for normalization.) Here, $q(t)$ is some arbitrary function of time that we'll determine later, and the ω will make more sense soon. By Maxwell's equations, this corresponds to a magnetic component in the y direction

$$cB_y(z,t) = \sqrt{\frac{2}{\varepsilon_0 V}}p(t)\cos kz,$$

where $p(t)$ is some other arbitrary function of time (related to $q(t)$ by Maxwell's equations). We can check this configuration more carefully, but for now the important thing is for us to think about the energy of such a system: since we're squaring the E and B fields and integrating over the whole box of volume V, the prefactors will actually disappear – this is because the average value of $\sin^2 kz$ and $\cos^2 kz$ is $\frac{1}{2}$, and this is a valid approximation for us to use if our box is large enough. Putting everything together, we'll find that our energy is

$$E = \frac{1}{2}\left(p(t)^2 + \omega^2 q(t)^2\right).$$

So now our ω makes a bit more sense – we're getting something that looks a lot like a harmonic oscillator, except we're missing the mass terms: this means that we have different units for p and q as we do for a usual harmonic oscillator.

Fact 209

Notice, though, that we couldn't have done any better – photons have no mass, and we're trying to describe an electromagnetic field with photons.

So we'll just resolve the units ourselves – p must have units $[p] = \sqrt{E}$, and q must have units $[q] = T\sqrt{E}$ (where the extra time factor T comes from ω having units of $\frac{1}{T}$). So at the end of the day, pq has the units of $[T][E]$, which are the units of $\hbar$ – that's a good sign! This perhaps motivates us, because there is a **natural correspondence** between a mode of vibration of a classical electromagnetic field and an energy functional that looks like the harmonic oscillator.

Proposition 210

We'll say that

$$E = \frac{1}{2}\left(p(t)^2 + \omega^2 q(t)^2\right)$$

is a Hamiltonian, where p and q are the **Heisenberg** operators of the electromagnetic field.

So now we can say that

$$H = \frac{1}{2}\left(\hat{p}^2 + \omega^2 \hat{q}^2\right)$$

is our time-independent Hamiltonian – even though p and q are functions of t, that's because we're taking those to be the Heisenberg versions of our operator – and while this might seem speculative, we can do some checks to make sure that this is indeed reasonable. First of all, we should look at the Heisenberg equations of motion and compare them to the classical equations of motion:

$$i\hbar \frac{d}{dt} p_H(t) = [\hat{p}_H, H]$$

for a time-independent Hamiltonian, and we can also plug in Maxwell's equations and see what relations we get for $q(t)$ and $p(t)$. It turns out (when we do this for homework), those two sets of equations are exactly equivalent! So it is indeed valid to think of our dynamical system with $\hat{q}$ and $\hat{p}$ as our quantum operators.

So remembering that we're using a harmonic oscillator, except replacing mass m go to 1 (this is okay because we found that p and q have units that multiply to $\hbar$), we now have **expressions for our two operators in terms of creation and annihilation operators**:

$$\hat{q} = \sqrt{\frac{\hbar}{2\omega}}(\hat{a} + \hat{a}^\dagger), \quad \hat{p} = \frac{1}{i}\sqrt{\frac{\omega\hbar}{2}}(\hat{a} - \hat{a}^\dagger)$$

just by setting $m = 1$. Indeed, the units match up over here, and then we can also write the Hamiltonian in terms of of our number operator:

$$H = \hbar\omega\left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right),$$

because m doesn't show up in this formula in the harmonic oscillator case anyway, and therefore we can also write this in terms of the number operator

$$H = \hbar\omega\left(\hat{N} + \frac{1}{2}\right).$$

We'll now physically interpret this as saying that **a state with some number of photons n has the energy $n\hbar\omega$** (plus the extra $\frac{1}{2}\hbar\omega$). This is actually a huge assumption, because what we're doing is taking $\hat{x}$ and $\hat{p}$ and replacing them

with $\hat{q}$ and $\hat{p}$, but they have nothing to do with the usual position and momentum – they should represent the electric and magnetic field. So really, $\vec{E}$ and $\vec{B}$ are becoming quantum operators! Quantum field theory is the whole idea that fields are operators, and it seems to be a valid idea in this case: a state with N photons is viewed as a state of a "harmonic oscillator" with mass 1.

So now let's go to our Heisenberg form for our operators: we have equations above that tell us $\hat{p}$ and $\hat{q}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$, and just replacing everything with its Heisenberg counterpart now tells us that

$$q(t) = \sqrt{\frac{\hbar}{2\omega}} \left(e^{-i\omega t}\hat{a} + e^{i\omega t}\hat{a}^\dagger\right).$$

(Each operator on the right hand side just gains a phase.) And now substituting this back into our electric field, we find that

$$\boxed{\hat{E}_x(z,t) = \mathcal{E}_0 \left(e^{-i\omega t}\hat{a} + e^{i\omega t}\hat{a}^\dagger\right) \sin kz},$$

where t is the time in a Heisenberg operator and $\mathcal{E}_0 = \sqrt{\frac{\hbar\omega}{\varepsilon_0 V}}$. And the main point here is that this is now an **electromagnetic field operator**!

Example 211

Let's find the expectation value of this electric field operator to get a bit more intuition.

Suppose we have some photon energy eigenstate $|n\rangle$, so now we have a state with n photons and a total enregy of $n\hbar\omega + \frac{1}{2}\hbar\omega$. We now want to compute

$$\langle E_x\rangle_{|n\rangle} = \mathcal{E}_0 \left(e^{-i\omega t}\langle n|\hat{a}|n\rangle + e^{i\omega t}\left\langle n\middle|\hat{a}^\dagger\middle|n\right\rangle\right)\sin kz,$$

and the idea is that this tells us how the electric field should look in this state $|n\rangle$. But $\hat{a}$ reduces $|n\rangle$ to $|n-1\rangle$, which is orthogonal to $|n\rangle$, and similarly $\hat{a}^\dagger$ raises $|n\rangle$ to an orthogonal state as well. **So the expectation value is zero**, but this isn't that surprising – in an energy eigenstate, the wavefunction doesn't change in time, so nothing interesting happens.

So let's pick a more imaginative state – we've said many times that **coherent states** act like classical states, so let's try putting in the state $|\alpha\rangle$ instead. Then

$$\langle E_x\rangle_{|\alpha\rangle} = \mathcal{E}_0 \left(e^{-i\omega t}\langle \alpha|\hat{a}|\alpha\rangle + e^{i\omega t}\left\langle \alpha\middle|\hat{a}^\dagger\middle|\alpha\right\rangle\right)\sin kz,$$

and this time things are better: $\langle\alpha|\hat{a}|\alpha\rangle = \alpha\langle\alpha|\alpha\rangle = \alpha$, and similarly the other term evaluates to α^* (we evaluate on the bra instead), and this all simplifies to

$$= \mathcal{E}_0 \left(e^{-i\omega t}\alpha + e^{i\omega t}\alpha^*\right)\sin kz,$$

and now this is great: the expectation value of the electromagnetic wave look like traveling or stationary waves that we see in 8.02! So a classical wave that resonates in a finite-volume cavity really is just a coherent state of the electromagnetic field: even though this state of photons is not an eigenstate for energy, position, or momentum, we still have a nice classical picture that looks like a normal wave. (And that also explains that lasers are coherent states of the electromagnetic field – if the number uncertainty is large, the phase uncertainty can be very small.)

And now we can do this more explicitly: this can also be written as

$$\langle\hat{E}\rangle_{|\alpha\rangle} = 2\mathcal{E}_0 \,\mathrm{Re}(\alpha e^{-i\omega t})\sin kz,$$

and now if we write $\alpha = |\alpha| e^{i\theta}$, this simplifies to

$$= 2\mathcal{E}_0 |\alpha| \cos(\omega t - \theta) \sin kz,$$

which is a **standing wave** with a fixed spatial distribution, and it has a nice classical description as well as a good quantum description. And if we want to find the energy of this state, it's the expectation value of the Hamiltonian:

$$\langle H \rangle = \hbar\omega \left(\langle \hat{N} \rangle + \frac{1}{2} \right),$$

and in a coherent state, we know that $\hat{N} = |\alpha|^2$. **So the coherent state α has $|\alpha|^2$ photons**.

This is basically all we will talk about with photon states – we could put together different superpositions of modes and discuss commutation relations of the field operators and so on, but that's what quantum field theory is for. In summary, the main point of this discussion is that **the harmonic oscillator has entered in an interesting way**, such that we have an uncertainty between the E and B fields. The different energy levels of this oscillator correspond to different numbers of photons, and we get a classical description by considering coherent states – this is how we can recover the classical wave oscillations that are familiar from 8.02.

We'll now spend the next few lectures on **two-state systems**, and the first topic of interest is that of **spin precession**. It seems like this is a very particular kind of problem when we have spins in magnetic fields, but it'll turn out that **any two-state system can be thought of as a spin in a magnetic field**, even if we're talking about an electron shared between two atoms or an ammonia molecule – mathematically, spins are what we've already become familiar with.

Recall that this whole concept of spin precession comes up when we try to relate a particle's magnetic moment with its angular momentum. We made an argument earlier on in class that

$$\vec{\mu} = \frac{q}{2m} \vec{S},$$

where $\vec{S}$ is the classical angular momentum. But we also claim that this is true in quantum mechanics as well, except for a few small modifications: we get a slightly different magnetic moment in the Hamiltonian, which gives us an additional g factor on the right side, and the $\vec{S}$ is now an **intrinsic spin angular momentum**. It's a bit abstract, and the best way for us to view this object is as an operator! The magnetic dipole moment is then also an operator (since it's a constant times the spin operator).

Recall that $g = 2$ for the electron – this is predicted both by Dirac's relativistic equation for the electron and by experimental results – and particles like the proton or neutron have different values of g. For example, a neutron has three quarks – two with some charge, one with the opposite – and it's possible that this can have a positive angular magnetic moment. At the end of the day, we'll simplify this with some notation and just write

$$\boxed{\vec{\mu} = \gamma \vec{S}},$$

where the constant γ summarizes all of the factors that we gain throughout this process. The Hamiltonian for such a system is just (subscript s for spin)

$$\hat{H}_s = -\vec{\mu} \cdot \vec{B},$$

and here $\vec{B}$ will typically be a **static** magnetic field, so that we don't have to quantize it and think of it as a quantum field (as discussed above). And we'll typically write this also as

$$= -\gamma \vec{S} \cdot \vec{B} = -\gamma \vec{B} \cdot \vec{S} = -\gamma [B_x \hat{S}_x + B_y \hat{S}_y + B_z \hat{S}_z].$$

Example 212

When the magnetic field only points in the z-direction (and is of the form $B\hat{z}$), our Hamiltonian simplifies to

$$\hat{H}_s = -\gamma B \hat{S}_z.$$

Then the unitary operator that generates time evolution of states (for a time-independent Hamiltonian) is

$$\exp\left(-\frac{iH_s t}{\hbar}\right) = \exp\left(\frac{-i(-\gamma B t)\hat{S}_z}{\hbar}\right).$$

Now we're going to use a property that we've justified in homework but will understand in more detail in the next few lectures: we talked about the operator

$$\hat{R}_{\vec{n}}(\alpha) = \exp\left(-\frac{i\alpha \hat{S}_n}{\hbar}\right),$$

where $\vec{n}$ is a unit vector and $\hat{S}_{\vec{n}} = \vec{n} \cdot \hat{S}$. This was called the **rotation operator** – we verified with some calculations that this rotates a spin state by an angle α around the axis $\vec{n}$. But any spin state also corresponds to a vector $\vec{n}'$ – we're going to verify that this vector $\vec{n}'$ is indeed rotated by an angle α.

So if we now look at the operators $\hat{H}_s$ and $\hat{R}_{\vec{n}}$, notice that the Hamiltonian just has $-\gamma B t$ playing the role α and $\hat{S}_z$ playing the role of $\hat{S}_{\vec{n}}$. So we must do some kind of rotation here as well, and that's the calculation we'll do now.

Example 213

Our magnetic field is still in the z-direction. Consider some arbitrary spin state in the direction in some direction $\vec{n}$ with spherical coordinates θ_0, ϕ_0 (note that this is not the same as the vector $\hat{z}$ around which we're rotating the states).

Our spin state is thus in the direction $\vec{n}$ at time $t = 0$, and its general formula is

$$|\psi, 0\rangle = \cos\frac{\theta_0}{2}|+\rangle + \sin\frac{\theta_0}{2} e^{i\phi_0}|-\rangle.$$

Now we'll apply the time-evolution operator to this state, but first we'll do a preliminary calculation:

$$H_s|+\rangle = -\gamma B S_z|+\rangle = -\gamma B\frac{\hbar}{2}|+\rangle,$$

and similarly

$$H_s|-\rangle = -\gamma B S_z|-\rangle = +\gamma B\frac{\hbar}{2}|-\rangle.$$

So now the state at any time is governed by our unitary time evolution operator:

$$|\psi, t\rangle = e^{-iH_s t/\hbar}|\psi, 0\rangle,$$

and now we can write $|\psi, 0\rangle$ out as a linear combination: because the exponent H acts on $|+\rangle$ with some eigenvalue, we can put that eigenvalue into the exponent instead! And thus

$$|\psi, t\rangle = \cos\frac{\theta_0}{2} e^{-i(-\gamma B\hbar/2)t/\hbar}|+\rangle + \sin\frac{\theta_0}{2} e^{i\phi_0} e^{-i(+\gamma B\hbar/2)t/\hbar}|-\rangle,$$

where we've just replaced H with its eigenvalues, and this simplifies to

$$|\psi, t\rangle = \cos\frac{\theta_0}{2} e^{i\gamma Bt/2}|+\rangle + \sin\frac{\theta_0}{2} e^{i\phi_0} e^{-i\gamma Bt/2}|-\rangle.$$

We have some extra phase terms, so we need to factor those out to get them into our generic phase state: factoring out $e^{i\gamma Bt/2}$ yields an irrelevant phase, and this is just

$$e^{i\gamma Bt/2}\left(\cos\frac{\theta_0}{2}|+\rangle+\sin\frac{\theta_0}{2}e^{i\phi_0}e^{-i\gamma Bt}|-\rangle\right).$$

So now the exponential term is $\exp(i(\phi_0-\gamma Bt))$, and now we know exactly what's going on here: **we have a spin state where $\boxed{\theta=\theta_0}$ is fixed, while $\boxed{\phi=\phi_0-\gamma Bt}$ is precessing** at some linear rate. Indeed, this is what we claimed with the rotation operator $R_{\vec{n}}$ earlier on in the class! And the negative sign means that ϕ decreases in time.

And now that we've done a calculation, we'll also present the general result so that this all becomes more clear. Spin precession is **both** a quantum and a classical phenomenon – in the classical case, if we have a magnetic moment $\vec{\mu}$ in a magnetic field $\vec{B}$, we have a torque

$$\vec{\tau}=\vec{\mu}\times\vec{B}$$

(this is the computation where we have a square wire not aligned with a magnetic field from 8.02). But the rate of change of angular momentum is this torque, so

$$\boxed{\frac{d\vec{S}}{dt}}=\vec{\tau}=\vec{\mu}\times\vec{B}=\gamma\vec{S}\times\vec{B}=\boxed{-(\gamma\vec{B})\times\vec{S}}.$$

This equation is a particular case of a famous equation in classical mechanics where we have a rotating vector

$$\frac{d\vec{x}}{dt}=\vec{\omega}\times\vec{x}:$$

the solution is that a vector $\vec{x}$ rotates with angular frequency ω around the axis defined by ω. So in the specific case we're talking about, $\vec{S}$ plays the role of $\vec{x}$, and $\gamma\vec{B}$ plays the role of $\vec{\omega}$. This gives us what's called the **Larmor frequency**

$$\vec{\omega}_L=-\gamma\vec{B}.$$

Indeed, this is the same Larmor frequency that we derived in the phase ϕ in the quantum state – we now have derivations in both cases! And this isn't a coincidence – we just made our classical variables into quantum operators, and none of the physics is changing. $\mu\cdot\vec{B}$, the energy, just became the Hamiltonian, and now we can rewrite our Hamiltonian in terms of the Larmor frequency:

$$\hat{H}_S=-\vec{\mu}\cdot\vec{B}=-\gamma\vec{B}\cdot\vec{S}=\vec{\omega}_L\cdot\vec{S}.$$

What's important to keep in mind here is the main form of this equation: if a Hamiltonian is some vector dotted with $\vec{S}$, that vector will be the Larmor frequency of rotation, and the spin states will rotate with a frequency of ω_L.

We'll finish by generalizing one level further so that we can understand why any system can be thought of as a spin system – this is maybe the best way to understand the physical effects of any Hamiltonian.

Example 214

Consider a time-independent Hamiltonian for a two-state system

$$H=\begin{bmatrix}g_0+g_3 & g_1-ig_2\\ g_1+ig_2 & g_0-g_3\end{bmatrix},$$

where $g_0,g_1,g_2,g_3\in\mathbb{R}$.

Remember that "two-state system" means we have "two basis states," so a Hamiltonian is a Hermitian 2×2 matrix

– indeed, the above matrix is the most general form allowed. But we've arranged our coefficients in such a way that we can rewrite

$$H = g_0 I + g_1\sigma_1 + g_2\sigma_2 + g_3\sigma_3,$$

because the Pauli matrices, along with the identity matrix, form a basis for all Hermitian 2×2 matrices. And now we can write this Hamiltonian as

$$H = g_0 I + \vec{g} \cdot \vec{\sigma},$$

where $\vec{g}$ is (g_1, g_2, g_3). And now if we write the $\vec{g}$ vector as

$$\vec{g} = g\vec{n}$$

for some unit vector, we're saying that a **general Hamiltonian** can be understood as

$$H = g_0 I + g\vec{n} \cdot \vec{\sigma}.$$

And we know how to work with this – we can diagonalize the matrix and find its eigenvalues and eigenvectors, but we've already done that work earlier on in the class! The eigenstates for such a Hamiltonian are

$$n \cdot \vec{\sigma} \left| n; \pm \right\rangle = \pm \vec{n; \pm},$$

and now we can replace $\vec{\sigma}$ with our spin operator $\vec{S}$ (just picking up a factor of $\frac{\hbar}{2}$) to get that

$$n \cdot \vec{S} \left| n; \pm \right\rangle = \pm \frac{\hbar}{2} \left| n; \pm \right\rangle .$$

These vectors $|n; \pm\rangle$ are exactly the basis in which H is diagonalized, so we've found our eigenstates! And the values of our energy are just

$$H \left| n; \pm \right\rangle = (g_0 I + g\vec{n} \cdot \vec{\sigma}) \left| n; \pm \right\rangle = (g_0 \pm g) \left| n; \pm \right\rangle .$$

So we've figured out both the energies and the eigenstates for the most general two-state system: we have a state $\boxed{|n; +\rangle}$ with energy $\boxed{g_0 + g}$, as well as a state $\boxed{|n; -\rangle}$ with energy $\boxed{g_0 - g}$. We don't have to do any diagonalization by hand, as long as we know the values of g_0, g_1, g_2, g_3.

Here, $|n; +\rangle$ is the **excited state** and $|n; -\rangle$ is the **ground state**: there is a **splitting** of $2g$, so the energy gap between our two eigenstates actually corresponds to the twice the length of the vector (g_1, g_2, g_3). And there's just one more thing we want to do with this: time-evolving the system. But we know that the second term of $H = g_0 I + g\vec{n} \cdot \vec{\sigma}$ can be identified with the $\vec{\omega}_L \cdot \vec{S}$ expression we had before: we can write the second term as

$$g\vec{n} \cdot \vec{\sigma} = \frac{2\vec{g}}{\hbar} \vec{S},$$

so our Larmor frequency in this case is

$$\boxed{\vec{\omega}_L = \frac{2\vec{g}}{\hbar}}.$$

So the non-identity part of the Hamiltonian does precession, and the identity part only produces a pure phase – it doesn't change the direction of our state! That pure phase will give us an extra factor of $e^{-ig_0 t/\hbar}$ through all of our states, but this $g_0 I$ term is generally almost never important.

In summary, we've taken our general Hamiltonian and identified it with the physical phenomenon of the Larmor frequency. And now knowing $\vec{g}$ for any system will tell us how our states evolve in time – we just take our two basis states as the $|+\rangle$ and $|-\rangle$ of some "spin," and we can then describe a physical picture of how the state is evolving in time.

24 March 30, 2020

Recitations are now online over Zoom. This is a bit unusual, but we'll see how we can proceed for the rest of the semester.

Because we have an exam in a few hours, we can discuss a few topics related to it. First of all, the test is going to be 3 hours long: the test opens at 12pm Eastern and stays open for 24 hours, and we have to do it in one sitting (so we should pick an uninterrupted time). Professor Zwiebach doesn't think it'll take us the whole time, but we can use the full time if we keep reviewing and checking our answers.

We might worry about partial credit on this exam – the computer will grade everything as being right or wrong. But we'll alleviate this worry by dividing the questions in a lot of pieces, where some pieces are quite independent from the parts before. So we should still sometimes be able to do later parts of the problem even if we can't do an earlier part.

The formula sheet is available for us – we can print it or have it on a different screen. It's not an exam with heavy use of the formula sheet, but it will be useful to have as a reference point. Usually, MITx will give us a red cross or a green button – this time, we will not know if we got the right answer or not. But when we enter a short answer into a box, it'll check the syntax to make sure it's valid. Until we finish the exam, we can change all of our answers – it's always better to save them all the time. (All of this is in the information page before we go into the exam.)

The exam will have 4 problems: one multiple choice, one about the "mathy" things we've discussed in the early part of the class, and two on things like oscillators, the variational principle, and spin states. A few topics that have been discussed recently – time evolution, Heisenberg operators, coherent states, photon states, and two-state systems – won't be relevant to this exam. Let's do a little bit of review:

- We've studied a lot about spin-1/2 systems, discussing Pauli matrices and their properties, explicit formula for spin states, and so on. In general, when we take the operator

$$\vec{\sigma} \cdot \vec{n} = \sigma_1 n_1 + \sigma_2 n_2 + \sigma_3 n_3$$

  for a vector $\vec{n}$ of unit length, we'll have eigenvalues of ± 1 corresponding to the two spin states $|n;+\rangle$ and $|n;-\rangle$.

- We've also discussed the matrix representation of an operator: when we act on the kth basis vector, we learn about the kth column of the matrix representation.

- An important idea was that of an **invariant subspace** – an example is that **eigenvectors** of our linear operators generate one-dimensional invariant subspaces. There may be others as well – in general, we find an invariant subspace U by looking at a general vector $v \in U$ and seeing if Tv is still in U. An important example of this is that degeneracies in the spectrum (that is, the set of eigenvalues) correspond to higher-dimensional invariant subspaces. For example, if there are three linearly independent eigenvectors with the same eigenvalue λ, those three eigenvectors generate a three-dimensional **invariant subspace**, corresponding to the set of vectors where $Tv = \lambda v$. (Basically, in this subspace, every vector gets multiplied by λ, so **every vector in the subspace is an eigenvector**.)

  On the other hand, if we take two eigenvectors v_1, v_2 with **different** eigenvalues, their span is indeed an invariant subspace – any linear combination of v_1 and v_2 will still be a linear combination of v_1 and v_2 after we apply our linear operator T. But this is not a nice invariant subspace, because not every vector will be an eigenvector! (In fact, only those along the direction of v_1 or v_2 will be.)

  And we can say something more concretely by thinking about our operators as matrices: suppose that the span of e_1 and e_2 is an invariant subspace in our vector space V. If we let a matrix (operator) act on our vector space,

then this condition tells us something about the first two columns of the matrix: they must have all zero entries except for the first two rows.

- One important topic is that of diagonalization. We discussed that certain classes of nice operators are unitarily diagonalizable – these are the **normal operators**, and they include the Hermitian, anti-Hermitian, and unitary operators. When talking about trying to diagonalize different operators, it's important that they **commute**. An example of this is a system with a (spherical symmetric) central potential: we often need to find a set of states for each value of ℓ, and the spectrum is degenerate in ℓ (there are multiple states with a given value of ℓ). Then if we want to distinguish those states with a given ℓ (corresponding to the energy) by comparing their values of a different operator, we need to make sure the new operator commutes with the first one, so that diagonalization of one operator doesn't mess up diagonalization of the other one.

  One idea that's worth reviewing is how we deal with degenerate sets of eigenvalues when trying to simultaneously diagonalize two different matrices A and B. For example, if A is diagonalized and looks like $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$ (so there is a degeneracy with the eigenvalue $\lambda = 2$), the matrix B will look like $\begin{bmatrix} \lambda & 0 & 0 \\ 0 & * & * \\ 0 & * & * \end{bmatrix}$. And to turn the $*$ parts into a diagonal matrix, we apply another unitary transformation to the invariant subspace for $\lambda = 2$.

- The variational principle says that we can estimate the ground state energy by calculating the expectation of the Hamiltonian in a test function: this tells us an **upper bound** on the true ground state energy.

- The trace of a matrix $\text{tr}(A)$ is an important linear operator: it is formally defined as

$$\text{tr}(A) = \sum_i A_{ii},$$

  the sum of the diagonal matrix entries. It turns out that this definition doesn't depend on the basis that we use – even though the diagonal entries can change between different matrix representations, it turns out that the sum of the diagonal entries is always constant. Note that when we have an orthonormal basis, we can also write this trace in bra-ket notation as

$$= \sum_i \langle i|A|i\rangle .$$

  The trace is **linear**: $\text{tr}(aA) = a\text{tr}(A)$, and $\text{tr}(A+B) = \text{tr}(A) + \text{tr}(B)$. We also have the nice property that $\text{tr}(AB) = \text{tr}(BA)$, which gives us something called **cyclicity of trace**:

$$\text{tr}(ABCD) = \text{tr}((ABC)(D)) = \text{tr}(DABC).$$

  This also means that the trace of any commutator is zero, because

$$\text{tr}([A,B]) = \text{tr}(AB - BA) = \text{tr}(AB) - \text{tr}(BA) = 0.$$

  For complex-valued vector spaces, a more intrinsic way to think about the trace is that it is the **sum of the eigenvalues**: it's not true in real vector spaces, because we have cases where operators don't have any eigenvalues at all.

25 Two State Systems, Part 2

Recall that last time, we talked about general Hamiltonians for a two-state system: they're specified by four real numbers and can be written in the form

$$H = g_0 I + \vec{g} \cdot \vec{\sigma} = g_0 I + \vec{\omega}_L \cdot \vec{S}.$$

Here, $\vec{\omega}_L = \frac{2\vec{g}}{\hbar}$ is the Larmor frequency – we mentioned last time that spins will rotate with an angular velocity $|\omega_L|$ around the vector $\vec{\omega}_L$. (In the case of a magnetic field,this looks like $\vec{\mu} = \gamma \vec{S}$.) There are at most two energy levels in a two-state system, because we have a two-dimensional vector space: then there are two energy levels $g_0 \pm g$, corresponding to the spin states $|\vec{n}; \pm\rangle$. And we can think of any system specified by such a Hamiltonian as having two basis vectors, corresponding to "spin up" and "spin down," even if the system itself has nothing to do with spins!

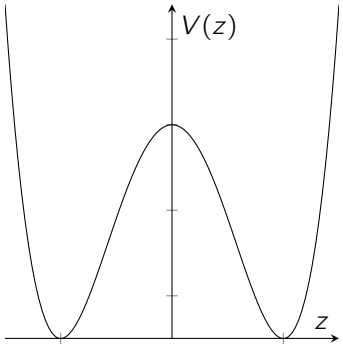
With that, we'll start talking about the **ammonia molecule**.

Fact 215

Ammonia is a molecule with chemical formula NH_3 – it's a colorless gas used as a fertilizer or in cleaning products. Its shape is a **flattened tetrahedron** with a nitrogen atom at one corner and a base of three hydrogen atoms.

If the atom were totally flat, the angles N–H–N would be 120 degrees, and if the atom were a regular tetraheron, that angle would be 60 degrees (because we'd have an equilateral triangle). The angle turns out to be 108 degrees in this particular molecule.

And we can think of this as a two-state system, because the nitrogen atom can be "up" above the hydrogen base or "down" below it. Thus, there are two configurations of this system – both states are stable – and we can think of this as having a potential $V(z)$ in the z-direction (where the equilateral triangle base of hydrogens is in the xy-plane) that looks something like this:



We'll try to describe this as a two-state system, and we'll need some notation for that. Let our **basis states** be $|1\rangle = |\uparrow\rangle$, corresponding to the nitrogen atom being up, and $|2\rangle = |\downarrow\rangle$, corresponding to the nitrogen atom being down. We can now write down a Hamiltonian for the system – this potential does not correspond to a two-state system because there can be many energy eigenstates, but we can use our quantum mechanics intuition here. The ground state is some wavefunction with two peaks (at the two points where $V = 0$), and the first excited state looks basically like that but with one of the peaks flipped, so that we have an odd function.

If the middle barrier is high enough, we can assume that the energy levels are close to each other – let's call the ground state energy E_0, and let's try to write down a Hamiltonian. If our basis states are $|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|\downarrow\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, our

Hamiltonian can't just look like $\begin{bmatrix} E_0 & 0 \\ 0 & E_0 \end{bmatrix}$: there aren't two degenerate energy eigenstates for this one-dimensional potential, so we need more to describe the physics here. Instead, we'll try

$$H = \begin{bmatrix} E_0 & -\Delta \\ -\Delta & E_0 \end{bmatrix},$$

where $\Delta > 0$. (The choice of sign doesn't change the physics that we're using: we could get a positive Δ if we replaced $|2\rangle$ with $-|2\rangle$.) But now $|\uparrow\rangle$ and $|\downarrow\rangle$ are no longer our energy eigenstates, so we should try to figure out how this compares to previous models. First, let's write the Hamiltonian as

$$H = E_0 I - \Delta\sigma_1.$$

Comparing this to our generic Hamiltonian above yields the $\vec{g}$ vector in the x-direction (because we have the matrix σ_1) with magnitude Δ:

$$\vec{g} = -\Delta\hat{e}_x \implies g = \Delta.$$

To find the ground and excited states, we just need to find the eigenvalues and eigenvectors of this matrix, and we'll see if this matches the actual physics of the system. It turns out that the energies are $g_0 \pm g = E_0 \pm \Delta$, and the energy gap here is 2Δ. So that's a good first step: we have two energy eigenstates, $E_0 + \Delta$ and $E_0 - \Delta$, and they correspond to eigenvectors of $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$ and $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$, respectively. In terms of our basis states, this means that the energy eigenstates are

$$|E\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - |\downarrow\rangle\right), \quad |G\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right).$$

So now we can think back to how this relates to our spin states: in this nitrogen atom, only one direction matters (the z-direction, corresponding to up and down orientation of the N atom), while for our spin states, three different dimensions matter. So we need to be a bit more abstract: remember that the vector $\vec{g} = -\Delta\hat{e}_x$ points in the x-direction, and the excited and lower states correspond to $|\vec{n};+\rangle$ and $|\vec{n};-\rangle$, respectively. So the excited state is supposed to correspond to a vector in the $+\vec{n}$ direction, while the ground state should correspond to a vector in the $-\vec{n}$ direction. So in spin language, we can say that

$$|E\rangle = (|+\rangle - |-\rangle)/\sqrt{2}, \quad |G\rangle = (|+\rangle + |-\rangle)/\sqrt{2}.$$

And indeed $|+\rangle + |-\rangle$ is along the positive x-direction in our original spin state model (pointing in the same direction as $\vec{g}$), and $|+\rangle - |-\rangle$ is along the negative x-direction (pointing opposite from $\vec{g}$).

Fact 216

Since this energy gap is 2Δ, the transition energy can be written as

$$2\Delta = \hbar\omega,$$

and this corresponds to a frequency of about $\nu = 23.827$ GHz, which corresponds to a wavelength of about 1.26 cm.

So we haven't introduced too much complexity, and we already have a nice model of the ammonia molecule.

Example 217

How does the $|\uparrow\rangle$ state evolve in time?

(Remember that this is not a stationary state, because it is not an energy eigenvector.) The fastest way for us to do thi in principle is to think of this with spins, though it is a little painful. Recall that the Larmor frequency vector $\vec{\omega}_L$ points in the direction of $\vec{g}$, so we have a starting vector $|\uparrow\rangle$ which begins in the z-direction and precesses around $\vec{g}$, which is in the $-\hat{x}$ direction. So **the state rotates in the yz-plane**, and now we can calculate a little bit by writing this in terms of energy eigenstates. The initial state is

$$|\psi, 0\rangle = |\uparrow\rangle = \frac{1}{\sqrt{2}}(|E\rangle + |G\rangle),$$

and we know how the energy eigenstates evolve in time (using the unitary time evolution operator $e^{-iHt/\hbar}$, we can then convert from $|E\rangle$ and $|G\rangle$ to the up and down states (which is the intuition that we wanted in the first place). The final result is that

$$\psi(t) = e^{-iEt/\hbar}\left(\cos\frac{t\Delta}{\hbar}|\uparrow\rangle + i\sin\frac{t\Delta}{\hbar}|\downarrow\rangle\right),$$

and we can also use this to find the probabilities of being in the up and down states: they're just the squared magnitudes, or $\cos^2\frac{t\Delta}{\hbar}$ and $\sin^2\frac{t\Delta}{\hbar}$ respectively. In other words, this nitrogen-up molecule will rotate even if we don't do anything, and this is happening 23 billion times a second, because it's not in a stationary eigenstate!

Note that the frequency of rotation here is $\frac{\Delta}{\hbar}$, while we have a Larmor frequency of $\frac{2g}{\hbar} = \frac{2\Delta}{\hbar}$, the frequency of the photons that we found above. But there's no contradiction between the Larmor frequency and the frequency of rotation: remember that in a spin state we had an expression with a $\cos\frac{\theta}{2}$. So the physical angle of rotation changes twice as fast as the angle corresponding to the up and down ket vectors, and this is the same confusion with the $\frac{1}{2}$ factors that we had when we first saw spin states!

We'll now move on to a different time-dependent problem, that of **nuclear magnetic resonance**. This problem begins when we have a magnetic field with a large component B_0 in the z-direction, plus some smaller magnetic field rotating with some angular frequency ω in the xy-plane. In other words, we have

$$\vec{B} = B_0\hat{z} + B_1(\cos(\omega t)\hat{x} - \sin(\omega t)\hat{y}).$$

Our goal is to see what spins do in this field – since $\vec{B}$ is time-dependent, it's possible that H is time-dependent. We know that

$$H_s(t) = -\gamma\vec{B}(t)\cdot\hat{S} = -\gamma\left[B_)\hat{S}_z + B_1\hat{S}_x\cos(\omega t) - \hat{S}_y\sin(\omega t)\right].$$

And indeed H is time-dependent, and in fact the Hamiltonian doesn't even commute at different times! (Sometimes we have $\hat{S}_z$ and $\hat{S}_x$, and at other times we have $\hat{S}_z$ and $\hat{S}_y$.) So we need to figure out this problem in a new way.

We'll start by trying to get the main intuition for what's going on. Our Schrodinger equation is very complicated – it has a time-dependent Hamiltonian, and we have the equation

$$i\hbar\partial_t|\psi\rangle = H|\psi\rangle.$$

We'll try to change the Hamiltonian while keeping the physics: one way we can do that is by trying to apply a unitary transformation U to our states $|\psi\rangle$, and we'll hope that the Hamiltonian on these new states $|\psi'\rangle$ will simplify the Hamiltonian. Unitary transformations are basically just a change of basis unless the unitary transformation has time-dependence, and then we even mess up the ∂_t term on the left side. But this is our only real chance of getting a time-independent Hamiltonian of the form $U^\dagger H_s U$, so we'll go ahead with this idea.

Example 218

Suppose we start with a system with a Hamiltonian of 0.

Since we have a rotating magnetic field in our original problem, we'll think about what happens to our physics in this "nothing is happening" system if we have the xy-plane rotating with angular velocity ω. In our "nothing" system, $H_s = 0$, and any spin state stays in place. But when we jump into our **rotating frame**, all of the spin states that started off being static are not rotating – they're precessing around the z-axis! So **there is some nonzero Hamiltonian in our rotating frame**: it should be such that the spins rotate around the z-axis with angular velocity ω, and this is done by the unitary (rotation) operator

$$U = e^{-i\omega t \hat{S}_z/\hbar}.$$

Thus, the rotating Hamiltonian must be

$$H_R = \omega \hat{S}_z$$

(to make the unitary operator $e^{-iHt/\hbar}$). Let's now think about how our Hamiltonian changes when we don't just start with 0, and we'll do this with a different calculation:

Example 219

Suppose we have a rotating wavefunction defined by

$$|\psi_R\rangle = U|\psi\rangle.$$

What is the Schrodinger equation for ψ_R if we know the equation for ψ?

We start with the usual equation

$$i\hbar\partial_t|\psi\rangle = H_s|\psi\rangle.$$

Evaluating the left hand side for ψ_R, we have

$$i\hbar\partial_t|\psi_R\rangle = i\hbar\partial_t(U|\psi\rangle) = i\hbar(\partial_t U)|\psi\rangle + i\hbar U\partial_t|\psi\rangle$$

by the product rule, and then we can simplify the first term by adding a $U^\dagger U$ between U and $|\psi\rangle$ and simplify the second by applying the Schrodinger equation:

$$= i\hbar(\partial_t U)U^\dagger|\psi_R\rangle + UH_s|\psi\rangle.$$

But now we put another $U^\dagger U$ in the second term and we'll find that we have a new Schrodinger equation:

$$\boxed{i\hbar\partial_t|\psi_R\rangle = i\hbar\left(UH_sU^\dagger + (\partial_t U)U^\dagger\right)|\psi_R\rangle}$$

This is essentially the "rotating Hamiltonian" that we've been trying to figure out, and this is what we hope is simpler than our original H_s! The first term $UH_SU^\dagger$ corresponds to a "similarity transformation" of the Hamiltonian, and the second term has to do with the time-change affecting the original left side of the Schrodinger equation. Recall the above argument: when $H_s = 0$, we want our new Hamiltonian to be $\omega\hat{S}_z$, so **we'll pick a U such that**

$$i\hbar(\partial_t U)U^\dagger = \omega\hat{S}_z \implies U = e^{-i\omega t\hat{S}_z/\hbar},$$

which is indeed the rotation transformation we had above! So our new Hamiltonian is

$$H_R = UH_sU^\dagger + i\hbar(\partial_t U)U^\dagger, \quad U = e^{-i\omega t\hat{S}_z/\hbar},$$

and our new state is

$$|\psi, t\rangle = e^{i\omega t\hat{S}_z/\hbar}|\psi_R, t\rangle$$

by taking the inverse of the unitary operator. So we now have a problem for $|\psi_R\rangle$ with a Schrodinger equation involving a Hamiltonian H_R where the second term is just $\omega\hat{S}_z$: our hope now is that we have a time-independent Hamiltonian in this new **rotating frame**.

Example 220

Before we look at time-independence, here's another way we can find the Schrodinger Hamiltonian for $|\psi_R, t\rangle$, our rotating wavefunction.

We can say that

$$|\psi_R, t\rangle = U(t)U_s(t)\,|\psi, 0\rangle\,,$$

where U_s is the unitary operator for the spin system itself (associated to the ordinary Hamiltonian). Then UU_s is the total unitary operator that evolves the state, and then we know that

$$H_R = i\hbar\partial_t(U(t)U_s(t))(U(t)U_s(t))^\dagger,$$

because the Hamiltonian associated to any unitary time-evolution operator A is $i\hbar(\partial_t A)A^\dagger$. Then we just evaluate the derivative by the product rule – this yields

$$= i\hbar(\partial_t U)U^\dagger + i\hbar\partial_t U(t)i\hbar(\partial_t U_s(t))U_s^\dagger U^\dagger(t).$$

And now the middle of this second term is the Hamiltonian associated to U_s, and either way this means we can write down the following formula which summarizes everything:

$$\boxed{H_R = H_U + U(t)H_s(t)U^\dagger(t)},$$

where H_R is the rotated Hamiltonian, H_U is the Hamiltonian associated to the unitary operator U, and H_s is our original Schrodinger Hamiltonian.

So let's bring this back to our original example. We chose $U = e^{-i\omega t\hat{S}_z/\hbar}$ so that H_U is just $\omega\hat{S}_z$, and now plugging everything in (including our original Hamiltonian), we find that

$$H_R = \omega\hat{S}_z = e^{-i\omega t\hat{S}_z/\hbar}\left[-\gamma(B_0\hat{S}_z + B_1(\cos(\omega t)\hat{S}_x - \sin(\omega t)\hat{S}_y))\right]e^{i\omega t\hat{S}_z/\hbar}.$$

To simplify this further, the $B_0\hat{S}_z$ term can go outside of the conjugation by $e^{-i\omega t\hat{S}_z/\hbar}$ (also called a **similarity transformation**) because both just have $\hat{S}_z$s, so they commute. This contributes a term of $-\gamma B_0\hat{S}_z$, and then the rest looks like

$$-\gamma B_1\boxed{e^{-i\omega t\hat{S}_z/\hbar}\left[\cos(\omega t)\hat{S}_x - \sin(\omega t)\hat{S}_y\right]e^{i\omega t\hat{S}_z/\hbar}}.$$

There are two ways we can simplify from here: since we have two exponentials, we can expand them and multiply or we can use the formula for $e^A B e^{-A}$. But here's another idea: we know the function $U(t)$, so knowing ψ means that we know ψ_R as long as we can make H_R less complicated. So we'll call that boxed term $m(t)$, and we'll take its time derivative (this is a good idea if we're in a rush). Then we use the product rule: the derivatives of the outside terms bring terms down from the exponentials, which gives us a commutator, and the other term is just evaluating the derivative in the middle:

$$\frac{d}{dt}M(t) = e^{-i\omega t\hat{S}_z/\hbar}\left(-\frac{i\omega}{\hbar}\left[\hat{S}_z, \cos(\omega t)\hat{S}_x - \sin(\omega t)\hat{S}_y\right] - \omega\sin(\omega t)\hat{S}_x - \omega(\cos\omega t)\hat{S}_y\right)e^{i\omega t\hat{S}_z/\hbar}.$$

Now we just evaluate the commutator with our known relations:

$$= e^{-i\omega t\hat{S}_z/\hbar}\left(-\frac{i\omega}{\hbar}(i\hbar S_y\cos(\omega t)+i\hbar S_x\sin(\omega t))-\omega\sin(\omega t)\hat{S}_x-\omega(\cos\omega t)\hat{S}_y\right)e^{i\omega t\hat{S}_z/\hbar}$$

and now all of the terms cancel, and we're just left with zero! This means that $M(t)$ has **no time dependence**, since its derivative is zero, and now we can just evaluate it at $t=0$. Then the exponentials disappear, and the whole boxed expression is just $\hat{S}_x$!

So plugging everything back in gives us our **final rotated Hamiltonian**:

$$\boxed{H_R=(-\gamma B_0+\omega)\hat{S}_z-\gamma B_1\hat{S}_x}.$$

This now just has two pieces: the $\hat{S}_z$ coefficient got an extra ω term from the rotation, and the rotating xy-magnetic field just became a static one in the x-direction (as it was at time 0).

To make this look nicer, $\omega_0=\gamma B_0$ is the Larmor frequency for B_0, so this can also be written as

$$=-\gamma\left[\left(B_0-\frac{\omega}{\gamma}\right)\hat{S}_z+B_1\hat{S}_x\right]=-\gamma\left[B_0\left(1-\frac{\omega}{\omega_0}\right)\hat{S}_z+B_1\hat{S}_x\right].$$

So now we can think of this Hamiltonian as being in the form $-\gamma\vec{B}_R\cdot\vec{S}$, where the magnetic field points in the direction

$$\vec{B}_R=B_0\left(1-\frac{\omega}{\omega_0}\right)\hat{z}+B_1\hat{x}.$$

So we can finally answer our additional problem: we wanted to know how a state time-evolves, and we just have

$$|\psi,t\rangle=U^\dagger|\psi_R,t\rangle=e^{i\omega t\hat{S}_z/\hbar}e^{-iH_Rt/\hbar}|\psi,0\rangle,$$

where the whole point of all of this is that the second exponential is very simple because H_R is time-independent! Plugging in the value we know for H_R, this gives us the equation

$$\boxed{|\psi,t\rangle=e^{i\omega t\hat{S}_z/\hbar}e^{i\gamma(\vec{B}_r\cdot\vec{S})t/\hbar}|\psi,0\rangle}.$$

(Remember that the states ψ_R and ψ are the same at $t=0$.) This is the complete solution for our rotating spin problem!

With this, it's time for us to talk about applications. In practical examples, we always have $B_1\ll B_0$.

Example 221

Let's look at the case where $\omega\ll\omega_0$.

The ω_0 frequency is the Larmor frequency, and because B_0 is very large, this means ω_0 is also very large. So it's reasonable for ω to be very small (the B field rotates very slowly compared to the rotation that it is creating) – in such a case, we can approximate

$$\vec{B}_R\approx B_0\hat{z}+B_1\hat{x}.$$

So this magnetic field is mostly along the z-axis, and let's also look at the case where **the spin is up in the** $+z$ **direction at time** $t=0$. This magnetic field will rotate our spins around the axis of $\vec{B}_R$, and since $\vec{B}_R$ is very close to $\hat{z}$, the path is a small cone near the z-axis. But we should make sure not to forget the $e^{i\omega t\hat{S}_z/\hbar}$ term, which is also producing a rotation around the z-axis. In this case, since $\omega\ll\omega_0$, the "rotating cone" behavior is much faster than the precession of the whole process around the z-axis.

Example 222

Let's now do the **resonance** case, where $\omega = \omega_0$.

Basically, we know what ω_0 looks like for the spins themselves, and then we set up our system so that ω completely lines up with ω_0. Then the $\hat{z}$ component of the magnetic field disappears: we just have $B_R = B_1\hat{x}$, which means that our spin state now precess around the x-direction. (Since we're actually missing a negative sign here, the spin rotates around the $-\hat{x}$ direction.) Now $B_1 \ll B_0$, meaning that the rotation operator $e^{i\omega t\hat{S}_z/\hbar}$ will rotate our spin around the z-axis faster than we can precess around the x-axis: thus we create a **spiral**!

And now as the spin fills out the spiral, it's an interesting question to time the signals: we care about when the spin is perpendicular to the original direction (so in the xy-plane for the first time). To do this, we'll choose

$$\omega_1 T = \frac{\pi}{2},$$

where $\omega_1 = \gamma B_1$ is the Larmor frequency. Thus $T = \boxed{\frac{\pi}{2\gamma B_1}}$ is called the **90 degree pulse**: after this much time, the spin has gone from the x-axis to the equator of the sphere, and the B_1 term is negligible for a while. (As an exercise, it's worth figuring out the spiral equation that comes out of all of this!)

This turns out to be the technique used for **magnetic resonance imaging** (MRIs), which is one of the interesting applications of quantum mechanics to technology. This device goes beyond what we can do with an x-ray: basically, a person is put inside a solenoid with a magnetic field of 2 Tesla. (It's not dangerous, but if we forget metal or have iron ink in a tattoo, that can cause some problems.)

The purpose of this MRI is to figure out the **local concentration of water**. The magnetic fields from the solenoid interact with the magnetic dipole moments in the protons of hydrogen atoms, and these protons get roughly aligned to this B_0 magnetic field. (Not all of the protons get aligned – maybe just one in a million – but that's enough.) But then this 90 degree pulse is sent, so the proton will start spiraling, and this rotating dipole moment will **generate electromagnetic waves**. The MRI's detectors then picks up this signal: the strength of that signal is proportional to the concentration of water (or other kinds of liquid) that we have.

This is useful because we can compare signals from different areas: we can then distinguish different kinds of tissues (some have more water than others).

But this rotation of the proton has a **relaxation time** T_2 for the rotation (in which the spin interacts with other spins), and there is also a time T_1 that it takes for the spin to return to its original position (in which the atom interacts with a set of neighboring atoms). These two measurements, T_1 and T_2, are very good for our applications, because we can measure any liquid's T_1 and T_2 and compare it to the numbers that we measure in our own MRI! For example, the value of T_2 is good enough to distinguish white matter, grey matter, and fluids in our brain.

And one final note: an MRI often makes large noises when we first go into the machine. This comes from **gradient magnets**: the value of B_0 is adjusted as a function of position, which also changes the ω_0 for our spins. This technology has gotten sophisticated enough that we can get **spatial resolution**: we can tell where a signal is coming from in our body, up to a resolution of half a millimeter. (This is a junior lab experiment as well!)

26 April 1, 2020

We've now finished with the first exam – it was mentioned in an email what we need to do to pass the class this semester with a PE grade (60 percent or above). There are lots of different parts of this class, and that boundary can

be possibly lowered but not raised.

In the next few days, we'll do an anonymous poll to see how we felt about the exam – feedback is always appreciated! Doing things online definitely requires different skills, so there's something new for all of us. The second midterm and final will be in this kind of format as well; the idea is to mitigate any difficulties before those tests.

In this recitation, we'll talk about some of the concepts needed to move forward with this class. There's several things we'll have to discuss, but let's talk about the main subject. Since we last discussed recent material, we've explored a lot about **unitary time evolution**: we know that we can write the wavefunction at a time t as

$$|\psi, t\rangle = U(t, t_0)\,|\psi, t_0\rangle\,.$$

It is important to emphasize that this works for all t and t_0, and in fact we can use **any wavefunction** ψ in our system and we'll have the same **unitary operator** U.

There are a few other important properties that we should remember about our unitary time-evolution operator:

- $U(t_0, t_0) = I$ is the identity operator.
- Composition of times works as nicely as we'd like:

  $$U(t_2, t_1)U(t_1, t_0) = U(t_2, t_0).$$

  (Going from time t_0 to t_1 to t_2 is the same as skipping over the middle time.) And we should remember that if we plug in $t_2 = t_0$, we have found that the inverse of $U(t_1, t_0)$ is $U(t_0, t_1)$, which makes sense. This can also be written (because a unitary operator has $U^\dagger = U^{-1}$) in the form

  $$(U(t_0, t_1))^\dagger = U(t_1, t_0)$$

- **We can find the Hamiltonian** associated to the unitary operator U:

  $$H = i\hbar \left(\frac{\partial U}{\partial t}(t, t_0)\right) U(t_0, t).$$

  (We might have seen this last term usually written as $U^\dagger(t_0, t)$.) Usually, we have a lot of intuition on how to write Hamiltonians, but we have less intuition on how to write unitary operators, so we often go from H to U. But if we know how the system evolves in time, then we can use this tool to reconstruct the Hamiltonian (go from U to H)! And we can use the last equation as a differential equation for U: multiplying both sides by $U(t, t_0)$ yields

  $$i\hbar \frac{\partial U}{\partial t}(t, t_0) = HU(t, t_0).$$

- There are some important special cases where it's easy to solve for the unitary time evolution operator. If H is time-independent, then we can write

  $$U(t, t_0) = e^{-\frac{i}{\hbar}H(t-t_0)},$$

  and if H isn't necessarily time-independent but still commutes at different times, we have

  $$U(t, t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'}.$$

  This property of the Hamiltonian makes it much simpler, so it's a good thing. The reason this formula doesn't work in general for a Hamiltonian that doesn't commute in time can be seen if we try to write out this expression

as an exponential: then we have terms of the form

$$\left(-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'\right)\left(-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'\right)\cdots\left(-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'\right).$$

Then when we take the derivative and use the product rule, we get $H(t)$ terms replacing one of the terms in this product. But in order for us to factor this nicely, we need to be able to move $H(t)$ past the integral, so we need H to commute at different times! The main idea is that in general, **we do not have**

$$\frac{d}{dt}e^{M(t)} = \dot{M(t)}e^{M(t)}$$

for a matrix $M(t)$.

Unitary operators are used to help us transition from the Schrodinger picture to the **Heisenberg picture** of quantum mechanics. The idea is to start with an expectation value (or a matrix element if we'd like to think of it that way)

$$\left\langle \psi_1, t\middle|\hat{A}_s\middle|\psi_2, t\right\rangle.$$

When we think about Schrodinger operators, we should just think $\hat{x}$, $\hat{p}$, and so on: usually these are time-independent, and we can have Schrodinger operators with time-dependence only if we write in a specific time t. By time evolution, we know that we can write the above expression as

$$\left\langle \psi_1, 0\middle|U^\dagger(t,0)\hat{A}_s U(t,0)\middle|\psi_2, 0\right\rangle.$$

We call this middle term the **Heisenberg operator**: it's a similarity transformation of our usual operator $\hat{A}_s$. This has a few nice properties for us to remember:

- $\hat{A}_H = \hat{A}_S$ at time $t = 0$.
- The "algebra of operators" is preserved, because of the way that U is acting on our operators. For example, the identity operator and the commutators stay the same. Specifically, if we have a Lie algebra, then $[A_s, B_s] = C_s$ means that $[A_H(t), B_H(t)] = C_H(t)$, and also that $(AB)_H = A_H B_H$. We can check this ourself:

$$(AB)_H = U^\dagger ABU = U^\dagger AUU^\dagger BU = A_H B_H.$$

- A Schrodinger Hamiltonian of the form $H(\hat{p}, \hat{x}; t)$ gives rise to a Heisenberg Hamiltonian $H_H = H(\hat{p}_H(t), \hat{x}_H(t); t)$. And this statement is true for any operator that depends on just these variables: basically, to get the Heisenberg Hamiltonian, we just plug in the Heisenberg versions of our operators.
- One special property for the Hamiltonian, though: if $[H_s(t), H_s(t')] = 0$ – that is, the Schrodinger Hamiltonian commutes at different times – then we actually have $H_H(t) = H_S$ for all t. In other words, they are identical operators – they are the same function, and in particular this means H_H doesn't actually have time-dependence.
- We have the important **Heisenberg equation of motion**

$$i\hbar\frac{d\hat{A}_H}{dt} = [\hat{A}_H(t), H_H(t)] + i\hbar\left(\frac{\partial\hat{A}_S}{\partial t}\right)_H.$$

The last term is often irrelevant – it means we're taking the Heisenberg version **of the time-derivative of our Schrodinger operator** (note that this is not the same as the time-derivative of the Heisenberg operator). And often $\hat{A}_S$ doesn't depend explicitly on time, so that last term just goes away. And an explanation for

An important example of this Heisenberg formulation is the simple harmonic oscillator. We derived that the

Heisenberg operators for $\hat{x}$ and $\hat{p}$ look like

$$\hat{x}_H = \hat{x}\cos(\omega t) + \frac{1}{m\omega}\hat{p}\sin(\omega t), \quad \hat{p}_H = \hat{p}\cos(\omega t) - m\omega\hat{x}\sin(\omega t).$$

We can check that this gives us Heisenberg operators for the creation and annihilation operators

$$\hat{a}(t) + e^{-i\omega t}\hat{a}, \quad \hat{a}^\dagger(t) = e^{i\omega t}\hat{a}^\dagger.$$

This is fairly fundamental, so we should make sure we can follow along with all of the logic here.

We'll close with a few remarks about coherent states: this concept arises out of the translation operator

$$T_{x_0} = e^{-i\hat{p}x_0/\hbar},$$

which is a unitary operator. (In general, any operator of the form e^{iA}, where A is Hermitian, is a unitary operator.) So T_{x_0}'s inverse is also its adjoint:

$$(T_{x_0})^\dagger = T_{-x_0},$$

and we can also combine exponentials because they all commute:

$$T_{x_0}T_{x_1} = T_{x_0+x_1}.$$

There are a few ways of justifying the name "translation operator": recall that

$$T_{x_0}^\dagger \hat{x} T_{x_0} = \hat{x} + x_0 I,$$

and therefore

$$\langle\hat{x}\rangle_{T_{x_0}\psi} = \langle\hat{x}\rangle_\psi + x_0, \quad \boxed{T_{x_0}|x\rangle = |x + x_0\rangle}.$$

(Note, though, that $\langle x|\,T_{x_0}$ is $\langle x - x_0|$ instead, because we can take the dagger of the above boxed expression and then replace x_0 with $-x_0$.) With this, we define the coherent state with label x_0 to be

$$|\tilde{x_0}\rangle = e^{-i\hat{p}x_0/\hbar}|0\rangle.$$

We can verify that the wavefunction is just the ordinary ground state wavefunction translated by x_0:

$$\psi_{\tilde{x_0}}(x) = \phi_0(x - x_0).$$

This is because the wavefunction is defined to be $\langle x|\tilde{x_0}\rangle$, and then we just expand this out with the definition:

$$= \langle x|T_{x_0}|0\rangle = \langle x - x_0|0\rangle = \phi_0(x - x_0).$$

We've only gotten through some of the new ideas, and we'll continue to work towards catching up on our concepts over the next few recitations.

27 Multiparticle States, Part 1

We're now shifting to more complicated systems: for example, suppose we have two particles in a system (it doesn't matter yet whether they're distinguishable or indistinguishable; that's more of an 8.06 topic). Then the two particles can be described with their own physics: particle 1 might have a complex vector space V for its state space, along with some operators T_1, T_2, and particle 2 might have some other vector space W, along with some operators S_1, S_2.

(These operators are things like position, momentum, and so on.) Our first question will be how to **describe the composite system** – that is, the system of the two particles together, especially when the two particles can interact with each other.

Since particle 1 is described by some $v \in V$, and particle 2 is described by some $w \in W$, it's reasonable to imagine that (v, w) describes the composite system. It turns out that this is a bit naive – it doesn't represent everything we want in our system just yet – but we do need to encode the two systems together.

So we'll use a specific notation: we'll encode those pairs of vectors as $v \otimes w$, where $\otimes$ represents a **tensor product**. Here, we're not multiplying the two vectors in any obvious way – we're just saying that this is an object that puts together our information from V and from W. This object $v \otimes w$ is going to be an element of the **new (complex) vector space** $V \oplus W$, called the **tensor product** of the two vector spaces.

Let's try to extract some properties for this object that we've just introduced. We know that states can have constants in front of them, so we'll allow ourselves to put constants in front of the v: this gives us $(\alpha v) \otimes w$. We want to relate this object to $v \otimes w$ – otherwise, we have a much larger space, and we get what's mathematically called a **direct product**. Essentially, we don't want $(\alpha v) \otimes w$ to be linearly independent to $v \otimes w$ (since αv and v are the same state in V), so we're going to say that the αs can come out of the product:

$$(\alpha v) \otimes w = \alpha(v \otimes w) = v \otimes (\alpha w).$$

(Notably, these don't come out with a complex conjugate.) We can impose this property on the object we defined, and now we can make some more progress: if $v_1 \otimes w_1$ and $v_2 \otimes w_2$ are two vectors in our tensor product vector space $V \otimes W$, any linear combination of them should also be in the space:

$$\alpha(v_1 \otimes w_1) + \beta(v_2 \otimes w_2) \in V \otimes W.$$

Notice now that we can't just treat our v and w separately from each other in the tensor product, because quantum mechanics now seems to require us to be in a superposition between $(v_1 \otimes w_1)$ and $(v_2 \otimes w_2)$, and there's some kind of connection between the two particles in general! This is where **entanglement** comes from, and we'll see that soon.

And there's one more constraint we need to impose: for the sake of linearity, we'll also say that

$$(v_1 + v_2) \otimes w = v_1 \otimes w + v_2 \otimes w.$$

The reason for this is that both sides of this equation represent the first particle being in a superposition of one of two possibilities, while the second particle is in some specific state. Again, this is different from the direct product, in which we just put the two vectors side by side – in that case, we would add the two ws together as well, which isn't what we want to do here. And similarly, we'll want to say that

$$v \otimes (w_1 + w_2) = v \otimes w_1 + v \otimes w_2,$$

and now we have all of the axioms we need for our tensor product: just read off the equations above.

To add a bit more intuition for this, the space $V \otimes W$ is spanned by vectors of the form $v_i \times w_i$. Specifically, if we choose a basis $(e_1, \cdots, e_n)$ for V and a basis $(f_1, \cdots, f_m)$ for W, then **we have a basis for $V \otimes W$ of the form $e_i \otimes f_j$.** Since there are mn such vectors of this form, we **multiply the dimensions** for a tensor product, not add them:

$$\dim(V \otimes W) = (\dim V)(\dim W).$$

Indeed, because of the axioms that we introduced, we can get any vector in V on the left and any vector in W on the right! (This, for example, wouldn't have been possible with a direct product.)

Fact 223

There are a lot of subtle facts about this tensor product, so it might feel at some points that we are taking a long time to explain things, and it might feel at others that something is confusing.

We'll now try to introduce **operators** to our spaces $V \otimes W$. Say that T is an operator on V, and S is an operator on W: we'll define an operator $T \otimes S \in \mathcal{L}(V \otimes W)$, and let's see what properties this must have. It suffice to show how $T \otimes S$ will act on any element of the form $(v \otimes w)$, and then we'll be able to extend it to any superposition of such vectors by linearity. We're going to make a definition, but it won't have very much to do with anything else we're talking about today: the most natural way is to say that

$$T \otimes S(v \otimes w) = (Tv) \otimes (Sw).$$

In other words, everything acts in the space where it can, and there isn't much more to say here. Since T and S are linear, $T \otimes S$ will be linear as well.

But now suppose $T_1 \in \mathcal{L}(V)$, and we want to get an operator on $V \otimes W$ without having an operator on W. Then we'll need to **upgrade our operator** by just using the identity operator on W: we end up with the object $T_1 \otimes I \in \mathcal{L}(V \otimes W)$. (Similarly, we can upgrade a vector $S_1 \in \mathcal{L}(W)$ by turning it into $I \otimes S_1$.) And now one important idea is that **these two operators will commute**:

$$(T_1 \otimes I)(I \otimes S_1)(v \otimes w) = (T_1 \otimes I)(v \otimes S_1 w) = T_1 v \otimes S_1 w,$$

and similarly

$$(I \otimes S_1)(T_1 \otimes I)(v \otimes w) = (I \otimes S_1)(T_1 v \otimes w) = T_1 v \otimes S_1 w.$$

Essentially, **operators that originate from different particles still commute** – "they don't know anything about each other." So this is helpful, because writing the Hamiltonian of the whole system H_T is just

$$H_T = H_1 \otimes I + I \otimes H_2,$$

where H_1, H_2 are the Hamiltonians of the original two systems.

We'll now show an example for all of this: it's famous and important, because it's how we can think about **combining angular momenta**.

Example 224

Consider two spin 1/2 particles: the first one has basis states $|+\rangle_1, |-\rangle_1$, while the second has basis states $|+\rangle_2, |-\rangle_2$.

To form the tensor product, we need the four basis vectors where we take the product of the basis vectors: our space is

$$\text{span}\left(|+\rangle_1 \otimes |+\rangle_2,\ |+\rangle_1 \otimes |-\rangle_2,\ |-\rangle_1 \otimes |+\rangle_2,\ |-\rangle_1 \otimes |-\rangle_2\right).$$

In other words, **two spin states form a four-dimensional complex vector space**: a general state in this space looks like

$$|\psi\rangle = \alpha_1(|+\rangle_1 \otimes |+\rangle_2) + \alpha_2(|+\rangle_1 \otimes |-\rangle_2) + \alpha_3(|-\rangle_1 \otimes |+\rangle_2) + \alpha_4(|-\rangle_1 \otimes |-\rangle_2).$$

We can do a simple computation with this: let's act with the "total z-component of angular momentum" on this state ψ. This total z-component is just the z-component of the first particle's angular momentum plus the z-component

of the second particle's angular momentum, so our operator is

$$\hat{S}_z^T = \hat{S}_z^{(1)} + \hat{S}_z^{(2)} = \hat{S}_z^{(1)} \otimes I + I \otimes \hat{S}_z^{(2)}.$$

Essentially, we're constructing a new operator $\hat{S}_z^T$ on the new (larger) vector space. And now we can calculate this term by term: since $\hat{S}_z^{(1)} \otimes I$ acts on our state, it acts on each term of the vector $|\psi\rangle$. We can pull out the constants and then just apply $\hat{S}_z^{(1)}$ to the v-vectors: thus,

$$(\hat{S}_z^{(1)} \otimes I)\,|\psi\rangle = \alpha_1 \hat{S}_z\,|+\rangle \otimes |+\rangle + \alpha_2 \hat{S}_z\,|+\rangle \otimes |-\rangle + \alpha_3 \hat{S}_z\,|-\rangle \otimes |+\rangle + \alpha_4 \hat{S}_z\,|-\rangle \otimes |-\rangle\,.$$

(We've dropped the subscripts for convenience.) And now we know that $\hat{S}_z\,|+\rangle = \frac{\hbar}{2}\,|+\rangle$, so the number comes out of the tensor:

$$(\hat{S}_z^{(1)} \otimes I)\,|\psi\rangle = \frac{\hbar}{2}\left(\alpha_1\,|+\rangle \otimes |+\rangle + \alpha_2\,|+\rangle \otimes |-\rangle - \alpha_3\,|-\rangle \otimes |+\rangle - \alpha_4\,|-\rangle \otimes |-\rangle\right).$$

We can do the other one pretty quickly as well:

$$(I \otimes \hat{S}_z^{(2)})\,|\psi\rangle = \frac{\hbar}{2}\left(\alpha_1\,|+\rangle \otimes |+\rangle - \alpha_2\,|+\rangle \otimes |-\rangle + \alpha_3\,|-\rangle \otimes |+\rangle - \alpha_4\,|-\rangle \otimes |-\rangle\right).$$

So if we add these together, we get the total operator $\hat{S}_z^T$, and thus

$$\hat{S}_z^T\,|\psi\rangle = \frac{\hbar}{2}\left(2\alpha_1\,|+\rangle \otimes |+\rangle + 2\alpha_4\,|-\rangle \otimes |-\rangle\right)$$

And now any state with total z-angular momentum $\hat{S}_z^T = 0$, we must have $\alpha_1 = \alpha_4 = 0$ (because those two vectors on the right hand side are independent). We will see soon that there is a state whose total angular momentum in all three directions is zero.

One thing that we haven't said very much about is the **zero vector** of this tensor space. We know that there is a zero vector in $V \otimes W$, and in this case, it looks a bit more complicated than usual. Consider the vector

$$0 \otimes w_i, \quad w_i \in W.$$

This is actually the zero vector for any vector w_i, and similarly $v_i \otimes 0$ is the zero vector for any $v_I \in V$. This is because we can pick $a = 0$ in the statement $a(v \otimes w) = av \otimes w$: then the left side is just 0, while the right side is $0 \otimes w$. This means that having 0 in either input guarantees that we have the zero vector.

We can now try to get numbers out of our tensor space: specifically, we can define a new inner product. As always, we should define this object to our best ability and hope it satisfies the axioms we want: we'll require the inner product to have

$$\left\langle \sum a_{ij} v_i \otimes w_j, \sum_{p,q} b_{pq} v_p \otimes w_q \right\rangle = \sum_{i,j} a_{ij}^* \sum_{p,q} b_{pq} \langle v_i \otimes w_j, v_p \otimes w_q \rangle.$$

Essentially, we're assuming the linearity on the right inputs and anti-linearity on the left-inputs, just like our usual inner product. To get a final number, the best thing for us to do is to use an inner product from v and an inner product from w:

$$\langle v_i \otimes w_j, v_p \otimes w_q \rangle = \langle v_i, v_p \rangle_V \langle w_j, w_q \rangle_W.$$

This last step is the most interesting one: we do need to multiply, because setting $v_i = 0$ must yield zero – in that case, we're taking the inner product of zero with some other vector. And this does indeed happen here, because $\langle v_i, v_p \rangle_V = 0$.

Example 225

Let's now return to the state

$$|\psi\rangle = \alpha(|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle).$$

(Sometimes we put subscripts 1 and 2 for the ket vectors, so we're careful that we're looking at the right vector spaces. In particular, $|+\rangle_{(1)} \otimes |-\rangle_{(2)}$ and $|-\rangle_{(2)} \otimes |+\rangle_{(1)}$ are the same things – commutativity isn't really a problem – and then we do care about the labels.) This is an example of an **entangled state** of spin 1/2 particles – we haven't quite defined that yet, but the idea is that we should try to normalize this state. Like with any other vector space, we take the inner product of the state with itself:

$$\langle \psi, \psi \rangle = \alpha^* \alpha \langle |+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle, |+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle \rangle.$$

But every term inside the inner product is now part of an orthonormal basis for the tensor space: the squared terms give $\langle +|+\rangle \langle -|-\rangle = 1$, while the other terms give nothing because $\langle +|-\rangle = \langle -|+\rangle = 0$. (One way to visualize this is that **we can turn all the kets on the left argument into bras**.) Either wway, this means that $\langle \psi, \psi \rangle = 2|\alpha|^2$, so normalizing the state yields

$$\psi = \frac{1}{\sqrt{2}}(|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle).$$

It turns out this state actually is the one with zero total angular momentum (in the x, y, and z directions). This state is **rotationally invariant** – if we apply a rotation operator to this state by rotating both spaces, the state that comes out is the same!

So now we're ready to talk about the concept of **entanglement**: **entangled states** are those where we cannot say that "the first particle does something and the second particle does something else." We know that $V \otimes W$ includes superpositions (that is, sums) of $\alpha_{ij} v_i \otimes w_j$. If we're given such a superposition, a good question to ask is whether we can write it in the form $v_* \otimes w_*$ for some $v_* \in V, w_* \in W$. If we could say that, then we would know that the first particle is in the state v_* and the second particle is in the state w_*: the two particles are not actually entangled **if we can factor our state**.

It seems like this is a complicated factorization problem – it might take some time to see whether a state is an entangled state or not. (Note that being entangled is a **basis-independent** problem!) Let's illustrate how this would work with an example:

Example 226

Suppose V, W are two-dimensional complex vector spaces with bases (e_1, e_2) and (f_1, f_2), respectively.

The most general state looks like

$$a_{11} e_1 f_1 + a_{12} e_1 f_2 + a_{21} e_2 f_1 + a_{22} e_2 f_2.$$

There are $2 \times 2 = 4$ basis states, and we want to ask whether we can write this as $(a_1 e_1 + a_2 e_2) \otimes (b_1 f_1 + b_2 f_2)$ (this is the most general way to write a vector in V and a vector in W). Luckily, it's pretty easy to see when these numbers $a_{11}, a_{12}, a_{21}, a_{22}$ exist: distributing out, this means that

$$a_{11} = a_1 b_1, \ \ a_{12} = a_1 b_2, \ \ a_{21} = a_2 b_1, \ \ a_{22} = a_2 b_2.$$

This gives us a consistency condition for the four equations: note that

$$a_{11}a_{22} = a_1b_1a_2b_2 = a_{12}a_{21},$$

so four numbers $a_{11}, a_{12}, a_{21}, a_{21}$ can only factor if the determinant of the matrix $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$ is zero. And with a quick argument, we can check that whenever the determinant is zero, there exists a solution! So in this case, **the determinant of the matrix is zero exactly when the two particles are not entangled**.

However, there are many entangled states, and there's "enough of them" that we can construct a basis of our tensor product space such that all basis vectors are entangled states. To do that, we'll use our spin 1/2 system again: let V be the state system for a spin 1/2 particle, and consider a two-particle system $V \otimes V$. We'll take

$$|\Phi_0\rangle = \frac{1}{\sqrt{2}}(|+\rangle|+\rangle + |-\rangle|-\rangle)$$

(note that we've dropped the $\otimes$ symbol, and eventually we're also going to make the ket simpler and just write $|{+}{+}\rangle$ – our notation will evolve as our calculations get more complicated). This is similar to the state that we just built – it's already normalized, and we can check that by taking the dual and directly evaluating the inner product. Indeed, this is an entangled state, because we have a matrix representation of $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, and the determinant is nonzero.

We still need four other basis states, and we'll write them in the following form:

$$|\Phi_i\rangle = (I \otimes \sigma_i)|\Phi_0\rangle.$$

For example,

$$\Phi_1 = (I \otimes \sigma_1)|\Phi_0\rangle = (I \otimes \sigma_1)\frac{1}{\sqrt{2}}(|+\rangle|+\rangle + |-\rangle|-\rangle),$$

and now the I acts on the first ket, while the σ acts on the second ket, and we're left with

$$\frac{1}{\sqrt{2}}(|+\rangle\sigma_1|+\rangle + |-\rangle\sigma_1|-\rangle) = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle + |-\rangle|+\rangle),$$

because σ_1 is the matrix $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. We can check that Φ_1 is orthogonal to Φ_0 – none of the terms have both labels matching, so the inner product is just zero. Similarly, we have that

$$|\Phi_2\rangle = \frac{i}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle),$$

and

$$|\Phi_3\rangle = \frac{1}{\sqrt{2}}(|+\rangle|+\rangle - |-\rangle|-\rangle).$$

We can indeed verify that these are all orthogonal to $|\Phi_0\rangle$, and we also need to do the calculation for $\langle\Phi_i|\Phi_j\rangle$. But this time, we don't need to do everything by inspection: since the Pauli matrices are Hermitian, we have

$$\langle\Phi_i|\Phi_j\rangle = \langle\Phi_0|(I \otimes \sigma_i)(I \otimes \sigma_j)\Phi_0\rangle$$

since "moving from one argument to the other" is the definition of a Hermitian operator in terms of the inner product. And now we can make progress using the Pauli identities: operators multiply in the most direct way, so II is just the

identity operator, while $\sigma_i\sigma_j$ is the identity plus a Pauli matrix: it'll be $I\delta_{ij} + i\varepsilon_{ijk}\sigma_k$. So plugging this in,

$$\langle\Phi_i|\Phi_j\rangle = \langle\Phi_0|(I\delta_{ij} + i\varepsilon_{ijk}\sigma_k)\Phi_0\rangle\,,$$

and now the $I\delta_{ij}$ term just gives us a δ_{ij}, while $\sigma_k\Phi_0 = \sigma_k$ is orthogonal to Φ_0 (as we just showed)! Thus,

$$\langle\Phi_i|\Phi_j\rangle = \delta_{ij},$$

and we've indeed shown that we have an **orthonormal basis** of the tensor product of two spin 1/2 particles! We can now write down our conventional basis states in terms of the entangled states:

$$|+\rangle\,|+\rangle = \frac{1}{\sqrt{2}}(|\Phi_0\rangle + |\Phi_3\rangle).$$

Similarly, we can find the others by a direct inspection:

$$|+\rangle\,|-\rangle = \frac{1}{\sqrt{2}}(|\Phi_1\rangle - i\,|\Phi_2\rangle),$$

$$|-\rangle\,|+\rangle = \frac{1}{\sqrt{2}}(|\Phi_1\rangle + |\Phi_2\rangle),$$

$$|-\rangle\,|-\rangle = \frac{1}{\sqrt{2}}(|\Phi_0\rangle - |\Phi_3\rangle).$$

The vectors $|\Phi_0\rangle\,, |\Phi_1\rangle\,, |\Phi_2\rangle$, and $|\Phi_3\rangle$ are known as the **Bell basis** for this system.

We'll now move on to the concepts of measurement and teleportation. Recall that that there is a postulate that in an orthonormal basis, we can find the probabilities of our states being along these basis states after a measurement. Before our experiment, the state is in a superposition of these basis states, but it will collapse into one of them, each with some probability. For example, in the Stern-Gerlach experiment, we picked two basis states, $|+\rangle$ and $|-\rangle$ and the device collapses our state into one of those two – what we're saying here is slightly more general. Specifically, if we have **any orthonormal basis** $(|e_1\rangle\,, \cdots, |e_n\rangle)$, we can construct a machine to measure a state $|\psi\rangle$ to be in the state $|e_i\rangle$ with probability $|\langle e_i|\psi\rangle|^2$, and then after that measurement, we'll be in some state $|e_k\rangle$.

The other point that we should note is that Pauli matrices are Hermitian and square to 1, so they're actually unitary, and thus they can govern time-evolution of a system! For example, multiplying a state by σ_1 doesn't need to be very mathematical – because it's unitary, we can construct a **suitable Hamiltonian** that evolves the state through some time. For example, with our spin states, we can take a magnetic field that exists for a few picoseconds, and that will implement σ_1! Indeed, we can check that

$$e^{i\frac{\pi}{2}(-1+\sigma_i)} = e^{-i\pi/2}e^{i\pi\sigma_1/2} = -i\left(I\cos\frac{\pi}{2} + i\sigma_i\sin\frac{\pi}{2}\right) = \sigma_i,$$

and thus we've written σ_i as the exponential of i times a Hermitian operator, so we can just pick a Hamiltonian H such that $\frac{\pi}{2}(-1+\sigma_i) = \frac{tH}{\hbar}$. In other words, we can physically realize σs with a machine.

So now we're ready to discuss teleportation: this is a hot topic of science fiction, and it was an idea that was impossible classically. But in quantum mechanics, we can do much better, and we'll be explaining this now!

Fact 227

This discovery actually came from 1993, so this hasn't been known for a long time. Quantum mechanics is a Renaissance of physics in some sense, because now we can do lots of cool experiments.

The following idea came from Bennett (IBM), Brassard, Crepeau, Jozsa (Montreal), Peres (Technion), and Wootters (Williams) – it was a big collaboration. Here's the setup:

Example 228

Two people, Alice and Bob, play a game. Alice has a quantum state – it's an unmeasured state of a spin 1/2 particle, $\alpha|+\rangle + \beta|-\rangle$. Her goal is to teleport the state to Bob, who is far away. (A spin state in this context is also sometimes called a **qubit**.)

First of all, we might ask why we don't just make a copy of our state. The issue is that there's a **no cloning** idea: we can't create a copy of a state like this. Similarly, we can't measure our state to find α and β, because she only has one copy of the state – the Stern-Gerlach experiment would just give us a single $|+\rangle$ or $|-\rangle$, and then our qubit is gone. So no matter what, Alice should not measure the state.

On the other hand, perhaps Alice created this state with a specific Hamiltonian, so she knows what α and β are. So she could tell Bob those numbers, but if α is some irrational number which requires an infinite string of information to transmit, that's not good either! So instead, we'll try to produce an experiment in which Bob will get the state on the other side – **our state will teleport**.

Basically, let's let this state space be C: we'll write that Alice's original state is

$$|\psi\rangle = \alpha|+\rangle_C + \beta|-\rangle_C.$$

The whole idea with teleportation is to use an **entangled state** here! We can product an entangled pair of two particles, where one particle is given to Alice and the other to Bob. Entanglement occurs instantaneously – there's no way to send information through entanglement in general. If we wanted to teleport a person, we'd have to create a reservoir of billions of entangled pairs in two different locations, and then we'd have to take these billions of pairs and do a bunch of measurements so that every quantum state in the person's body is measured with some entangled state. And that's essentially what's happening here – Alice will do a measurement so that the particle will become the state we wanted to teleport initially!

Fact 229

Alice will need to send some additional information as well: suppose Alice has a console with four lights, labeled $0, 1, 2, 3$. Alice will need to send two bits of information – which of those four lights lit up during the measurement – and then Bob will use that information to send B into one of four machines, labeled $0, 1, 2, 3$.

It turns out that after this replication, Alice's state will be destroyed, but Bob will have a copy of the state, and that's what we'll explain now. We'll start with the **AB pair** (this explains the name C for the teleported state), which is the entangled state

$$|\phi_0\rangle_{AB} = \frac{1}{\sqrt{2}}(|+\rangle_A|+\rangle_B + |-\rangle_A|-\rangle_B).$$

Even though the particles Alice and Bob have can be very far apart, they're still entangled. So we can take the total tensor product of the particles from A, B, and C: this yields

$$|\phi_0\rangle_{AB} \otimes (\alpha|+\rangle_C + \beta|-\rangle_C).$$

Here's the key point: Alice will do a sneaky measurement with the particles A and C. (Remember that the particle A and the state A are different, because A and B are entangled.) Since Alice has these two particles, she can pick any orthonormal basis of the two-particle state space, because of the earlier notion that we can measure with any orthonormal basis! We'll use the **Bell basis** for A and C. First, we can rewrite our above tensor product as

$$|\psi_T\rangle = \frac{1}{\sqrt{2}}(|+\rangle_A|+\rangle_B + |-\rangle_A|-\rangle_B) \otimes (\alpha|+\rangle_C + \beta|-\rangle_C),$$

and now we can multiply everything out: this evaluates to

$$= \frac{1}{\sqrt{2}}[\alpha |+\rangle_A |+\rangle_C |+\rangle_B + \beta |+\rangle_A |-\rangle_C |+\rangle_B + \alpha |-\rangle_A |+\rangle_C |-\rangle_B + \beta |-\rangle_A |-\rangle_C |-\rangle_B]$$

(the order of multiplication doesn't matter, as long as we keep the labels). We've written this so that we have A-and-C vectors that are orthonormal to each other. However, our basis isn't entangled between the particles A and C yet – instead, we'll mathematically rewrite it using the formulas for $|\pm\rangle |\pm\rangle$ in terms of the $|\Psi_i\rangle$s that we derived above. This is a bit of algebra, but our result is

$$\frac{1}{2}(|\Phi_0\rangle_{AC} + |\Phi_3\rangle_{AC})\alpha |+\rangle_B + \frac{1}{2}(|\Phi_1\rangle_{AC} - i|\Phi_2\rangle_{AC})\beta |+\rangle_B$$

$$+\frac{1}{2}(|\Phi_1\rangle_{AC} + i|\Phi_2\rangle_{AC})\alpha |-\rangle_B + \frac{1}{2}(|\Phi_0\rangle_{AC} - |\Phi_3\rangle_{AC})\beta |-\rangle_B ,$$

and now we can collect terms across the Φs to find

$$= \frac{1}{2}|\phi_0\rangle_{AC}(\alpha |+\rangle_B + \beta |-\rangle_B) + \frac{1}{2}|\phi_1\rangle_{AC}(\beta |+\rangle_B + \alpha |-\rangle_B) + \frac{1}{2}|\phi_2\rangle_{AC}(i\alpha |-\rangle_B - i\beta |+\rangle_B) + \frac{1}{2}|\phi_3\rangle_{AC}(\alpha |+\rangle_B - \beta |-\rangle_B).$$

Remember that we haven't done anything yet – we're just rewriting the state mathematically. But something funny has happened – the state that we wanted to transmit, which was originally in particle C, not shows up in particle B in various funny linear combinations. Specifically, we have a $|\psi\rangle_B$ term for the $|\Psi_0\rangle$ coefficient (where ψ was the original $\alpha |+\rangle + \beta |-\rangle$ that we wanted), and we also have a $\sigma_3 |\Psi\rangle_B$ term for the $|\Psi_3\rangle$ coefficient, because σ_3 is of the form $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ – it gives a $+1$ eigenvalue for the $|+\rangle$ state and a -1 eigenvalue for the $|-\rangle$ state. Similarly, the other states simplify too: we actually just have that the **total state** is

$$|\psi_T\rangle = \frac{1}{2}|\phi_0\rangle_{AC}|\psi\rangle_B + \frac{1}{2}|\phi_1\rangle_{AC}\sigma_1|\psi\rangle_B + \frac{1}{2}|\phi_2\rangle_{AC}\sigma_2|\psi\rangle_B + \frac{1}{2}|\phi_3\rangle_{AC}\sigma_3|\psi\rangle_B .$$

And now comes the physics! **Alice measures in the Bell space of A and C** – specifically, we measure one of the four basis states in the equation above. The wave function will collapse into one of these basis states – the 0 basis state makes the 0-labeled light light up, the 1 basis state makes the 1-labeled light light up, and so on. In any case, we now have an entangled set of particles $|\psi\rangle_{AC}$ which have no memory at all of the original state C, but now B has the information instead! Whenever light i lights up, this means that Bob now has the particle in the state $\sigma_i |\psi\rangle_B$, and now Bob just needs to apply the σ_i operator to his state (remember that $\sigma_i^2 = I$). This just means that Bob puts his system into the ith machine, which has some specific Hamiltonian, and the state will time-evolve into $|\psi\rangle_B$. Indeed, we've now teleported our state from Alice to Bob – all we needed to send was the information of which light shined.

28 April 6, 2020

There are a few announcements regarding grades – the main thing to keep in mind is that each of our tests is now 15 percent of the total grade, and the homework and lecture questions are now more heavily weighted. This should make passing the course more focused on our weekly work, but hopefully we'll still take the tests seriously.

Remark 230. *There's two ways to approach practice problems: some are better for doing better in exams, and others are better for giving physics insight. It's unfortunately hard to find problems of the former type, except for the unused edX problems. But Griffiths (3rd edition) is the best source for problems in general, though not all of them are relevant. Another set of good books are Cohen-Tannoudji's "Quantum Mechanics," volumes 1 and 2, which have a lot of worked exercises – every problem is done very slowly, but it's very well explained.*

We'll spend some time today putting together the ideas about two-state systems, being a bit more direct and to the point.

We should always remember that two-state systems have **two basis states**, not two states in general! A good way to summarize a system like this is with a magnetic dipole moment

$$\vec{\mu} = \gamma \vec{S},$$

where γ is positive for a positive charge and negative for a negative charge – for example, $\vec{\mu} = -\frac{e}{m_e c}\vec{S}$ for an electron (where we're using Gaussian units – the c in the denominator is a matter of convention). The Hamiltonian for such a system looks like

$$H = -\vec{\mu} \cdot \vec{B} = -\gamma \vec{B} \cdot \vec{S},$$

where B is the magnetic field that the dipole moment is in. Further simplifying for our purposes in the case where the field B is **constant**, we can write $\vec{B} = B\vec{n}$, where $B = |\vec{B}|$ is the (nonnegative) magnitude of our magnetic field – this gives us yet another expression

$$H = -\gamma B \vec{n} \cdot \vec{S}.$$

We can then write down the unitary time-evolution operator:

$$e^{iHt/\hbar} = \boxed{e^{-i(-\gamma B t)(\vec{n}\cdot\vec{S})/\hbar}}.$$

To understand how this affects our states, recall that there is a rotation operator

$$R_{\vec{n}}(\alpha) = \boxed{e^{-i\alpha \vec{n}\cdot\vec{S}/\hbar}}.$$

parameterized by a rotation axis $\vec{n}$ and an angle α – we rotate counterclockwise (with the right-hand rule) around $\vec{n}$ with angle α. But these last boxed expressions can be identified with each other: we can use the same $\vec{n}$s, and our angle of rotation is now $\alpha = -\gamma B t$. α is a number – it doesn't have a direction – and thus we can describe our states as rotating around $\vec{n}$ with angular velocity

$$\vec{\omega} = \frac{d\alpha}{dt}\vec{n} = -\gamma B \vec{n}.$$

Rewriting $B\vec{n}$ as the vector $\vec{B}$, this is the **Larmor frequency** $\vec{\omega}_L = -\gamma \vec{B}$, and we can use this to rewrite our Hamiltonian as

$$\boxed{H = \vec{\omega}_L \cdot \vec{S}}.$$

To make this more explicit, we can consider the most general Hamiltonian for a two-state system

$$H = g_0 I + \sum_i g_i \sigma_i = g_0 I + \vec{g} \cdot \vec{\sigma}.$$

where g_0, g_1, g_2, g_3 in general can be time-independent. Then the Larmor frequency can be written by replacing $\vec{\sigma}$ with $\frac{2}{\hbar}\vec{S}$: this tells us that

$$\vec{\omega}_L = \frac{2}{\hbar}\vec{g}$$

for our general-form Hamiltonian. Similarly to the magnetic field, we can write $\vec{g} = g\vec{n}$, where g is the magnitude of $\vec{g}$: remember that the operator $\vec{n} \cdot \vec{\sigma}$ has energy eigenstates $|n; \pm\rangle$, so the Hamiltonian

$$H = g_0 I + g(\vec{n} \cdot \vec{\sigma})$$

will have energy eigenstates of $g_0 + g$ and $g_0 - g$, corresponding to $|n; +\rangle$ and $|n; -\rangle$ respectively. (Here, we should

think of the $g_0 I$ term as not really doing anything, except **shifting all of the energies**. We do have to be careful, though: adding a $g_0 I$ term to a Hamiltonian will add a phase e^{ict} to our wavefunction. This is not something we can observe if the $g_0 I$ term shows up in the whole system, but it can be relevant if this is only a subsystem!)

We'll spend some time trying some exercises now:

Problem 231

Recall the expression for our coherent state

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |0\rangle .$$

Use this expression to calculate the overlap $\langle\beta|\alpha\rangle$.

We have that

$$\langle\beta|\alpha\rangle = \langle 0| \left(e^{-|\beta|^2/2} e^{\beta a^\dagger}\right)^\dagger e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |0\rangle .$$

Since $e^{-|\alpha|^2}$ and $e^{-|\beta|^2}$ are both real numbers, we can pull them out of the bra-ket expression (the dagger doesn't affect the $e^{-|\beta|^2/2}$ term), leaving

$$= e^{-|\alpha|^2/2 - |\beta^2|/2} \left\langle 0 \middle| e^{\beta^* a} e^{\alpha a^\dagger} \middle| 0 \right\rangle .$$

We can now expand the exponentials as

$$\sum_{i,j} \frac{(\beta^*)^i}{i!} \frac{\alpha^j}{j!} \langle 0 | \hat{a}^i (\hat{a}^\dagger)^j | 0 \rangle ,$$

and then we can put a factor of $\sqrt{i!}$ and $\sqrt{j!}$ into the denominators of the bra-ket so that we get orthonormal energy eigenstates: thus this expansion will yield

$$= \sum_{i,j} \frac{(\beta^*)^i}{\sqrt{i!}} \frac{\alpha^j}{\sqrt{j!}} \delta_{ij}.$$

Working a bit more will yield an answer of $\boxed{e^{-|\alpha|^2/2 - |\beta^2|/2 + \beta^* \alpha}}$.

Problem 232

Suppose we have a two-body Hamiltonian $H = H_1 \otimes I + I \otimes H_2$. Show that we can write the time-evolution operator $e^{-iHt/\hbar}$ can be written as a tensor product.

Note that a Hamiltonian can't really look like $H_1 \otimes H_2$, because that would have units of squared energy. So the above expression is actually the natural Hamiltonian for two particles that don't talk to each other!

The idea is to first plug in directly, yielding

$$e^{-\frac{it}{\hbar}(H_1 \otimes I) - \frac{it}{\hbar}(I \otimes H_2)}.$$

The operators in the exponent here **do commute**: they act on different worlds, so we can rewrite this as a product of exponentials

$$= e^{-\frac{it}{\hbar}(H_1 \otimes I)} e^{-\frac{it}{\hbar}(I \otimes H_2)}.$$

This is an **ordinary product** – both expressions are operators on the tensor product space, so we should not take their tensor product. We can then rewrite this as

$$\left(e^{-iH_1 t/\hbar} \otimes I\right) \cdot \left(I \otimes e^{-iH_2 t/\hbar}\right),$$

and now we can multiply the two operators by composition to yield $\boxed{\left(e^{-iH_1 t/\hbar} \otimes e^{-iH_2 t/\hbar}\right)}$. This is a fundamental result: we just tensor product the time-evolution operators for the two spaces! (It's good to make sure we can understand the logic here – that means we're on our way to understanding tensor product spaces.)

29 Multiparticle States, Part 2

Last lecture, we started discussing the **singlet state**

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle_1 |-\rangle_2 - |-\rangle_1 |+\rangle_2).$$

This state has a few interesting properties: its total angular momentum is zero (in the x, y, and z directions), so it is a **rotationally invariant** state. It is also an entangled state (which we used when discussing quantum teleportation), and it isn't hard to realize physically.

Example 233

Particles can decay in such an entangled state physically: for example, a **meson** called an η_0 is an interacting particle, which decays into a μ^+ and a μ^- particle.

Since η_0 has zero angular momentum (it doesn't spin), conservation of angular momentum tells us that the $\mu^\pm$ particles will be in a state like $|\psi\rangle$, as long as there is no orbital angular momentum. So it's pretty easy to create such an entangled state!

We have also showed that

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\vec{n};+\rangle_1 |\vec{n};-\rangle_2 - |\vec{n};-\rangle_1 |\vec{n};+\rangle_2)$$

for **any direction** $\vec{n}$ because of rotational invariance. We can use this to talk about probability:

Definition 234

Let $\mathbb{P}(\vec{a}+, \vec{b}+)$ be the probability that we find the first particle to be in state $|\vec{a};+\rangle$ and the second particle to be in state $\left|\vec{b};+\right\rangle$ when we measure the **singlet state** along the $\vec{a}, \vec{b}$ directions respectively.

Calculating such a probability is nontrivial, but we can use the fact that our state $|\psi\rangle$ is rotationally invariant. Picking our normal vector to be $\vec{a}$, we know that

$$\boxed{|\psi\rangle = \frac{1}{\sqrt{2}}(|\vec{a};+\rangle_1 |\vec{a};-\rangle_2 - |\vec{a};-\rangle_1 |\vec{a};+\rangle_2)},$$

and now finding the probability comes from computing the numerical overlap and squaring:

$$\mathbb{P}(\vec{a}+, \vec{b}+) = \left|\langle\vec{a};+| \otimes \left\langle\vec{b};+\right| \left(\frac{1}{\sqrt{2}}(|\vec{a};+\rangle_1 |\vec{a};-\rangle_2 - |\vec{a};-\rangle_1 |\vec{a};+\rangle_2)\right)\right|.$$

We can evaluate each of these terms – remember that we evaluate the inner product for a tensor product by doing the inner products in the individual spaces. The second term drops out, because $\langle\vec{a};+|\vec{a};-\rangle$ is zero, and this just leaves us with

$$\mathbb{P}(\vec{a}+, \vec{b}+) = \left|\frac{1}{\sqrt{2}}\left\langle\vec{b};+\middle|\vec{a};-\right\rangle\right|^2 = \frac{1}{2}\left|\left\langle\vec{b};+\middle|\vec{a};-\right\rangle\right|^2.$$

To finish simplifying this, we can calculate the overlap between two spin states $\vec{n}$ and $\vec{n}'$: recall from early on in the class that this is $\cos^2\frac{\gamma}{2}$, where γ is the angle between the two spin states. Since we have a minus sign above, we should use the $-\vec{a}$ vector instead, meaning that our angle is $\pi - \theta_{ab}$ instead of θ_{ab} (the angle between the two vectors). Thus, our final answer is

$$\mathbb{P}(\vec{a}+, \vec{b}+) = \frac{1}{2}\cos^2\frac{1}{2}(\pi - \theta_{ab}) = \boxed{\frac{1}{2}\sin^2\frac{\theta_{ab}}{2}}.$$

For example, if the second particle is being measured along $\vec{b} = -\vec{a}$ (they point in completely opposite directions), then the overlap should be $\frac{1}{2}$, because we can look at the boxed expression for $|\psi\rangle$ above: the first term, $|\vec{a};+\rangle_1 |\vec{a};-\rangle_2$, corresponds to $\vec{a}$ and $\vec{b}$ **both being positive**, while the second term corresponds to them both being negative. And indeed, $\pi_{ab} = \pi$ in this case, and our probability is $\frac{1}{2}$.

Another interesting case is to consider $\mathbb{P}(\hat{z}+, \hat{x}+)$: these two vectors have $\pi_{ab} = \frac{\pi}{2}$, so the probability that they are both measured to be positive is $\frac{1}{2}\sin^2\frac{\pi}{4} = \boxed{\frac{1}{4}}$.

With this, we can discuss the **EPR paradox** – we might have seen this in 8.04, but now we have the mathematics to appreciate it more completely. And this will lead to the Bell inequalities soon after.

Fact 235

The EPR story began when Einstein, Podolsky, and Rosen wrote a paper about **local realism**.

This sounds like philosophy, and people thought the question was undecidable for a while. While it's difficult to pin down the actual definition of local realism, one main idea regards **two assumptions that we make about measurement results**:

- When we measure something and get a number, this measurement corresponds to "some aspect of reality." In other words, there is something real about our object.
- Measurements that we do (for example, in a lab) are not affected by measurements or other actions that are done far away (for instance, on the moon) **at the same time**, because there's no time for the information to propagate between the two actions.

Einstein was very vocal about insisting that physics must satisfy both of these assumptions – while he was correct and insightful about the photoelectric effect and relativity, he was unfortunately wrong in this case.

It seems very reasonable that the first assumption would be true – Einstein would perhaps say that a spin up particle is always spin up, and we discover that fact through measurement. Then a way to get around us not knowing whether a particle exits the Stern-Gerlach machine spin up or down is to try using **hidden variables**: perhaps there are some properties of our particles that we just don't know, but if we knew those properties, we could predict the result of our experiment. This might sound like an untestable hypothesis, but it isn't – we'll see this soon!

And the second assumption breaking seems even more disturbing – we've gotten used to the idea that simultaneous events cannot affect each other because light cannot be exchanged between them. It then seems that we could send information faster than light if this assumption were false – people have discussed many questions here, and it's worth thinking about. But it turns out at the end of the day that there isn't a way to get real information faster than the speed of light.

So let's now review the EPR thought experiments and try to see how they relate to the two assumptions we're trying to make.

Example 236

Suppose Alice and Bob are measuring states, both along the z-axis, in such a way that if Alice measures spin up, Bob measures spin down and vice versa.

This is some kind of a **correlation** between Alice and Bob's experiments, and it seems like we'd know information from Alice's experiment about Bob's experiment. But EPR claims that when we do this experiment, we've already created entangled particles with **definite spin vectors**. Specifically, the claim would be that 50 percent of Alice's particles are definitely spin up (so Bob's corresponding particles are spin down), and the other 50 percent of her particles are spin down. This does indeed give us correlation, and what EPR says is that there is no quantum superposition there!

Mathematically, there isn't a problem here – we're just claiming that the (definite) spins depend on some hidden variables that we don't know. So let's look at a more complicated example:

Example 237

Suppose Alice and Bob each have two Stern-Gerlach machines, one in the z and one in the x-direction.

Einstein would say that in such an example, we shouldn't talk about making one measurement after the other: we can measure either in z or in x, and there will be a definite answer for each particle's spin. Let's say for example that we have a particle $(\hat{z}+, \hat{x}-)$ – in other words, if we measure the z-spin, we get $+$, and if we measure the x-spin, we get $-$. So EPR is saying here that the particles look like this instead of a strange superposition of $|+\rangle$ and $|-\rangle$: there is some reality, and we measure that reality for each particle.

So suppose we have entangled particles for Alice and Bob: say that Alice's particle is $(\hat{z}+, \hat{x}+)$. Then Bob's corresponding entangled particles must look like $(\hat{z}-; \hat{x}-)$. Indeed, we'd find that we would have correlation if we measure in either the z- or the x-direction. Similarly, if Alice's particle is $(\hat{z}-, \hat{x}+)$, Bob's would be $(\hat{z}+, \hat{x}-)$, and we can also produce pairs of particles with $(\hat{z}+, \hat{x}-)$ and $(\hat{z}-, \hat{x}+)$ or with $(\hat{z}-, \hat{x}-)$ and $(\hat{z}+, \hat{x}+)$. There are **four different possibilities here**, and what EPR is saying is that 25 percent of the entangled pairs that are formed are of each type.

And now we can ask EPR some questions: for example, the probability

$$\mathbb{P}(z+_A, z-_B)$$

(which is the probability Alice measures $+$ and Bob measures $-$) is **50 percent**, because there are two of the four cases which correspond to this reality. (And this is the same prediction that we would make from the entangled state formulation.) Similarly, we can ask for the probability

$$\mathbb{P}(z+_A, x+_B),$$

and this time there is only one of the four cases that works: thus the probability is **25 percent**. Again, this matches our quantum results, and it seems like everything is consistent.

So everything so far has not required quantum mechanics at all: it wasn't until Bell that we tried three directions and made a breakthrough towards disproving the EPR theory!

Example 238

Now Alice and Bob have three Stern-Gerlach machines in directions a, b, c, and our particles now need to be labeled with a $+$ or $-$ label for each of x, y, z.

So an example of a label for a particle would be $(a+, b-, c+)$: in other words, measuring in the a-direction yields an spin of $\frac{\hbar}{2}$, measuring in the b-direction yields $-\frac{\hbar}{2}$, and measuring in the c-direction yields $\frac{\hbar}{2}$. So we're doing a **single measurement** here (not doing anything with simultaneity), and we'll always ask for probabilities of events like "Alice measures $a+$ and Bob measures $c+$."

Let's quickly list the different possibilities for our entangled particles:

Particle 1 (Alice)	Particle 2 (Bob)
$(a+, b+, c+)$	$(a-, b-, c-)$
$(a+, b+, c-)$	$(a-, b-, c+)$
$(a+, b-, c+)$	$(a-, b+, c-)$
$(a+, b-, c-)$	$(a-, b+, c+)$
$(a-, b+, c+)$	$(a+, b-, c-)$
$(a-, b+, c-)$	$(a+, b-, c+)$
$(a-, b-, c+)$	$(a+, b+, c-)$
$(a-, b-, c-)$	$(a+, b+, c+)$

(The particles that Alice and Bob have always have different measurements along each of a, b, c – that's the way that they're correlated.) It might seem like we want to put $\frac{1}{8}$ of the particles in each of these states, but the argument that we'll be making here doesn't require this: let's say that there are N total particle pairs in our system, and there are $N_1, N_2, \cdots, N_8$ particle pairs in the eight states of our table above.

What we're going to do is run into a contradiction: we need to make our quantum mechanical formula $\frac{1}{2}\sin^2\frac{\theta_{ab}}{2}$ go wrong in this model with all of the different measurements we can try. The idea is to try to **combine the three directions** into a single equation. First of all,

$$\mathbb{P}(a+, b+) = \frac{N_3 + N_4}{N},$$

because only the third and fourth cases have the first particle in the $a+$ state and the second particle in the $b+$ state. Similarly,

$$\mathbb{P}(a+, c+) = \frac{N_2 + N_4}{N},$$

and

$$\mathbb{P}(c+, b+) = \frac{N_3 + N_7}{N}.$$

Now we can make a silly-looking inequality: because $N_3 + N_4 \leq N_3 + N_7 + N_4 + N_2$, we can divide that by N, and we now know that **under the assumption of local realism**, we have

$$\boxed{\mathbb{P}(a+, b+) \leq \mathbb{P}(a+, c+) + \mathbb{P}(c+, b+)}.$$

This is **Bell's inequality** – we've turned an assumption of realism into a mathematical fact! We didn't write down specific probabilities here, but what's interesting is that we can pick any populations that we want here, and we can try to use any a, b, c to get a contradiction. But we know that quantum mechanics has a formula for each of these expressions in Bell's inequality! If quantum mechanics is true, then the left hand side is equal to

$$\mathbb{P}(a+, b+) = \frac{1}{2}\sin^2\frac{\theta_{AB}}{2},$$

while the right hand side is

$$\mathbb{P}(a+, c+) + \mathbb{P}(c+, b+) = \frac{1}{2}\left(\sin^2\frac{\theta_{AC}}{2} + \sin^2\frac{\theta_{BC}}{2}\right).$$

And it's actually pretty easy to find vectors a, b, c such that the left hand side here is larger than the right hand side:

put them all in the same plane with c between a and b, such that there is an angle θ between a and c, as well as between c and b. Then **local realism claims** that

$$\frac{1}{2}\sin^2\theta \overset{??}{\leq} \frac{1}{2}\sin^2\frac{\theta}{2}\cdot 2 = \sin^2\frac{\theta}{2}.$$

And if we make θ **sufficiently small**, this inequality is not satisfied: the left side is approximately $\frac{\theta^2}{2}$, while the right hand side is approximately $\frac{\theta^2}{4}$. In general, this inequality fails for any $\theta \leq \frac{\pi}{2}$! So we now have a measurement that we can do in quantum mechanics with correlated entangled particles, and this actually **contradicts local realism**.

Therefore, what this tells us is that **there's no way to use hidden variables** to get around the issues of quantum mechanics – local realism is incorrect.

Fact 239

And Alain Aspect and others did the physical experiments in the 1980s, and this confirmed that Bell's inequality is indeed violated.

We'll finish this lecture by discussing **angular momentum** and an elegant vector notation that will help us understand this better. Let's summarize some of the things that we already know about it! The **orbital angular momentum** operators are defined to be

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \quad \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x.$$

In many cases, it's better to use labels $\hat{x}_1, \hat{x}_2, \hat{x}_3$ instead of $\hat{x}, \hat{y}, \hat{z}$ (and analogously for $\hat{p}$). That's because we can write commutation relations like

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0.$$

But the main idea we want to explore here is using **vector notation**. There are two ways to do this – we can construct triplets of objects, which are vectors, or we can form the vectors ourselves. This second option often leads to objects that are a bit confusing, but we try our best to avoid this. For example, instead of thinking of the $\vec{r}$ operator as $(\hat{x}, \hat{y}, \hat{z})$, we'll write

$$\vec{r} = \hat{x}\vec{e}_1 + \hat{y}\vec{e}_2 + \hat{z}\vec{e}_3 = \hat{x}_1\vec{e}_1 + \hat{x}_2\vec{e}_2 + \hat{x}_3\vec{e}_3.$$

We should understand that the basis vectors $\vec{e}_i$ are useful for writing expressions instead of triplets, but that they're not really interacting with the $\hat{x}, \hat{y}, \hat{z}$ operators. Similarly, we can define a momentum operator

$$\vec{p} = \hat{p}_1\vec{e}_1 + \hat{p}_2\vec{e}_2 + \hat{p}_3\vec{e}_3,$$

as well as the angular momentum operator

$$\vec{L} = \hat{L}_1\vec{e}_1 + \hat{L}_2\vec{e}_2 + \hat{L}_3\vec{e}_3.$$

These vectors are unusual, because **their components are vectors, not numbers**. So we need to understand how these operator vectors can be modified – we'll define the **dot product** and **cross product** like we usually do, though we need to be careful not to make mistakes.

Definition 240

Let $\vec{a}, \vec{b}$ be vector operators. The **dot product** of the two operators is defined to be

$$\vec{a} \cdot \vec{b} = \sum a_i b_i.$$

Similarly, the **cross operator** of the two operators is a vector operator defined via

$$(\vec{a} \times \vec{b})_i = \varepsilon_{ijk} a_j b_k.$$

The order matters here – a and b are operators, so they might not commute.

Definition 241

For a vector-valued operator, define $\vec{a}^2 = \vec{a} \cdot \vec{a} = \sum a_i a_i$.

We can now start doing some calculations. For example,

$$\vec{a} \cdot \vec{b} \neq \vec{b} \cdot \vec{a},$$

because our vectors now have non-commuting operators: specifically, we know that

$$\vec{a} \cdot \vec{b} = a_i b_i = [a_i, b_i] + b_i a_i,$$

where we're using the repeated index convention. But $b_i a_i$ is $b \cdot a$, so we get a formula

$$\boxed{\vec{a} \cdot \vec{b} = \vec{b} \cdot \vec{a} + [a_i, b_i]}.$$

Example 242

Plugging in the operators $\vec{r}, \vec{p}$, we find that

$$\boxed{\vec{r} \cdot \vec{p} = \vec{p} \cdot \vec{r} + 3i\hbar}.$$

(We should remember that the commutator $[x_i, p_i]$ is summed over i, so we pick up a factor of 3.) This means that the dot product is no longer symmetric, and similarly the cross product is no longer antisymmetric! Indeed,

$$(\vec{a} \times \vec{b})_i = \varepsilon_{ijk} a_j b_k = \varepsilon_{ijk}([a_j, b_k] + b_k a_j).$$

The first term here stays put, and we can swap the indices j and k in the ε_{ijk} on the second term, picking up a minus sign: thus

$$\boxed{(\vec{a} \times \vec{b})_i} = \varepsilon_{ikj} b_k a_j - \varepsilon_{ijk}[a_j, b_k] = \boxed{-(\vec{b} \times \vec{a})_i + \varepsilon_{ijk}[a_j, b_k]}.$$

In other words, the cross product will no longer be antisymmetric unless we're lucky.

Example 243

If we try to compute $\vec{r} \times \vec{r}$, we can plug it into our identity above to find that

$$\vec{r} \times \vec{r} = -\vec{r} \times \vec{r} + \varepsilon_{ijk}[\hat{x}_j, \hat{x}_k] = -\vec{r} \times \vec{r} + 0,$$

so we do have $\vec{r} \times \vec{r} = 0$.

We can similarly find that $\vec{p} \times \vec{p} = 0$, but something like $\vec{L} \times \vec{L}$ will not be zero! This is because $[\hat{L}_j, \hat{L}_k]$ is nonzero, and we'll end up finding that

$$\vec{L} \times \vec{L} = i\hbar \vec{L}.$$

On the other hand, if we try computing

$$(\vec{r} \times \vec{p})_i = -(\vec{p} \times \vec{r})_i + \varepsilon_{ijk}[\hat{x}_j, \hat{p}_k] = -(\vec{p} \times \vec{r})_i + \varepsilon_{ijk}\delta_{jk},$$

the last term is zero. It's true because δ requires j and k to be the same while ε requires them to be different, but a more general principle is that multiplying an antisymmetric and a symmetric object will yield zero! (To show that, we can just relabel j and k by swapping: then we get the same quantity with a negative sign.) Therefore, we actually have

$$(\vec{r} \times \vec{p})_i = -(\vec{p} \times \vec{r})_i \implies \boxed{\vec{r} \times \vec{p} = -\vec{p} \times \vec{r}},$$

and this is the object that we call the angular momentum.

Example 244

We know that the angular momentum $\vec{L}$ is classically perpendicular to both $\vec{r}$ and $\vec{p}$ – is this true in the quantum mechanical case?

We'll first compute $\vec{r} \cdot \vec{L}$. By definition, we know that

$$\vec{r} \cdot \vec{L} = \vec{r} \cdot (\vec{r} \times \vec{p}) = \hat{x}_i \varepsilon_{ijk} \hat{x}_j \hat{p}_k = \varepsilon_{ijk} \hat{x}_i \hat{x}_j \hat{p}_k,$$

and now the operators $\hat{x}_i$ and $\hat{x}_j$ commute, but ε_{ijk} is antisymmetric, so the whole expression will collapse to 0. Therefore, $\vec{r} \cdot \vec{L}$ is indeed 0.

On the other hand, let's find $\vec{p} \cdot \vec{L}$. There's two ways to do this problem, and we'll do it by writing out the indices:

$$\vec{p} \cdot \vec{L} = \hat{p}_i \varepsilon_{ijk} \hat{x}_j \hat{p}_k.$$

There is a temptation to say that the operator part of this is symmetric in i and k, because there are two operators $\hat{p}_i$ and $\hat{p}_k$, but this is incorrect! We have to move the $\hat{p}$ operators together, and there's an $\hat{x}$ operator in the middle that might screw things up. So we'll be a bit more careful: this evaluates to

$$\varepsilon_{ijk} \hat{p}_i \hat{x}_j \hat{p}_k = \varepsilon_{ijk} \hat{x}_j \hat{p}_i \hat{p}_k$$

because the commutator of $\hat{p}_i$ and $\hat{x}_j$ vanishes, and now it is okay to say that ε_{ijk} is antisymmetric in i and k, while the rest of the expression is symmetric in i and k: thus everything vanishes and we're left with zero again.

Remark 245. *Note that we could have also used that $L = -\vec{p} \times \vec{r}$, which would have simplified things a lot.)*

So now we know that $\vec{r} \cdot \vec{L} = \vec{p} \cdot \vec{L} = 0$, and doing a few analogous calculations allows us to find that $\vec{L} \cdot \vec{r} = \vec{L} \cdot \vec{p} = 0$ as well.

30 April 8, 2020

Concepts of multiparticle states and tensor products have been coming at us pretty quickly! We'll try to talk about some of the important ideas.

The idea of a **tensor product** is both physical and mathematical – there's lots of physical ideas that are reflected in the way we construct the mathematical axioms. Recall that we are trying to create a new space $V \otimes W$ from two vector spaces V, W, and the initial idea is that we want to just write down ordered pairs (v, w), where $v \in V$ and $w \in W$, and make these the objects of our new vector space. But on its own, this doesn't give us very much insight, and it doesn't actually reflect the physics that we care about here – here, we get what is called the **direct product** instead.

One of the main problems is the multiplicative structure of this new vector space: in a direct product, the vectors (v, w) and (av, w) are linearly independent. But in quantum mechanics, we have a single wavefunction for any system – even if we have two or three particles, there's still just one wavefunction. So picking up multiplicative factors of a independently in the v- and w-entries means we're constructing "separate" wavefunctions for v and w, which we don't like.

So that motivates us to say that

$$a(v, w) = (av, w) = (v, aw)$$

for any complex number a (there's no complex conjugation here – we treat V and W the same, so this isn't like having a dual space). And now we introduce the notation $v \otimes w$ instead of (v, w) to emphasize that we're putting the vectors in V and W together with a kind of structure.

And once we introduce linearity in the form

$$(v_1 + v_2) \otimes w = v_1 \otimes w + v_2 \otimes w,$$

$$v \otimes (w_1 + w_2) = v \otimes w_1 + v \otimes w_2,$$

we have a rigorous definition of the tensor product space! In general, if $v \otimes w$ is an element of $V \otimes W$, then we can have objects of the form

$$\sum_i v_i \otimes w_i \in V \otimes W.$$

Fact 246

In relativity, there are objects called **tensors** (which have indices and transform in specific ways). They have some relations with tensor products, but it's not very immediate – the tensor products we're writing here represent objects with two indices.

To be more specific, we can form a basis for our tensor product space $V \otimes W$ of the form $\{e_i \otimes f_j\}$, where the e_i are basis elements of V and the f_J are basis elements of W. So **a general vector in this space** will look like

$$\sum_{i,j} h^{ij}(e_i \otimes f_j),$$

and now the object h^{ij} can be thought of as a two-index tensor. (The position of the indices being "up" instead of "down" is more important when we discuss transformations, though it's not important for our purposes here.) And if we rotate the basis vectors, that will affect the components of h^{ij}, and then we'll need to think a bit more about how tensors transform.

Recall from last lecture that we defined the operator

$$H_T = H_1 \otimes I + I \otimes H_2,$$

and we found that we could write the time-evolution operator

$$e^{-itH_T/\hbar} = e^{-iH_1 t/\hbar} \otimes e^{-iH_2 t/\hbar}.$$

Let's consider some wavefunction in our tensor product space: naively, it might be of the form $\psi_1 \otimes \psi_2$. (Practically, we end up dropping the tensor symbol.) If we apply the time-evolution operator, it seems like the first factor acts on the first wavefunction, and the second factor acts on the second wavefunction. But this isn't quite precise because of **entanglement**! A general wavefunction might look like

$$\sum_i \psi_1^i \otimes \psi_2^i,$$

constructed in such a way that we might not be able to rewrite it as $\psi_1 \otimes \psi_2$ at all. So it doesn't make sense for an operator to act on the individual components of the tensor product, even when we have a Hamiltonian which is acting separately on the two parts.

And tensor products are often used to combine different properties of a single particle: for example, an electron with a position wavefunction might also be a spin 1/2 particle, so we'd have to deal with terms like $\psi(\vec{x}) \otimes \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$. It's good to remember that Hamiltonians on this tensor product space might make the spin and the position function interact in complicated ways!

Let's take a moment now to look at Bell's inequality, statistical mixtures, and EPR. Everything starts when we start with our **singlet spin state**

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|+\rangle|-\rangle - |-\rangle|+\rangle)$$

This is going to show up when we study angular momentum soon: what's important about it is that the total angular momenta S_x, S_y, S_z are all zero (this requires a bit of computation), which means that we can write it as

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\vec{n};+\rangle|\vec{n};-\rangle - |\vec{n};-\rangle|\vec{n};+\rangle)$$

for **any** direction $\vec{n}$ – since we're getting the same state in any direction, it's a rotationally invariant state! So it's very nice to work with and analyze, and now let's turn to the quantity

$$\mathbb{P}(\vec{a}, \vec{b}).$$

To explain what this means, suppose Alice and Bob have the two particles of the singlet state, and Alice measures along $\vec{a}$ while Bob measures along $\vec{b}$. Then we're defining that probability above to be the probability that Alice measures a state along $+\vec{a}$ (instead of $-\vec{a}$), and Bob measures a state along $+\vec{b}$ (instead of $-\vec{b}$). We've derived the value of this before – it's $\boxed{\frac{1}{2}\sin^2\frac{\theta_{ab}}{2}}$, where θ_{ab} is the angle between the vectors $\vec{a}$ and $\vec{b}$.

For example, if the angle is 180°, so that Alice and Bob measure along $\vec{a}$ and $-\vec{a}$ respectively (which is basically measuring along the same axis), the two particles will always be in opposite directions, so either they will both measure $(+)$ or they will both measure $(-)$ (because their orientations are different). As a different example, if Alice and Bob measure along the $\hat{x}$ and $\hat{z}$ directions, we have that $\mathbb{P}(\hat{x}, \hat{z}) = \frac{1}{2}\sin^2\frac{\pi}{4} = \frac{1}{4}$. In this case, the measurements are essentially independent for Alice and Bob.

The statistical mixtures idea from Einstein is basically claiming that we don't actually need any of this probability idea: when we have a bunch of entangled states of this singlet state form, EPR claims that the results that we see are already inherent in the particles before measurement. For example, a $(\hat{z}, -\hat{x})$ particle has attributes that are deterministically prepared, and whenever we put it into a z-direction Stern-Gerlach machine, it will always come out

with a $+\frac{\hbar}{2}$.

To make this consistent with an equation like $\mathbb{P}(\hat{x}, \hat{z}) = \frac{1}{4}$ (which is **experimentally verified**), we need to give a different explanation than quantum mechanics does: instead, we say that one-quarter of the particle pairs in our ensemble of entangled states have particle 1 in the $(\hat{z}, \hat{x})$ direction and particle 2 in the $(-\hat{z}, -\hat{x})$ direction. And this is consistent with the fact that whenever we measure the two particles along some given axis, they are in **opposite** directions (the signs are **correlated**). And we'll also need to have another quarter of our particle pairs have particle 1 in the $[\hat{z}, -\hat{x}]$ state and particle 2 in the $[-\hat{z}, \hat{x}]$ state, and so on. If we set up such an ensemble, this EPR model is indeed consistent with our quantum mechanical observations: there's only one of these four groups such that Alice would measure $-z$ and Bob would measure $+x$, and so on.

The EPR model holds up well whenever we look in two dimensions: we can set up an ensemble of particle pairs along any two directions $\vec{a}, \vec{b}$. It's not until we introduce a third dimension that the problem comes up!

we'll finish with an idea regarding operators on a tensor product space: **we claim that**

$$\mathcal{L}(U \otimes V) = \mathcal{L}(U) \otimes \mathcal{L}(V).$$

This will require a lot of thinking if we haven't seen a tensor product space before. One point that might be puzzling: if $\dim U = \dim V$, we can consider the swap operator

$$S(u \otimes v) = v \otimes u.$$

If the two vector spaces have the same dimension, this is a valid operator. But how can an operator in $\mathcal{L}(U) \otimes \mathcal{L}(V)$ swap vectors between the vector spaces?

31 Angular Momentum, Part 1

Last time, we introduced the quantity of angular momentum, which we showed could be written as

$$\vec{L} = \vec{r} \times \vec{p} = -\vec{p} \times \vec{r}.$$

When we work with angular momentum, we often think about how a vector behaves with rotations.

Definition 247

A vector operator $\vec{u}$ is a **vector under rotation** if

$$[\hat{L}_i, u_j] = i\hbar \varepsilon_{ijk} u_k.$$

We've verified that $\vec{r}$ and $\vec{p}$ are indeed vectors under rotation in our homework. This gives us an important theorem:

Theorem 248

If $\vec{u}, \vec{v}$ are vectors under rotations, then $\vec{u} \cdot \vec{v}$ is a scalar and $\vec{u} \times \vec{v}$ is a vector, both under rotation.

Recall here that $\vec{u} \cdot \vec{v}$ being a scalar means that

$$[\hat{L}_i, \vec{u} \cdot \vec{v}] = 0.$$

This, for example, shows that if we plug in $u, v = \vec{r}$ or $\vec{p}$, we have that

$$[\hat{L}_i, \vec{r}^2] = [\hat{L}_i, \vec{p}^2] = [\hat{L}_i, \vec{r} \cdot \vec{p}] = 0.$$

We can also plug in $\vec{r}$ or $\vec{p}$ into the equation

$$[\hat{L}_i, (u \times v)_j] = i\hbar\varepsilon_{ijk}(u \times v)_k.$$

For example, we can plug in $u = \vec{r}, v = \vec{p}$ (to yield the vector $\vec{L}$), and we'll find that

$$[\hat{L}_i, \hat{L}_j] = i\hbar\varepsilon_{ijk}\hat{L}_k.$$

This time, we didn't need to verify the complicated calculations by moving the xs and ps past each other – we just used the theorem above! And now that $\vec{L}$ is a vector under rotations, we know that

$$\boxed{[\hat{L}_i, \vec{L}^2] = 0}$$

(because $\vec{L} \cdot \vec{L}$ is a scalar). This last property is very important, and we can indeed check that it works by using the algebra directly (we're encouraged to try this out ourselves).

Remark 249. *We know that the spins have basically the same algebra:*

$$[S_i, S_j] = i\hbar\varepsilon_{ijk}S_k,$$

and in that case $\hat{S}^2$ *is just* $S_x^2 + S_y^2 + S_z^2 = 3\left(\frac{\hbar}{2}\right)^2 I$. *So in that case, it was clear that* S_i *always commutes with* $\vec{S}^2$.

The point is that whenever we look at **any** kind of angular momentum, we'll use a generic name J. We'll always have the **algebra of angular momentum**

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k,$$

and that will let us extract the properties of this algebra alone, rather than the specific physics of the system – we'll always have

$$[J_i, \vec{J}^2] = [J_i, J_1^2 + J_2^2 + J_3^2] = 0.$$

This algebra also tells us (in fact equivalently) that

$$\vec{J} \times \vec{J} = i\hbar\vec{J},$$

and **in fact** a vector $\vec{u}$ being a vector under rotation tells us that

$$\boxed{\vec{J} \times \vec{u} + \vec{u} \times \vec{J} = 2i\hbar\vec{u}}.$$

(To derive this, we just expand out the left hand side using index notation.)

Now that we've established some basic identities for vectors under rotations, let's move on to the question of computing

$$(\vec{a} \times \vec{b}) \cdot (\vec{a} \times \vec{b}).$$

We have classical formulas for this, but there are some correction terms: it's not $\vec{a}^2\vec{b}^2 - (\vec{a} \cdot \vec{b})^2$, which is the quantity that we get if we do things classically. To understand what the extra terms are, we'll look at the special case of $\vec{a} \times \vec{b} = \vec{r} \times \vec{p}$: indeed, we have

$$\vec{L}^2 = \vec{r}^2\vec{p}^2 - (\vec{r} \cdot \vec{p})^2 + i\hbar\vec{r} \cdot \vec{p}.$$

We can then solve for $\vec{p}^2$ to find

$$\vec{p}^2 = \frac{1}{\vec{r}^2}\left((\vec{r} \cdot \vec{p})^2 - i\hbar(\vec{r} \cdot \vec{p}) + \frac{1}{\vec{r}^2}\vec{L}^2.$$

(Note here that we've multiplied $\frac{1}{\vec{r}^2}$ by having it multiplied on the **left** instead of the right.) But now remember that

$\vec{p} = \frac{\hbar}{i}\vec{\nabla}$, which means that $\vec{r}\cdot\vec{p} = \frac{\hbar}{i} r\frac{\partial}{\partial r}$ (since we plug in $\vec{r} = r\hat{r}$). We can then simplify the first term on the right hand side above, and we end up with

$$\vec{p}^2 = -\hbar^2 \frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{\vec{r}^2}\vec{L}^2.$$

(We can verify that this is the correct operator by it to a test function $f(r)$). But we also know that this function

$$\vec{p}^2 = -\hbar^2\nabla^2$$

is the Laplacian, which we can expand out as

$$= -\hbar^2\left(\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right).$$

Comparing these two expressions for $\vec{p}^2$ gives us an explicit formula for $\vec{L}^2$: we have the **scalar operator**

$$\vec{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

This means $\vec{L}^2$ only depends on the angular variables, and this makes sense intuitively – it's a rotation, so it shouldn't change $\vec{r}$, and we can say that it acts on functions on the unit sphere! And this isn't something that we can easily find by direct computation: we would have had to write this out in terms of $\hat{L}_x^2, \hat{L}_y^2, \hat{L}_z^2$ and then subsequently write this in terms of $\hat{x}$ and $\hat{p}$ and simplify to angular variables.

What's important is that this gives us an understanding of the Hamiltonian for a central potential

$$H = \frac{\vec{p}^2}{2m} + V(r)$$

(here the potential only depends on $r = |\vec{r}|$). We know the expression for $\vec{p}^2$, and plugging it in here gives us

$$H = \frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{2mr^2}\vec{L}^2 + V(r)$$

This will be the starting point for helping us write the Schrodinger equation for our central potentials – it does indeed depend on our operator $\vec{L}^2$.

Remark 250. *No parentheses in an operator means that an operator acts on* **everything to its right**. *For example,*

$$r\frac{\partial}{\partial r} = \frac{\partial}{\partial r} r - 1$$

(by using it on a test function $f(r)$).

We can now discuss the concept of a **set of commuting observables**. Forming such a set helps us understand the physics attached to a particular Hamiltonian: the **first thing in the list should be the Hamiltonian H itself**, since we do care about the energy of our states.

Now, we know that the $\hat{x}_1, \hat{x}_2, \hat{x}_3$ operators commute with each other, but they don't commute with the Hamiltonian – there's a $\vec{p}^2$ term. Similarly, we can't use $\hat{p}_1, \hat{p}_2, \hat{p}_3$, because there's an x-dependence in the potential and there's no reason in general for this to commute. Similarly $\vec{r}^2$ or $\vec{p}^2$ or $r\cdot p$ are bad, but the operator $\vec{r}\times\vec{p}$ is interesting: let's try using the operators

$$\hat{L}_1, \hat{L}_2, \hat{L}_3.$$

We can check that the angular momentum commutes with the Hamiltonian: remember that the $\hat{L}_i$s commute with $\vec{p}^2$ from the discussion above, and $V(r)$ is a function of $\vec{r}^2 = |\vec{r}|^2$. So anything that is a function of r must commute with all of the $\hat{L}_i$s, so **our Hamiltonian commutes with the angular momentum operators**. This is then an **angular**

momentum conservation statement, because we know that

$$\frac{d}{dt}\langle \hat{L}_i \rangle = \langle [H, \hat{L}_i] \rangle = 0.$$

So now we want to add $\hat{L}_1, \hat{L}_2, \hat{L}_3$ to our list of observables, but they don't commute with each other! We can only add one, and the convention is to use $\boxed{\hat{L}_3}$. Finally, we can add the operator $\boxed{\vec{L}^2}$: this indeed commutes with all of the $\hat{L}_i$s.

Proposition 251

The universal set of commuting observables for a central potential is

$$\{H, \hat{L}_3, \vec{L}^2\}.$$

And we can always add funny observables to this set, like spin, if that's a property of the particles themselves. (We'll see that there are many states with the same $\hat{L}_3$ but different total angular momenta, so we do indeed need $\vec{L}^2$ to describe our system. But it's important to note that we can't actually measure different components of the angular momentum at once, because the operators don't commute!)

We want to learn about the **kind of states** that can exist in a system with the action of operators that behave like J_i, which are also **Hermitian**. We'll be able to derive powerful results, even in the case where systems have nothing to do with angular momentum. The first step is to introduce the operators

$$\hat{J}_\pm = J_1 \pm i J_2,$$

and note that

$$\boxed{J_+ J_-} = (J_1 + iJ_2)(J_1 - iJ_2) = J_1^2 + J_2^2 + i[J_2, J_1] = \boxed{J_1^2 + J_2^2 + \hbar J_3}.$$

Similarly, we have that

$$\boxed{J_- J_+ = J_1^2 + J_2^2 - \hbar J_3},$$

and we can use these to find the commutator

$$[J_+, J_-] = (J_1^2 + J_2^2 + \hbar J_3) - (J_1^2 + J_2^2 - \hbar J_3) = 2\hbar J_3,$$

as well as

$$\vec{J}^2 = J_1^2 + J_2^2 + J_3^2 = J_+ J_- + J_3^2 - \hbar J_3.$$

These kinds of identities are pretty simple – we're deciding that we like J_+ and J_- more than J_1 and J_2, and we're trying to figure out everything we can about them. Two other nice results we can find are

$$[J_3, J_+] = [J_3, J_1 + iJ_2] = i\hbar J_2 + \hbar J_1 = \hbar J_+,$$

and similarly

$$[J_3, J_-] = -\hbar J_-.$$

This should look similar to the harmonic oscillator commutator

$$[N, a^\dagger] = a^\dagger, \quad [N, a] = -a.$$

(Here, we've used the fact that our operators J_1, J_2 are Hermitian, so J_+ and J_- are actually adjoints of each other.) In the harmonic oscillator case, $a^\dagger$ increased the number eigenvalue of N, and a decreased it – we'll see something

similar in our new system – J_+ will increase the z-component of angular momentum, and J_- will decrease it.

Here's where we need to make a physical declaration: **there exist states** in this setup that we've been creating. In the harmonic oscillator case, we create infinitely many states above the ground state – this is connected to the idea that the operators $\hat{x}$ and $\hat{p}$ cannot be represented with finite-dimensional matrices. But in the angular momentum case, we're actually going to find that there are **finite-dimensional matrix representations!**

So our set of commuting Hermitian operators contains (replacing J_3 with J_z now)

$$J^2, J_z.$$

Since these are Hermitian commuting operators, they are simultaneously diagonalizable, and we're saying that **there are states** that represent this diagonalization: our vector space should contain a list of orthogonal vectors that are eigenstates of both operators, and in fact we can make an **orthonormal basis** for the whole vector space.

Definition 252

Define the orthonormal basis states $|j, m\rangle$ such that

$$\vec{J}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle , \quad \vec{J_z} |j, m\rangle = \hbar m |j, m\rangle ,$$

where $j, m \in \mathbb{R}$.

It seems reasonable at first to put

$$\vec{J}^2 |j, m\rangle = \hbar^2 j^2 |j, m\rangle , \quad \vec{J_z} |j, m\rangle = \hbar m |j, m\rangle .$$

But this isn't very convenient – we'll see later why our definition makes the algebra work out better. And we'll see soon also that j, m will get quantized.

To understand our definition a little more, we can evaluate

$$\langle j, m | J^2 | j, m \rangle = \hbar^2 j(j+1).$$

(We're sort of assuming that our states will be quantized so we don't need a delta function normalization factor.) But we also know that

$$\langle j, m | J^2 | j, m \rangle = \sum_i \langle j, m | J_i J_i | j, m \rangle = \sum_i ||J_i |j, m\rangle||^2 \geq 0,$$

where we've used the fact that J_i is Hermitian, so by definition we must have

$$j(j+1) \geq 0,$$

which means that we can label (parameterize) our states uniquely by either restricting our domain to $j \geq 0$ or $j \leq -1$.

The next step is to understand how J_+ and J_- act on these states: first, note that J_+ and J_- commute with J^2, because J_1, J_2, J_3 commute with J^2 and we just have linear combinations of them, which means that J_+, J_- **do not change the eigenvalue of J^2 for a given state**:

$$J^2(J_\pm |j, m\rangle) = J_\pm(J^2 |j, m\rangle) = \hbar^2 j(j+1) J_\pm |j, m\rangle .$$

So $J_\pm |j, m\rangle$ is also a state with the **same (eigen)value of J^2**, which means it must correspond to the same value of j:

$$J_\pm |j, m\rangle \sim |j, m'\rangle .$$

So we want to see how $J_\pm$ affect m, and here's where we have a bit of a calculation. Introducing a J_z into the expression,

$$J_z J_\pm |j,m\rangle = ([J_z, J_\pm] + J_\pm J_z)|j,m\rangle ,$$

and we've calculated the commutator before, and we can let J_z act on the state, to find that

$$= (\pm\hbar J_\pm + \hbar m J_\pm)|j,m\rangle = \hbar(m\pm 1)J_\pm |j,m\rangle .$$

Therefore, the operator J_z acts on $J_\pm |j,m\rangle$ to get an eigenvalue of $\hbar(m\pm 1)$, which means by definition of J_z that our state satisfies

$$J_\pm |j,m\rangle = c_\pm(j,m)|j,m\pm 1\rangle$$

for some constant of proportionality $c_\pm(j,m)$ to be determined. (We can label our states so that the js line up.) To find these constants, we take the dagger of the equation above:

$$\langle j,m| J_\mp = c_\pm^*(j,m)\langle j;m\pm 1| ,$$

and now putting these together to yield an inner product tells us that

$$\langle j,m|J_\mp J_\pm|j,m\rangle = |c_\pm(j,m)|^2 \cdot 1.$$

The left hand side can be calculated by using the formulas we've derived before:

$$|c_\pm(j,m)^2|^2 = \langle j,m\big|J^2 - J_3^2 \mp \hbar J_3\big|j,m\rangle = \hbar^2(j(j+1) - (m^2 \pm m)).$$

We've now found our constants, and taking the square root yields

$$c_\pm(j,m) = \hbar\sqrt{j(j+1) - m(m\pm 1)}$$

(we can ignore the extra phase terms, since they don't do anything physically). And **this is the reason** why we use $j(j+1)$ – it makes it easier to compare ms and js – and now what's important is that this quantity $j(j+1) - m(m+1)$ **must be nonnegative**, so that $||J_+|j,m\rangle||^2$ is a nonnegative number. This means

$$j(j+1) - m(m+1) \geq 0 \implies m(m+1) \leq j(j+1).$$

The right hand side of this is some nonnegative number, and the left hand side is a quadratic function of m. We have equality when $m = j$ but also when $m = -j-1$, so the required condition is that m must be between the two points:

$$-j-1 \leq m \leq j.$$

Similarly, the states $J_- |j,m\rangle$ must also have nonnegative norm, which means that

$$j(j+1) - m(m-1) \geq 0.$$

An analogous argument tells us that we must have

$$-j \leq m \leq j+1,$$

and now **both inequalities must hold**:

$$\boxed{-j \leq m \leq j}.$$

But we can say a little more than that: J_+ is supposed to increase m, so we run into trouble at some point. (Intuitively,

we should think of j as the "length" of the J^2 vector, and m is the J_z component.) Indeed, when $m = j$, we have that $j(j+1) - m(m+1) = 0$, which means that our state vanishes completely beyond that point! The same thing is true for $m = -j$ – we can't get to smaller values of m.

And now, we can think of this as having a ladder of states from $m \in [-j, j]$, where J_+ and J_- increase or decrease m by 1. Any state in our system created in this way must terminate at $-j$ or j on the ends for consistency, which in particular means that the distance $j - (-j) = 2j$ **must be an integer**. And now we've gotten the discretization of our states – this indeed tells us that our particles can have spin or angular momentum of 0, $\frac{1}{2}$, 1, and so on! And now we've arrived at the main result of angular momentum:

Theorem 253

The values of the angular momentum can be $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$, with a total of $1, 2, 3, 4, \cdots$ possible values for m, respectively.

For example, the only state for $j = 0$ is $|0, 0\rangle$, the only two states for $j = \frac{1}{2}$ are $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$ and $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$, the only three states for $j = 1$ are $|1, -1\rangle, |1, 0\rangle, |1, 1\rangle$, and so on.

The punchline of this is that we were working with an infinite-dimensional vector space, but it breaks down into states of half-integer j, and we need to figure out which values of j are actually possible. Central potentials will have $0, 1, 2, 4$, spins will have $\frac{1}{2}$, and so on.

Example 254

Consider a two-dimensional simple harmonic oscillator, where we have $a_x, a_y, a_x^\dagger, a_y^\dagger$ as our operators.

This may seem strange – we have a two-dimensional oscillator even though we've been talking about three-dimensional angular momentum. But we're going to get an angular momentum that pops out here – it's abstract, but it has important properties!

We can start by looking at the spectrum: we have the ground state $|0\rangle$, the first excited states $a_x^\dagger |0\rangle$ and $a_y^\dagger |0\rangle$, the second excited states $a_x^\dagger a_x^\dagger |0\rangle$, $a_x^\dagger a_y^\dagger |0\rangle$, and $a_y^\dagger a_y^\dagger |0\rangle$, and so on. In general, there are $(n+1)$ states in the nth excited level

$$(a_x^\dagger)^n |0\rangle, \quad (a_x^\dagger)^{n-1} a_y^\dagger |0\rangle, \quad \cdots, \quad (a_y^\dagger)^n |0\rangle.$$

And this actually relates to having $1, 2, 3, 4, \cdots$ states in the varying levels of j – let's see how that plays out. We can start by introducing the operators

$$a_R = \frac{1}{\sqrt{2}}(a_x - i a_y), \quad a_L = \frac{1}{2}(a_x + i a_y),$$

as well as the number operators

$$N_R = a_R^\dagger a_R, \quad N_L = a_L^\dagger a_L.$$

These new "left" and "right" operators don't mix, and now we can rewrite our excited states: we have the ground state $|0\rangle$, the first excited states $a_R^\dagger |0\rangle$ and $a_L^\dagger |0\rangle$, the second excited states $a_R^\dagger a_R^\dagger |0\rangle$, $a_R^\dagger a_L^\dagger |0\rangle$, and $a_L^\dagger a_L^\dagger |0\rangle$, and so on. (This is completely analogous to the result above.) But remember that we can compute the angular momentum in the z-direction

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = \hbar(N_R - N_L),$$

and now we can see what values of $\hat{L}_z$ we have here. The ground state $|0\rangle$ has $\hat{L}_z = 0$, the first excited states have $\hbar$ and $-\hbar$ respectively, the second excited states have $2\hbar, 0, -2\hbar$ respectively, and so on. This isn't exactly the

correct values of m that we derived earlier, but we can turn to another aspect of this theory: remember that J_+ keeps increasing the angular momentum until we annihilate our state $|j,j\rangle$, so we should see if something similar happens here. So our corresponding J_+ operator should actually be

$$L_+ = a_R^\dagger a_L,$$

which kills the top state $(a_R^\dagger)^n |0\rangle$ for any n, and then the corresponding dagger operator is

$$L_- = a_L^\dagger a_R.$$

Indeed, this kills the bottom state $(a_L^\dagger)^n |0\rangle$ for any n, and now we have all of the important parts except for one conceptual step: there is no angular momentum in the two-dimensional plane, so we'll instead introduce an **abstract angular momentum**

$$\hat{J}_z = \frac{\hbar}{2}(N_R - N_L).$$

And now things seem to fit: the magnitude of of J_z is 0 on our ground state, $-\frac{\hbar}{2}$ and $\frac{\hbar}{2}$ on the first excited states, and $-\hbar, 0, \hbar$ on the second excited states. This now means we can introduce our other angular momentum operators

$$J_+ = \beta a_R^\dagger a_L, \quad J_- = \beta a_L^\dagger a_R,$$

such that we have J_x, J_y, J_z satisfying the **algebra of angular momentum**. Once we verify that we can find such a β, our states do indeed need to organize themselves into representations of that angular momentum! So our two-dimensional harmonic oscillator has **all spin representations**: $j = 0, \frac{1}{2}, 1, \cdots$. And the only thing we have to check is that the J_is commute with the Hamiltonian $N_L + N_R$. This is the first example of a hidden symmetry in a physical problem that we've encountered, and it allows us to explain how the degeneracies in energy levels can fall into angular momentum representations.

32 April 13, 2020

We've been discussing tensor products recently, and there's a lot of properties that we'll want to go over and understand well. Because of the homework due tomorrow, we'll finish some of the discussion from last time first.

As a reminder, we were discussing operators on tensor product spaces last time: for example, the operator $H \otimes I \in \mathcal{L}(V \otimes W)$ acts on a vector in our space via

$$(H \otimes I)(v \otimes w) = Hv \otimes w.$$

Last time, we stated a general result:

Proposition 255

$\boxed{\mathcal{L}(U \otimes V) = \mathcal{L}(U) \otimes \mathcal{L}(V)}$: The vector space of linear operators can be written as the tensor product of the individual linear operator spaces of V and W.

This might be a bit disorienting, but it's important if we (for example) care about finding the most general operator on a vector space.

We'll explain this in the case of a finite-dimensional vector space. We can think of linear operators on a vector

space U of dimension N as matrices, spanned by the basis matrices:

$$\mathcal{L}(U) = \text{span}\left\{\left|e_i^U\right\rangle\left\langle e_j^U\right|\right\}, \quad 1 \le i, j \le N.$$

Here, $\left|e_i^U\right\rangle\left\langle e_j^U\right|$ represents the matrix with a 1 in the (i, j) entry and a 0 everywhere else. Similarly, we can write

$$\mathcal{L}(V) = \text{span}\left\{\left|e_k^V\right\rangle\left\langle e_\ell^V\right|\right\}, \quad 1 \le k, \ell \le M.$$

And now if we try to write down the basis vectors for $\mathcal{L}(U) \otimes \mathcal{L}(V)$, recall that we should tensor the basis vectors for $\mathcal{L}(U)$ and $\mathcal{L}(V)$ together: this gives us MN basis vectors in total. Thus,

$$\mathcal{L}(U) \otimes \mathcal{L}(V) = \text{span}\left\{\left|e_i^U\right\rangle\left\langle e_j^U\right| \otimes \left|e_k^V\right\rangle\left\langle e_\ell^V\right|\right\}, 1 \le k, \ell \le M, 1 \le i, j \le N.$$

So the most general linear operator in $\mathcal{L}(U) \otimes \mathcal{L}(V)$ is a linear combination of the basis vectors, meaning it is of the form

$$\boxed{S = \sum_{i,j,k,\ell} c_{i,j,k,\ell}\left|e_i^U\right\rangle\left\langle e_j^U\right| \otimes \left|e_k^V\right\rangle\left\langle e_\ell^V\right|},$$

where the $c_{i,j,k,\ell}$ are numbers.

That accounts for the right hand side in the proposition above, and now let's try to look at the left side. An example we gave last time of an operator on $U \otimes V$ is the **swap operator** in the case where $U = V$.

$$T(u \otimes v) = v \otimes u.$$

A good way to understand linear operators is to let them act on basis vectors: thus, let's apply T to $\left|e_p^U\right\rangle \otimes \left|e_q^V\right\rangle$. Then

$$T\left|e_p^U\right\rangle \otimes \left|e_q^V\right\rangle = \left|e_q^U\right\rangle \otimes \left|e_p^V\right\rangle$$

basically just swaps the indices, which means that in general, we have

$$T(u \otimes v) = T\left(u^p\left|e_p^U\right\rangle \otimes v^q\left|e_q^V\right\rangle\right)$$

(where we're summing over p, q) and then we can bring the constants u^p, v^q outside and swap the indices to get

$$= u^p v^q T\left(\left|e_p^U\right\rangle \otimes \left|e_q^V\right\rangle\right) = u^p v^q\left|e_q^U\right\rangle\left|e_p^V\right\rangle.$$

Looking at the two inner terms, notice that $v^q\left|e_q^U\right\rangle$ represents a vector v in the vector space V. Similarly, the two outer terms $u^p\left|e_p^V\right\rangle$ represents the vector u in the vector space U, and now we indeed have $T(u \otimes v) = v \otimes u$, as desired!

What this illustrates is that we indeed only need to define T on the basis vectors, which (we'll soon show) means we just need to define our linear operator on U and V separately. The punchline now is that because the operator $A = |j\rangle\langle i|$ gets us from $|i\rangle$ to $|j\rangle$, we can write

$$\boxed{T = \sum_{p,q}\left|e_q^U\right\rangle \otimes \left|e_p^V\right\rangle\left\langle e_p^U\right| \otimes \left\langle e_q^V\right|}.$$

But comparing this to the boxed equation for S above might make this look more familiar: we can rearrange this as

$$= \sum_{p,q}\left|e_q^U\right\rangle\left\langle e_p^U\right| \otimes \left|e_p^V\right\rangle\left\langle e_q^V\right|$$

(by the definition of composition of linear operators). But now we've understood what's going on: (1) the boxed

equation for T represents our linear operator as an element of $\mathcal{L}(U \otimes V)$, because we put a ket basis vector next to a bra basis vector and sum over all possibilities. But (2) the line immediately below that has rewritten the linear operator so that we're actually tensoring together a linear operator in $\mathcal{L}(U)$ and a linear operator in $\mathcal{L}(V)$ (and taking linear combinations)! In generality, any operator

$$S = \sum_{i,j,k,\ell} c_{i,j,k,\ell} \left|e_i^U\right\rangle \left\langle e_j^U\right| \otimes \left|e_k^V\right\rangle \left\langle e_\ell^V\right|,$$

which lives in $\mathcal{L}(U) \otimes \mathcal{L}(V)$, can be rewritten as

$$S = \sum_{i,j,k,\ell} c_{i,j,k,\ell} \left(\left|e_i^U\right\rangle \otimes \left|e_k^V\right\rangle\right) \left(\left\langle e_j^U\right| \otimes \left\langle e_\ell^V\right|\right),$$

and now the $\otimes$ symbol is "tensoring our vectors, not our operators," so this now lives in $\mathcal{L}(U \otimes V)$.

Fact 256

Remember that when we write $\mathcal{L}(U) \otimes \mathcal{L}(V)$, we mean that we take **linear combinations** of (operators in U) tensored with (operators in V). We can't always write any operator as $S \otimes T$ for $S \in \mathcal{L}(U)$ and $T \in \mathcal{L}(V)$, just like in the case with entangled particles.

An interesting question: **what are the coefficients** $c_{i,j,k,\ell}$ for our swap operator T here? Remember that coefficients correspond to matrix entries, so we'll write our swap operator T in matrix form. Let's do the case $d = 2$, so our basis vectors are $|+\rangle$ and $|-\rangle$. We know that one term of T looks like

$$\boxed{|+\rangle \otimes |+\rangle \langle +| \otimes \langle +|} = |+\rangle \langle +| \otimes |+\rangle \langle +|,$$

and the other three terms look like (dropping the $\otimes$ on the left side now)

$$\boxed{|-\rangle |+\rangle \langle +| \langle -|} = |-\rangle \langle +| \otimes |+\rangle \langle -|,$$

$$\boxed{|+\rangle |-\rangle \langle -| \langle +|} = |+\rangle \langle -| \otimes |-\rangle \langle +|,$$

$$\boxed{|-\rangle |-\rangle \langle -| \langle -|} = |-\rangle \langle -| \otimes |-\rangle \langle -|.$$

Adding these four things together gives us the whole operator T – remember that this is telling us the action on each of the $2 \times 2 = 4$ basis vectors, so it determines everything. And now we can write everything in matrix form using the right hand sides:

$$T = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix},$$

and we have a definition for the **tensor product of matrices** (which is consistent with the way we define our tensor product): the idea is that $A \otimes B$ can be thought of as multiplying in copies of B with each entry of A. This gives us

$$= \begin{bmatrix} 1 & 0 & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix} + \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot \end{bmatrix} + \begin{bmatrix} \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & 1 & 0 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix} + \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & 0 & 1 \end{bmatrix}.$$

where the dots represent A having component 0, so the whole copy of B vanishes. So

$$T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

and thus this tells us that four of the sixteen coefficients $c_{i,j,k,\ell}$ are 1s, while the other twelve are 0s.

To finish, we can talk a bit about **cloning**: we've studied teleportation in lecture, in which Alice can teleport a quantum state to Bob by just sending two bits. In such a case, Alice does not have the state anymore – Bob's state is rearranged at the same time that Alice's state is damaged beyond repair. So if we want to talk about a cloning machine, we would take a state $|\psi\rangle = a|+\rangle + b|-\rangle$, put it through a machine, and end up with two copies of that state.

Well, the machine cannot create new particles out of thin air, so we must start with a second particle in some fixed blank state $|\alpha\rangle$ (just like with a photocopy machine). So this machine takes in two particles $|\psi\rangle$ and $|\alpha\rangle$, and we need a **linear operator** U such that we end up with two identical states:

$$U|\psi\rangle \otimes |\alpha\rangle = |\psi\rangle \otimes |\psi\rangle.$$

Then the **no cloning theorem** tell us that there is no such unitary operator U that can do this for all states! We'll discuss this more later on.

33 Angular Momentum, Part 2

Last lecture, we discussed (with an algebraic analysis) states $|j,m\rangle$, which we'll now label with $|\ell,m\rangle$ because we're talking about **orbital** angular momentum. With orbital angular momentum, we can't actually have half-integer values of j. In fact, systems like spin states don't have wavefunctions in this sense; only states of integer angular momentum have wavefunctions, and those are the spherical harmonics we'll be discussing today.

Remember that our indexing $|\ell,m\rangle$ has $\ell \geq 0$ and $-\ell \leq m \leq \ell$, both integers: then we know that

$$L^2|\ell,m\rangle = \hbar^2\ell(\ell+1)|\ell,m\rangle, \quad L_z|\ell,m\rangle = \hbar m|\ell,m\rangle.$$

To approach the problem of finding these wavefunctions, remember that we already did some work in constructing the L^2 operator. Specifically, we have

$$\vec{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

and (we didn't do this explicitly, but it's a similar derivation)

$$L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = \frac{\hbar}{i}\frac{\partial}{\partial\phi}.$$

(We should think of this as rotating around the z-axis, so it changes phi but not theta.) We also defined the operators $L_\pm$ last time, and we can also write those in angular form:

$$L_\pm = \hbar e^{\pm i\phi}\left(i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi} \pm \frac{\partial}{\partial\theta}\right).$$

This takes a bit of algebra, but we can find it in various books, and the whole point is that we have differential operators

that act on theta and phi and **don't care about the radius**. So mathematical physicists invent **spherical harmonics** of the form $Y_{\ell m}(\theta, \phi)$, defined such that

$$L^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m}$$

and

$$L_z Y_{\ell m} = \hbar m Y_{\ell m},$$

where we think of L^2 and L_z as the differential operators in θ, ϕ. We can think of these functions as being wavefunctions for our states $|\ell, m\rangle$, and this is the natural way to think of them:

$$Y_{\ell m} = \langle \theta, \phi | \ell, m \rangle ,$$

which is the analogous idea of saying that $\psi(x) = \langle x|\psi\rangle$, only with angular coordinates. In order to extract some more properties so that the identification here is natural, we can start with the **completeness relation**. In three dimensions, we know that

$$\int d^3\vec{x} \, |\vec{x}\rangle \langle \vec{x}| = 1$$

is a completeness relation for position states, and our goal is to do this for spherical coordinates: we find that

$$\int dr(r d\theta)(r \sin\theta d\phi) \, |r\theta\phi\rangle \langle r\theta\phi| = 1.$$

We want to ignore the part that happens with r, so we'll write this as

$$\int d\theta \sin\theta d\phi \, |\theta\phi\rangle \langle\theta\phi| \int dr r^2 \, |r\rangle \langle r| = 1,$$

where we're basically "splitting up" the states in the orthogonal angular directions and the radial direction. But the two integrals here don't talk to each other, so we can say that the first integral acts as a completeness relation for things that just depend on θ and ϕ: in other words, we'll **postulate** that we have a completeness relation

$$\int d\theta \sin\theta d\phi \, |\theta\phi\rangle \langle\theta\phi| = 1.$$

Rewriting, since we know that

$$\int_0^\pi d\theta \sin\theta d\phi \int_0^{2\pi} d\phi = -\int_1^{-1} d(\cos\theta) \int_0^{2\pi} d\phi,$$

we can rewrite the term $\int_{-1}^1 d(\cos\theta) \int_0^{2\pi} d\phi = \int d\Omega$ as the **integral over solid angle**, and now we just know that

$$\int d\Omega \, |\theta\phi\rangle \langle\theta\phi| = 1.$$

So when we're trying to define spherical harmonics – the $|\ell, m\rangle$ states – we know they are orthogonal, meaning

$$\langle \ell' m' | \ell m \rangle = \delta_{\ell\ell'} \delta_{mm'}.$$

Remember that orthogonality is guaranteed here because we have Hermiticity and distinct eigenvalues. Specifically, we can always ask the overlap to be

$$\langle \ell' m' | \ell m \rangle = \int d\Omega \, \langle \ell' m' | \theta\phi \rangle \langle \theta\phi | \ell m \rangle = \int d\Omega Y^*_{\ell' m'}(\theta, \phi) Y_{\ell m}(\theta, \phi) = \delta_{\ell\ell'} \delta_{mm'}.$$

And from here, we can construct the wavefunctions in various ways from the quantum mechanical intuition: we can start by building the state $Y_{\ell\ell}$, because L_+ kills this state, meaning the differential equation is particularly simple.

From there, we can find $Y_{\ell,\ell-1}$ and so on, using the lowering operator repeatedly. But the formulas are messy and normalization is annoying, so we won't talk about that much – if we ever need a special harmonic, we can just look in a textbook.

So now we can discuss the **radial equation**: suppose we have a Hamiltonian

$$H = \frac{\vec{p}^2}{2m} + V(r),$$

which we can rewrite as

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2} + \frac{1}{2mr^2}\vec{L}^2 + V(r).$$

We'll solve the Schrodinger equation for this Hamiltonian using **separation of variables**: we'll write our wavefunctions satisfying $H\psi = E\psi$ as

$$\psi_{E,\ell,m}(\vec{x}),$$

in terms of its energy and two angular momentum parameters. This isn't going to be exactly correct, but we'll do the following idea first: we want to rewrite this as a product

$$f_{E,\ell,m}(r)Y_{\ell m}(\theta,\phi).$$

This is our initial ansatz, and we can try plugging this into the Schrodinger equation: **we can cancel a $Y_{\ell m}$ term throughout**, and we're left with

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(rf_{E\ell m}) + \frac{\hbar^2}{2mr^2}\ell(\ell+1)f_{E\ell m} + V(r)f_{E,\ell,m} = Ef_{E\ell m}.$$

where the second term comes from the definition of $Y_{\ell m}$. But now this differential equation doesn't depend on m at all (the m in the denominator is a mass, not the label m for our states), so ψ is a function of r, indexed by E and ℓ, and now we can multiply through by r to find that

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}(rf_{E\ell}) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}(rf_{E\ell}) + V(r)(rf_{E\ell}) = E(rf_{E\ell}).$$

This motivates the definition of

$$U_{E\ell}(r) = rf_{E\ell}(r),$$

and now our differential equation is

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2u_{E\ell}}{dr^2} + \left(V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)U_{E\ell} = EU_{E\ell}}.$$

This is known as the **radial equation**, and the expression $\left(V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)$ is often called the **effective potential**. The function f is now of the form $\frac{U_{E\ell}(r)Y_{\ell m}(\theta,\phi)}{r}$, and we can find U by solving a one-dimensional Schrodinger equation with **effective potential depending on ℓ**. So the central potential question is actually infinitely many Schrodinger equations!

From here, the first thing we'll discuss is the question of **normalization and boundary conditions**. If we want to normalize a wavefunction, we want

$$\int d^3x|\psi_{E\ell m}(\vec{x})|^2 = 1,$$

and we can convert this into angular variables and plug in our separated functional form f to get

$$\int d\Omega \int r^2 dr \frac{|U_{E,\ell}|^2}{r^2}Y^*_{\ell m}(\theta,\phi)Y_{\ell,m}(\theta,\phi) = 1.$$

(The r^2 in the denominator comes from squaring $\frac{U(r)}{r}$.) But now the angular integral is just 1 by orthonormality – it corresponds to the case where $\ell = \ell'$ and $m = m'$. And the r^2s cancel out, and we have a nice condition for normalization:

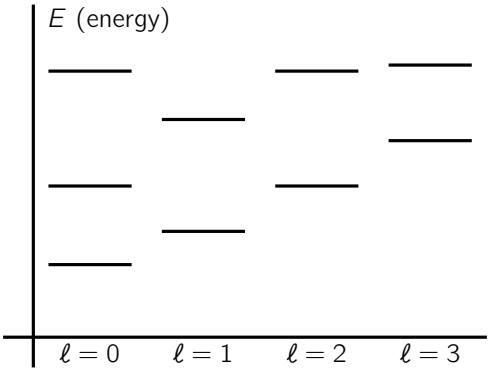
$$\int_0^\infty dr |U_{E\ell}(r)|^2 = 1.$$

So in a way, U does really play the role of a wavefunction on a line – its squared integral should be 1.

Proposition 257

This leads us to a main point, which is something that should stick in our head: when we want to organize our spectrum for such a problem, we should draw a plot with ℓ on the horizontal axis and E on the vertical.

Most of the time, we'll have bound states, and that means we'll have states for values of ℓ, m and some energies E. For each of $\ell = 0, 1, 2, 3, \cdots$ (which we can draw along the horizontal axis as a histogram), we'll typically have E being quantized, and we won't have any degeneracies because we have a **nondegenerate spectrum for bound states**. This means that we can draw a discrete set of lines for each value of ℓ, with each one corresponding to an eigenstate: we'll end up with a sequence of horizontal lines above each value of ℓ.



For the first column $\ell = 0$, we can then label the energies starting from the ground state as $E_{1,0}, E_{2,0}, \cdots$, and we find these energies by solving the Schrodinger equation with $\ell = 0$. And then we can do the same with the second column, $\ell = 1$: since the ℓ potentials are larger, the energies will be higher (or at least the ground state energy will be higher). We can then label them $E_{1,1}, E_{2,1}, \cdots$, and then we can repeat with higher and higher levels of ℓ. And no two lines will coincide in each column, because no two bound states with the same value of ℓ will have the same energy as well.

But that doesn't mean that there's only one state for each line that we draw! For example, remember that $\ell = 1$ comes with three different possible values of m, and the energy doesn't depend on m. So the energy of the $E_{1,1}$ multiplet actually corresponds to **three states**. Similarly, $E_{1,2}$ corresponds to five states, and so on.

Fact 258

From here, our next question will be studying the behavior of the wavefunction more carefully: we'll see what happens when $r \to 0$.

It seems like normalization is the main thing we care about – perhaps, as long as the function doesn't diverge near 0, anything will be okay. But it turns out this is false, and we actually need $\boxed{\lim_{r\to 0} U_{E\ell}(r) = 0}$ as well. To understand why this is the case, let's look at a simple case where something goes wrong: **suppose that**

$$\lim_{r\to 0} U_{E\ell}(r) = c.$$

Normalization isn't a problem here, so something else must be the problem – let's look at the case where $\ell = 0$ for simplicity, and now our wavefunction corresponding to U_{E0} looks like

$$\psi_{E00} = c\frac{U_{E0}}{r}$$

($m = 0$ if $\ell = 0$), where we've used the fact that Y_{00} is just a constant. But now ψ looks like $\frac{c'}{r}$ as ψ approaches 0, and this is bad: the Schrodinger equation tells us that $H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + \cdots$, and the Laplacian term is $\nabla^2\frac{1}{r} = -4\pi\delta(\vec{x})$. An there's no reason to expect there to be a delta function in the potential, because that gives us infinitely many bound states. Thus we can't cancel that term in the Schrodinger equation, and thus we can't get wavefunctions to work out in this case.

We can say something more about these potentials, too:

Fact 259

We're going to look at cases where **centrifugal barrier**, which is the $\frac{\hbar^2\ell(\ell+1)}{2mr^2}$ term of the effective potential, must dominate when r goes to 0.

So $V(r)$ might look like $\frac{1}{r}$, but it's not $\frac{1}{r^3}$ or something worse. Then we can look at the differential equation, and now $V(r)$ and U are less important than $\frac{U}{r^2}$ as r goes to 0. Thus, **at leading order**, we just keep the kinetic term:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}U_{E\ell} + \frac{\hbar^2\ell(\ell+1)}{2mr^2} = 0.$$

Simplifying constants, we end up with

$$\frac{d^2U_{E\ell}}{dr^2} = \frac{\ell(\ell+1)}{r^2}U_{E\ell}.$$

It turns out that the solution here is of the ansatz $U_{E\ell} = r^s$, and plugging this in yields either $s = \ell + 1$ or $s = -\ell$. But the latter case looks like $U_\ell \sim \frac{1}{r^\ell}$, and this does not go to 0 as $r \to 0$ as long as $\ell \geq 1$.

Proposition 260

When the centrifugal barrier dominates, the wavefunction will look like $\boxed{U_{E\ell} \sim r^{\ell+1}}$ near $r = 0$.

And because our wavefunction is in terms of $f = \frac{U}{r}$, this means that

$$f_{E\ell} \sim r^\ell,$$

which means that f behaves like a constant for $\ell = 0$. Physically, this means that when we have zero orbital angular momentum, there is some chance of having the particle near the origin. However, **for any** $\ell > 0$, f must vanish, and this explains the name **centrifugal barrier** – we can't get too close to $r = 0$.

Fact 261

Next, we can consider the case where r goes to infinity: again, we need to be careful what we're assuming, and the analysis here is richer than we can state quickly.

We'll just consider some simple cases: **in the case where** $V(r) = 0$ **for all** $r > r_0$**, or when** $rV(r) \to 0$ **as** r **goes to infinity**, we can ignore the contribution for V at large r.

Remark 262. *These two cases do not account for the hydrogen atom, which has a potential of* $\frac{1}{r}$*, so we'll need to figure out how to deal with that separately (and we will soon).*

The point of this special case is that $V(r)$ dependence is less important than the centrifugal term, and now we just have

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}U_{E\ell} = EU_{E\ell}.$$

There are now two cases: when $E < 0$, we have a decaying exponential

$$U_{e\ell} \sim \exp\left(-\sqrt{\frac{2m|E|}{\hbar^2}}r\right)$$

(it turns out that the hydrogen atom will get a power of r multiplied in here somewhere), and when $E > 0$, we have oscillating solutions

$$U_E = \exp\left(\pm ikr\right), \quad k = \sqrt{\frac{2mE}{\hbar^2}}.$$

With this, it's easy to make qualitative plots of how our solutions look: we know how it looks at the origin (proportional to r^ℓ), and far away (they then decay exponentially), and this is the kind of study that we do in 8.04.

Example 263

We'll now start to solve the radial equation with specific potentials: we'll begin with the free particle.

This is more nontrivial in spherical coordinates than it is in the Cartesian case! We know that particles in the usual case have a fixed energy and momentum, so we usually label them by three momenta or with an energy and direction. But we won't be using momentum eigenstates for our spherical coordinates, and this method will help us solve more complicated problems too.

To be more precise, we can label the states of a free particle with three numbers: sometimes we use p_1, p_2, p_3 (for the momentum) or E, θ, ϕ (for the energy). **In our case**, we'll be using (E, ℓ, m), and it turns out that we'll end up with the same number of states anyway.

Our differential equation here looks like

$$-\frac{\hbar^2}{2m}\frac{d^2U_{E\ell}}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2mr^2}U_{E\ell} = EU_{E\ell}.$$

(Remember that the V term is just zero, but the effective potential is still nonzero.) Canceling the constants, this just becomes

$$\boxed{-\frac{d^2U_{E\ell}}{dr^2} + \frac{\ell(\ell+1)}{r^2}U_{E\ell} = k^2U_{E\ell}},$$

where E is a positive energy, meaning k is defined as above. This equation is interesting – it looks like a typical one-dimensional Schrodinger equation, so the energy seems like it should be quantized. But we also know that the energy shouldn't be quantized because we have a free particle, and the way to resolve this is that **energy doesn't actually appear in the differential equation**. To explain this, we define a new variable $\boxed{\rho = kr}$, and this will clear out all of the energy terms: changing variables yields

$$-\frac{d^2U_{E\ell}}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2}U_{E\ell} = U_{E\ell},$$

and our rescaling has removed the energy E from the equation! It still makes its way into our solution, because $\rho = kr$ does still depend on energy, but we get no quantization in solving the differential equation itself.

But then we can look more carefully at the differential equation, and it turns out this is pretty nasty. Without any of the terms here, the equation is easy, but whenever we have two derivatives of a function f, a $\frac{1}{x^2}f$ term, and an f term, we're in the **Bessel function** world.

And spherical Bessel functions are not that bad, but they're a little bit complicated. It's easiest to find solutions of the form

$$U_{E\ell} = r \cdot j_\ell(kr)$$

where we don't care about the constant difference between $\rho = kr$ and r because of normalization, and j_ℓ is the **spherical Bessel function**. This means that a complete solution looks like

$$\psi_{E\ell m} = j_\ell(kr) Y_{\ell m}(\theta, \phi),$$

where we've just divided U by r to get the familiar form of ψ.

Remark 264. *There is a J-type and an N-type Bessel function, but the latter is singular at the origin, so it doesn't matter here.*

From this, we can extract some well-known behavior: as $\rho \to 0$, one property of the Bessel function is that

$$\rho \cdot j_\ell(\rho) \sim \frac{\rho^{\ell+1}}{(2\ell+1)!!}.$$

This is indeed consistent with $U_{E\ell}$ behaving as $r^{\ell+1}$ for small r. We also know that as $r \to \infty$, the Bessel function behaves as

$$\rho \cdot j_\ell(\rho) \sim \sin\left(\rho - \frac{\ell\pi}{2}\right).$$

So this behaves like a trigonometric function, because this is the superposition of a sine and cosine. And the $\frac{\ell\pi}{2}$ factor here is just a phase, which is fixed by the fact that our function needs to vanish at the origin.

This gives physicists a lot of opportunities – the free particle should behave like $\sin\left(kr - \frac{\ell\pi}{2}\right)$ for large r, so we can consider a **localized potential**. The solution far away from that localized potential is a superposition of sines and cosines, so it's a phase difference away from the $U_{e,\ell}$ we're talking about here. Therefore, we'll have

$$U_{E\ell} = \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell(E)\right),$$

and thus we can see the effect of our potential through the phase shift δ! In particular, if we do an experiment with particle scattering, we can use that shift to understand more about the potential that sends waves affecting our potentials.

Example 265

If we have an attractive potential, this "pulls the wave function in," so it corresponds to a positive δ. On the other hand, if the potential is repulsive, we "push the wave function out" and get a negative δ.

We'll finish by introducing another example, which is the **square well**. We studied the infinite square well in the one-dimensional case – it's easy, and it's just a combination of sines and cosines. Then the analogous idea in the three-dimensional case is to take a spherical cavity, in which the particle is free to move for all $r < a$ but has infinite potential past that point. So

$$V(r) = \begin{cases} 0 & r < a \\ \infty & r > a, \end{cases}$$

and we can solve this by just imposing boundary conditions: inside the cavity, solutions will look like

$$U_{E\ell} \sim r \cdot j_\ell(kr),$$

and we just need to make sure we satisfy the boundary condition

$$j_\ell(ka) = 0.$$

This seems like the most symmetric potential possible, but there isn't really much to say about this physical system: we won't get a lot of energy deneracies. On the other hand, if we look at something like

$$V(r) = \beta r^2,$$

we'll end up with lots of degeneracies in energy: we'll understand in the coming lectures why that's true!

34 April 15, 2020

There's been a lot of new ideas with the multiparticle states and tensor products, and we've most recently been talking about angular momentum. We'll still spend time today talking about the former topic, and then angular momentum is basically the main topic of the rest of the semester.

There will be two more problem sets for this class: one due next Friday (Bell inequalities, EPR, some angular momentum) and one due two weeks after that (on addition of angular momentum). We'll have a second test in two weeks – it'll be similar to the first one.

Fact 266

There will be an anonymous survey about the changes made to this class, and we should fill that out if we have any comments.

We started discussing the **no cloning theorem** last time. Recall that the idea is that we start with an arbitrary spin state: here, we'll call it $a_+ |+\rangle + a_- |-\rangle$. We're trying to make a photocopy of this state, so we'll also put in a generic $|+\rangle$ spin state. Then a cloning machine would start with these two particles, and we'd end up with two particles that are both in the $a_+ |+\rangle + a_- |-\rangle$ state. This is a deterministic machine, and the no cloning theorem states that under the assumption that our **cloning machine is unitary time evolution**, we will **not be able to clone our particle** in general, other than a few select states. (It's true that we can also do measurements, and that would be an interesting research project to look at. But then we start introducing probabilities, and our output becomes nondeterministic.)

If V is the vector space of spin states for each particle, our initial and final states are both in $V \otimes V$, so our cloning machine must be a linear operator in $\mathcal{L}(V \otimes V)$. Specifically, if we call the blank state $|b\rangle$, we must have

$$U : |\psi\rangle \otimes |b\rangle \to e^{i\phi} |\psi\rangle \otimes |\psi\rangle$$

be the action of our machine U **for all** $|\psi\rangle \in V$. (Here, we might as well assume our states are well-normalized: $\langle\psi|\psi\rangle = \langle b|b\rangle = 1$.) The ϕ here is a phase – it can depend on $|\psi\rangle$ or $|b\rangle$, but it won't end up being very helpful here.

Let's state the result we're trying to prove:

Theorem 267 (No cloning)

There is no unitary operator U sending $|\psi\rangle \otimes |b\rangle \to |\psi\rangle \otimes |\psi\rangle$ (for some ϕ a function of $|\psi\rangle$ and $|b\rangle$) for all $|\psi\rangle \in V$.

Proof. We'll stop writing the tensor product $\otimes$ symbol from here. Suppose that there is a single state which can be

cloned: that means our operator U looks like

$$U : |\psi_1\rangle |b\rangle \to |\psi_1\rangle |\psi_1\rangle e^{i\phi_1}.$$

Take norms of the initial and final states: we start with

$$\langle\psi_1|\psi_1\rangle \langle b|b\rangle = 1,$$

and we end up with

$$e^{-i\phi_1} \langle\psi_1|\psi_1\rangle \langle\psi_1|\psi_1\rangle e^{i\phi_1} = 1.$$

(We found both of these by writing the bra versions next to the ket versions and doing some rearrangement.) So there's no crazy obstacle here – this preserves the norm in our tensor product space.

Now, there's **always a unitary operator** which takes a vector $|e_1\rangle$ of length 1 to another vector $|f_1\rangle$ of length 1. The idea here is that we can construct a unitary operator out of this: the operator $|f_1\rangle \langle e_1|$, which will send $|e_1\rangle$ to $|f_1\rangle$, is not quite unitary yet, but we can use Gram-Schmidt to get orthonormal bases $|e_1\rangle, \cdots, |e_n\rangle$ and $|f_1\rangle, \cdots, |f_n\rangle$. Now the operator

$$U = \sum_i |f_i\rangle \langle e_i|$$

is indeed unitary, because it's a change of basis between two orthonormal bases! And we can also check that

$$U^\dagger U = \sum |e_i\rangle \langle e_i| = I.$$

And now we can generalize this: suppose we have two orthonormal states $|e_1\rangle, |e_2\rangle$, and we want to send them to two orthonormal states $|f_1\rangle, |f_2\rangle$ respectively. The same Gram-Schmidt argument tells us, again, that extending the bases gives us a unitary operator that does the job. In our original problem, this means that we can indeed clone two orthonormal states in V:

$$\boxed{|\psi_1\rangle |b\rangle \to |\psi_1\rangle |\psi_1\rangle e^{i\phi_1}, \quad |\psi_2\rangle |b\rangle \to |\psi_2\rangle |\psi_2\rangle e^{i\phi_2}}.$$

Further generalizing, this means that we can have n orthonormal basis vectors in a space of dimension n, and **we can clone all of these n states** (because they are an orthonormal set and are being mapped to an orthonormal set). So now we're getting to the punchline: suppose the two states that are boxed above are **arbitrary**, so they're not necessarily orthonormal. We know that the unitary operator should preserve inner products: since $\langle Uv, Uw\rangle = \langle v, w\rangle$, we should have that the inner product of $|\psi_1\rangle |\psi_1\rangle e^{i\phi_1}$ with $|\psi_2\rangle |\psi_2\rangle e^{i\phi_2}$ (the final states) is the same as the inner product of $|\psi_1\rangle |b\rangle$ with $|\psi_2\rangle |b\rangle$ (the initial states). This means that

$$\langle\psi_1|\psi_2\rangle \langle b|b\rangle = e^{-\phi_1} e^{\phi_2} \langle\psi_1|\psi_2\rangle^2 \implies \boxed{\langle\psi_1|\psi_2\rangle (1 - e^{-i(\phi_1-\phi_2)} \langle\psi_1|\psi_2\rangle) = 0},$$

so this only works if ψ_1 and ψ_2 have overlap **zero** (this is the orthonormal case we're already talking about) or if

$$\langle\psi_1|\psi_2\rangle = e^{i(\phi_1-\phi_2)} \implies |\langle\psi_1|\psi_2\rangle|^2 = 1.$$

But the Schwarz inequality tells us that

$$|\langle\psi_1|\psi_2\rangle|^2 \leq |\langle\psi_1|\psi_1\rangle| |\langle\psi_2|\psi_2\rangle| = 1$$

only has saturation when ψ_1 and ψ_2 are different by a constant e^{ix}, which means that **they are the same state**! And now we have our result: any two states that can both be cloned must be orthogonal, so vector spaces can only allow us to clone up to n orthonormal basis vectors. (We can pick any n such states, but then the cloning machine

won't work for any others.) □

Corollary 268
In a vector space of dimension n, there are only n states that can be cloned.

We'll conclude with an application to quantum computation. Normally, we use two bits 0 and 1, but quantum bits (or **qubits**) are quantum states in a two-state system spanned by $|0\rangle$ and $|1\rangle$.

Consider the classical **CNOT quantum gate**, which takes in two (classical) states (x, y) and outputs $(x, y \oplus x)$, where $\oplus$ denotes addition mod 2. (In other words, if $x = 0$, nothing happens, and if $x = 1$, we flip the state of y: the top bit x "controls the gate.")

The analogous quantum gate does something similar: for the basis states $x, y \in \{0, 1\}$, we take in two states $|x\rangle$ and $|y\rangle$ and we output $|x\rangle$ and $|y \oplus x\rangle$. In other words, **there is some unitary operator U such that**

$$U : |x\rangle \otimes |y\rangle \to |x\rangle \otimes |y \oplus x\rangle .$$

So now imagine feeding in the state

$$(a_0 |0\rangle + a_1 |1\rangle) \otimes |0\rangle$$

into our state. It looks like the CNOT gate might actually clone the first particle (if we naively write it out like in the classical case, saying that the second state is now $|y \oplus x\rangle = |x\rangle$), but we can't use that logic! We have to instead write out the initial state as

$$a_0 |0\rangle |0\rangle + a_1 |1\rangle |0\rangle ,$$

and now the gate replaces the first expression with $a_0 |0\rangle |0\rangle$ and the second with $a_1 |1\rangle |1\rangle$. So now this gate doesn't copy what's in the top – it gives us an **entangled state**! Indeed, this circuit only clones the $|0\rangle$ and $|1\rangle$ vectors, but it cannot clone anything else.

35 Angular Momentum, Part 3

Today, we'll start by solving the square spherical wall problem. Recall that this means we want to solve the radial equation

$$-\frac{\hbar^2}{2m}\frac{d^2U_{E\ell}}{dr^2} + V_{\text{eff}}(r)U_{E\ell} = EU_{E\ell},$$

where $U = rf(r)$, for the potential

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}, \quad V(r) = \begin{cases} 0 & r < a \\ \infty & r > a. \end{cases}$$

The first step is to look at the inside of the well – the particle is free in the region $r < a$, which is why we considered the free particle as our first example last time. in the range $r < a$, defining $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $\rho = kr$, our differential equation simplifies to

$$-\frac{d^2U_{E\ell}}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2}U_{E\ell} = U_{E\ell}.$$

(We've just changed the constants a bit, so that the rescaling gets rid of the explicit energy-dependence.) As we mentioned last time, this equation has Bessel function solutions – it's not a simple sinusoidal or power solution. **We'll look at the special case $\ell = 0$**, because this is the only case where we don't need Bessel functions: then our equation

is

$$-\frac{d^2U_{E0}}{d\rho^2} = U_{E0} \implies U_{E0} = A\sin\rho + B\cos\rho.$$

Remember from last time that $U_{E\ell}$ must behave like $r^{\ell+1}$ near the origin, which indeed happens here as long as the **cosine term disappears**. And thus

$$U_{E0}(r) \sim \rho = \sin(kr).$$

Because the potential goes to infinity at $r = a$, we need to satisfy the boundary condition $U_{E0}(a) = 0$. This means that $kr = n\pi$, so

$$k = k_n = \frac{n\pi}{a}$$

for some positive integer n. So far, everything here is analogous to the one-dimensional infinite square well, and the energies will look like (solving the equation $k = \sqrt{\frac{2mE}{\hbar^2}}$ for E)

$$E_{n,0} = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2ma^2}(k_n a)^2 = \frac{\hbar^2}{2ma^2}(n\pi)^2.$$

(These are the energy levels for the $\ell = 0$ state.) Most of these constants are irrelevant, and the important thing to remember is that the constant fraction is the "typical energy" for a system of length scale a, and we're just scaling by $(n\pi)^2$. This motivates the rescaling:

Definition 269

Define the unitless quantity (for any n, ℓ)

$$\varepsilon_{n,\ell} = \frac{E_{n,\ell}}{\left(\frac{\hbar^2}{2ma^2}\right)}.$$

This tells us how much bigger an energy level is compared to the natural energy scale for our system.

From here, let's look at the general case: we'll now need to know the zeros of the spherical Bessel function. For example, $j_1(\rho)$ has zeros when $\tan\rho = \rho$, which requires a numerical calculation to solve, and in general the Bessel function zeros can be found online if we need them. We'll use the notation

$$z_{n,\ell} = n\text{th zero of } j_\ell,$$

where all z's are nonzero and n is indexed by positive integers. And now, the energy eigenstates corresponding to an angular momentum ℓ yield a boundary condition of

$$U_{E\ell}(a) = 0 \implies k_{n,\ell}a = z_{n,\ell}.$$

So our energies look like

$$E_{n,\ell} = \frac{\hbar^2 k_n \ell}{2ma^2} = \frac{\hbar^2(k_{n,\ell}a)^2}{2ma^2},$$

so

$$\varepsilon_{n,\ell} = (k_{n,\ell}a)^2 = z_{n,\ell}^2,$$

which are just the squares of the zeros of the Bessel function! Here's a small table of $\varepsilon_{n,\ell}$ values for small n and ℓ:

	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$
$n = 0$	9.87	20.2	33.2	48.83
$n = 1$	39.48	59.7	82.7	108.5
$n = 2$	88.82	119	$\cdots$	$\cdots$

The purpose of looking at all of these numbers is to compare the energies in a plot: remember that we do this by plotting one column for each ℓ, and drawing horizontal marks at various energy levels for each one. Indeed, the ground state energy levels (corresponding to $n = 2$) do get larger for larger ℓ, as we predicted, but there are **never matching energies** for two different pairs (n, ℓ), which may be surprising for a round, seemingly-symmetric potential!

Example 270

The next system we'll solve is the three-dimensional (isotropic) harmonic oscillator.

This system has the potential

$$V = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) = \frac{1}{2}m\omega^2 r^2.$$

It turns out that there is much more symmetry in this system than there was in the spherical well! To start building our spectrum, note that the Hamiltonian looks like

$$H = \hbar\omega\left(\hat{N}_1 + \hat{N}_2 + \hat{N}_3 + \frac{3}{2}\right),$$

where $\hat{N}$s are the number operators in the three directions. Note that the **state space** of our system can be derived from $\mathcal{H}_1$, the state space of the one-dimensional harmonic oscillator. Conceptually, a 3-D SHO comes from the creation and annihilation operators for x, y, and z, so building a state of a three-dimensional oscillator depends on finding the number of $a_x^\dagger$s, $a_y^\dagger$s, and $a_z^\dagger$s: thus, we actually have a **tensor product**

$$\mathcal{H}_{\text{3D SHO}} = \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \mathcal{H}_1,$$

where any basis vector comes from picking some number of $a_x^\dagger$s, $a_y^\dagger$s, and $a_z^\dagger$s. So even though we introduced tensor products as corresponding to multiparticle systems, we're **tensoring different attributes for the same particle** here – this is just the correct way to combine data in quantum mechanics.

But now we can understand the energies $E_{n,\ell}$ by plotting them in an energy diagram.

- Our ground state $|0\rangle$ has number eigenvalues $N_1 = N_2 = N_3 = 0$, and the energy is $E = \frac{3}{2}\hbar\omega$: this is the single ground state with the lowest possible energy, and because it is spherically symmetric, it must come from the angular momentum equation. We want to know what the value of ℓ is, but there's a **single** state here – there's no multiplicity, while (for example) $\ell = 1$ corresponds to three linearly independent states for $m = -1, 0, 1$. So our ground state energy must have angular momentum $\boxed{\ell = 0}$.
- For the next energy level, there are three different states: $a_x^\dagger|0\rangle, a_y^\dagger|0\rangle, a_z^\dagger|0\rangle$. Each of these states has energy $\hbar\omega\left(1 + \frac{3}{2}\right) = \frac{5}{2}\hbar\omega$, and the multiplicity of 3 means we can argue that this corresponds to $\boxed{\ell = 1}$. After all, $\ell = 0, 1, 2, 3, \cdots$ have a $1, 3, 5, 7, \cdots$-fold degeneracy in m, so the only way to get three states is the second of these options.
- The level after that, with $E = \frac{7}{2}\hbar\omega$, has six states:

  $$(a_x^\dagger)^2|0\rangle, \quad (a_y^\dagger)^2|0\rangle, \quad (a_z^\dagger)^2|0\rangle, \quad a_x^\dagger a_y^\dagger|0\rangle, \quad a_x^\dagger a_z^\dagger|0\rangle, \quad a_y^\dagger a_z^\dagger|0\rangle.$$

  Each of these has $N = N_1 + N_2 + N_3 = 2$, and the six states must organize themselves into various different values of ℓ. We can't use $\ell = 3$ (that yields seven states), so we must either have two different sets of $\ell = 1$ states (3+3) or a set of $\ell = 2$ and a set of $\ell = 0$ states (5+1). But we can't build with two $\ell = 1$ states, because that means we'd need to put two horizontal lines at the same spot on our energy diagram for the same value of ℓ, and this is not allowed! So we instead split our states of $N = 2$ into five of $\boxed{\ell = 2}$, and one state of $\boxed{\ell = 0}$.

(We can write this as a direct sum of the two spaces.) So this is already interesting: we get an identical energy in different columns of ℓ. (We'll understand where this matching comes from later on in the course.)

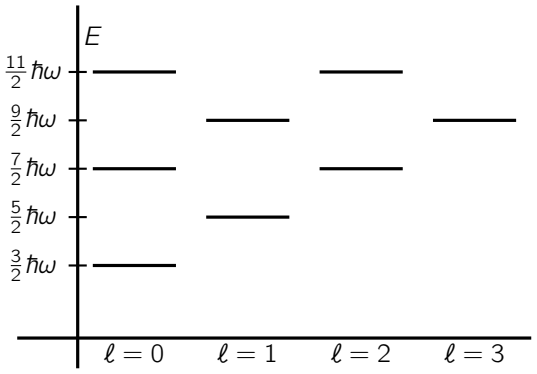
- Finally, let's consider $N = 3$. This case has ten possible states: we can cube one of the raising operators (3 options), use one of each raising operator (1 option), or use two of one and one of another (6 options) to get a state of energy $\frac{9}{2}\hbar\omega$. This can either originate out of $(\ell = 4) \oplus (\ell = 0)$ (with $9+1$ states) or $\boxed{(\ell = 3) \oplus (\ell = 1)}$ (with $7+3$ states). It turns out to be the latter (the best way to understand this is to look at the lowest energies for each value of ℓ, which go up in step).

- If we want to count the number of states for $N = 4$ or higher N, note that we just need to find nonnegative integers n_x, n_y, n_z with $n_x + n_y + n_z = N$. (This corresponds to the state $(a_x^\dagger)^{n_x}(a_y^\dagger)^{n_y}(a_z^\dagger)^{n_z}|0\rangle$.) Doing casework on the value of n_z, this yields a total of

$$1 + 2 + \cdots + (N+1) = \frac{(N+1)(N+2)}{2}$$

states of a given sum of number operators N. And we can carry out the same argument to understand that $N = 4$ most likely corresponds to $\ell = 4, 2, 0$, $N = 5$ corresponds to $\ell = 5, 3, 1$, and so on.

So the above analysis told us the ℓ-values at a given energy, and we can also use this to see the energy levels at a given ℓ. Basically, we do two jumps of $\hbar\omega$ between energy levels at a given ℓ:



To understand this system better, remember that we discussed that we can replace the operators a_x, a_y with a_R, a_L, which allows us to write

$$L_z = \hbar(N_R - N_L)$$

(we derived this for a two-dimensional oscillator, but it's still true in three dimensions). It's a bit harder to find the angular momentum operators L_x, L_y, but we can do that, and this time this is an actual momentum, not an abstract one like in the 2D case.

From here, we'll build states in the same way as before, doing casework on the value of $N = N_L + N_R + N_3$.

- For $N = 1$, there are three states: $a_R^\dagger|0\rangle, a_z^\dagger|0\rangle, a_L^\dagger|0\rangle$, which correspond to angular momenta L_z of $\hbar, 0, -\hbar$ respectively. So that gives us all of the structure for the $\ell = 1$ multiplet: we get the three states with m values of $+1, 0, -1$.

- Looking at the extreme cases, for $N = 2$, we have $a_R^\dagger a_R^\dagger|0\rangle$ with an angular momentum $L_z = 2\hbar$, and this is the highest possible value of L_z – in general, $L_z = N\hbar$ is the maximum possible value for a state with total number N, because each $a_R^\dagger$ adds $1\hbar$ to L_z, each $a_L^\dagger$ removes $1\hbar$, and each $a_z^\dagger$ does nothing. So there are going to be $2N + 1$ different values of L_z for each N (from $-N\hbar$ to $N\hbar$).

- So the only state with maximum angular momentum is $(a_R^\dagger)^N|0\rangle$, the only state with one unit less of angular momentum is $(a_R^\dagger)^{N-1}a_z^\dagger|0\rangle$, and then the next unit of angular momentum has two states: $(a_R^\dagger)^{N-2}(a_z^\dagger)^2|0\rangle$, as well as $(a_R^\dagger)^{N-1}a_L^\dagger|0\rangle$. But the point is that because we have some state with maximum angular momentum, we'll get a multiplet corresponding to $\ell = N$: this uses up the state of $L_z = n\hbar$, $L_z = (N-1)\hbar$, and one of the states of $L_z = (N-2)\hbar$. And now the highest angular momentum left is $L_z = (N-2)\hbar$, so that corresponds to $\ell = N-2$: **this explains the jump by two energy levels!**

Indeed, we'll find two states that we can write at $L_z = (N-3)\hbar$, three states at $L_z = (N-4)\hbar$ (which explains why we have an $\ell = N-4$, and so on. And we can conclude study of this system by understanding how we could have come up with this from the beginning without building it up: the answer is that certain operators commute with the Hamiltonian (meaning they don't change energy) and indeed move us from one value of ℓ to another (in other words, moves us to the right or the left by two values of ℓ in our above diagram). As a hint, the operators of the form $a_x^\dagger a_y$ does not change the energy, because it destroys one level in the y-direction and adds one in the x-direction. There's lots of hidden symmetries in the operators of this form!

Example 271

Our next system is that of the **hydrogen atom**: we have

$$H = \frac{p^2}{2m} - \frac{e^2}{r}.$$

Here, m is the reduced mass of the proton-electron system: it's roughly equal to m_e (the mass of the electron). There is a natural length scale in this system, known as the **Bohr radius**. We find this by setting $p = \frac{\hbar}{a_0}$ for some length a_0, and then we set the two terms of the Hamiltonian equal (ignoring constants because we care about units):

$$\frac{\hbar^2}{ma_0^2} = \frac{e^2}{a_0} \implies \boxed{a_0 = \frac{\hbar^2}{me^2}} \approx 0.529 \times 10^{-10} \text{ m}.$$

The $\frac{1}{e^2}$ is important: this means that if we make the interaction between the electron and proton small, then the hydrogen atom's radius gets large. The corresponding energy scale is $\frac{e^2}{a_0}$, and half of that quantity, $\frac{e^2}{2a_0}$, is a famous number – 13.6 eV.

Our main question here will be finding the (energy) spectrum: there's an elegant method for finding the ground state. We can write (for some specific constants γ, β) the Hamiltonian as

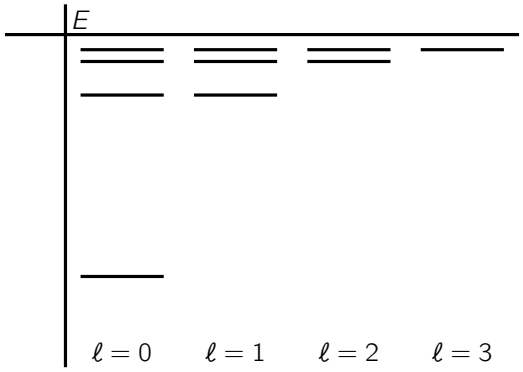
$$H = \gamma + \frac{1}{2m}\sum_{k=1}^{3}\left(\hat{p}_k + i\beta\frac{\hat{x}_k}{r}\right)\left(\hat{p}_k - i\beta\frac{\hat{x}_k}{r}\right):$$

this is basically a factorized version of our above expression. (Remember that we need to be careful, because the operators $\hat{x}_k$ and $\hat{p}_k$ don't commute.) But now we can view the second term $\left(\hat{p}_k - i\beta\frac{\hat{x}_k}{r}\right)$ as an operator and the first term $\left(\hat{p}_k + i\beta\frac{\hat{x}_k}{r}\right)$ as its dagger: in a way analogous to the harmonic oscillator, the ground state should be killed by our operator, meaning

$$\left(\hat{p}_k - i\beta\frac{\hat{x}_k}{r}\right)|\psi_{\text{gs}}\rangle = 0,$$

and the energy of this ground state is just the constant γ. (This looks like three equations, but it's just a single equation if we have a spherically symmetric state.)

Looking at the whole spectrum, there are interesting degeneracies just like in the 3-dimensional harmonic oscillator: we'll claim this result for now, and we'll show where this structure comes from later in the class.



If we label the states for each ℓ with $\nu = 0, \nu = 1, \cdots$ from bottom to top, notice that the states with the same $\boxed{n = \nu + \ell}$ have the same energy. That energy turns out to be

$$E_{n,\ell} = -\frac{e^2}{2a_0} \cdot \frac{1}{n^2}, \quad n = \nu + \ell,$$

where $0 \leq \ell \leq n-1$, and in order to understand more of the structure here, we're going to need to introduce the idea of the **Runge-Lenz vector**.

Example 272

The Runge-Lenz vector comes from classical mechanics: consider a Hamiltonian for an elliptical orbit

$$H = -\frac{p^2}{2m} + V(r),$$

where the (classical) force is $\vec{F} = -V'(r)\frac{\vec{r}}{r}$.

In this classical situation, we know that

$$\vec{F} = \frac{d\vec{p}}{dt} = -V'(r)\frac{\vec{r}}{r},$$

and because we have a central potential $V(r)$,

$$\frac{d\vec{L}}{dt} = 0$$

(there is no torque on the particle). It turns out that there is a (surprising) quantity here that is conserved: we start with the quantity $\vec{p} \times \vec{L}$ (this is a bit unmotivated, but it yields an interesting result), and then we can do some algebra to find

$$\frac{d}{dt}(\vec{p} \times \vec{L}) = mV'(r)r^2 \frac{d}{dt}\left(\frac{\vec{r}}{r}\right).$$

So this gives us a conservation law when $V'(r)r^2$ is a constant, which we'll call e^2. And this occurs exactly when

$$V'(r) = \frac{e^2}{r^2} \implies V(r) = -\frac{e^2}{r},$$

which is the potential of the hydrogen atom: it's a $\frac{1}{r^2}$ force field. **In such a situation**, there is a conservation law

$$\frac{d}{dt}\left(\vec{p} \times \vec{L} - \frac{me^2\vec{r}}{r}\right) = 0.$$

For the sake of convenience, defining

$$R = \frac{\vec{p} \times \vec{L}}{me^2} - \frac{\vec{r}}{r},$$

we know that $\frac{dR}{dt} = 0$, and we have a conserved quantity that is unitless. This R turns out to be conserved in the

quantum mechanical case too: R is an operator that **commutes** with the Hamiltonian H. (We'd have to hermiticize $\vec{p} \times \vec{L}$ for things to work out.) But what's important here is that this conservation law helps us understand the degeneracies in the hydrogen atom!

If we first consider a circular orbit, $\vec{p}$ is tangential and $\vec{L}$ is out of the plane of the orbit, so $\frac{\vec{p}\times\vec{L}}{me^2}$ points radially out of the circle. Combining this with the radial vector means that R is some vector that points radially outward, and it must be conserved: thus, R must actually be the zero vector in the circular case.

But R isn't zero in an elliptical orbit: if we repeat the same argument, it turns out that the vector will always point along the **major axis** of the ellipse! (And this always happens in a $\frac{1}{r}$ potential, though it's good to note that Einstein's theory of gravity has a different potential, so the ellipse precesses.) And the magnitude of this unitless $\vec{R}$ turns out to be exactly the eccentricity of our ellipse.

36 April 22, 2020

Our second midterm will be in a week – some materials, including past tests and a formula sheet, have been posted for us to work on. We'll discuss test review next recitation, and it's recommended that we look at the formula sheet to study – there's a lot more formulas than last time. (Basically, we should be able to realize what each one means and what it can be used for.) Logistics will be pretty similar to the first test, and we'll experiment a bit more with partial credit.

Fact 273

Everything we've learned up to **today's lecture** and Friday's problem set is fair game for the test. Monday's lecture will begin discussing addition of angular momentum, but it won't be on the test.

Each midterm, as well as the final, are now worth 15 percent of our grade. (And the final will not be uniformly covered, because we just don't have enough time.) We should expect a set of true/false questions on each test as well.

With that, we'll move to class material: first of all, to answer a question posed, we'll consider the identity

$$L^2 = r^2p^2 - (r\cdot p)^2 + i\hbar r\cdot p.$$

The Hamiltonian of the hydrogen atom looks like

$$H = \frac{p^2}{2m} + V(r), \quad V(r) = -\frac{e^2}{r},$$

so we need to write p^2 in terms of L^2 in the identity above to get the Laplacian term (involving p^2). We want to divide by r^2, and the idea is that the operator $\frac{1}{r^2}$ acts on the wavefunction ψ by just multiplying by the operator $\frac{1}{r^2}$ **on the left**, since r, p do not commute. This yields

$$\frac{1}{r^2}\left(L^2 + (r\cdot p)^2 - i\hbar r\cdot p\right) = p^2,$$

and we can then substitute that into the Hamiltonian, which yields

$$\frac{p^2}{2m} = \frac{1}{2mr^2}\left(L^2\right) + \frac{1}{2mr^2}\left((r\cdot p)^2 - i\hbar r\cdot p\right).$$

Remark 274. *When we see a fraction of operators $\frac{A}{B}$, this is usually ill-defined: it could either mean $B^{-1}A$ or AB^{-1}, so we shouldn't write fractions unless we have something like $\frac{L^2}{r^2}$, because the operators L^2 and $\frac{1}{r^2}$* **commute**. *Similarly,*

we should be careful with things like

$$\frac{1}{(AB)} = (AB)^{-1} = B^{-1}A^{-1} = \frac{1}{B} \cdot \frac{1}{A}.$$

We'll discuss some aspects of EPR now, using work by Greenberg, Horne, and Zeilinger (GHZ).

Example 275

Suppose we have three particles A, B, C in an entangled state (emerging from some kind of a elementary particle decay), and they go to Alice, Bob, and Charlie.

EPR's logic would tell us that these particles have attributes – we can measure the x-component or y-component of some particle, and we always get the same result for a given particle because these observables are properties. Even if we don't know why the particles have these values for the observables, there are some hidden variables or attributes that determine all physical properties of the state. Call these hidden variables λ.

Suppose, for example, that Alice measures the spin of her particle along the $\vec{x}$ state: then the result she will get looks like

$$A(\vec{x}; \lambda) \in \{\pm 1\},$$

where we're measuring σ_x instead of S_x. Here, we're saying that **given λ, the value of A is determined**: there's no probability going on. Similarly, Alice can measure $A(\vec{y}; \lambda) \in \{\pm 1\}$, and Bob and Charlie can also measure along the $\vec{x}$- and $\vec{y}$-directions to get answers of 1 or -1, depending on λ.

The main result we care about is that we can produce an entangled state such that we have the following $\vec{x}\vec{y}\vec{y}$ correlations:

$$A(\vec{x}, \lambda)B(\vec{y}, \lambda)C(\vec{y}, \lambda) = 1.$$

$$A(\vec{y}, \lambda)B(\vec{x}, \lambda)C(\vec{y}, \lambda) = 1.$$

$$A(\vec{y}, \lambda)B(\vec{y}, \lambda)C(\vec{x}, \lambda) = 1.$$

In other words, when one of our particles is measured in the x-direction and the other two particles are measured in the y-direction, their product is always 1 (either all $+1$s, or one $+1$ and two -1s). But now we can multiply these equations together to find

$$A(\vec{x}, \lambda)B(\vec{x}, \lambda)C(\vec{x}, \lambda) = 1,$$

since the square of any measurement we make here is always 1, so the y-terms all go away. But let's see what quantum mechanics predicts about this: consider the state

$$\Phi = \frac{1}{\sqrt{2}} \left(|+\rangle |+\rangle |+\rangle - |-\rangle |-\rangle |-\rangle \right).$$

We can see the analog of the $\vec{x}\vec{y}\vec{y}$ correlations now: if we consider the operator

$$\sigma_x^A \otimes \sigma_y^B \otimes \sigma_y^C,$$

this operator acts on Φ (because it acts on the three particles), and it is Hermitian (because each of the three operators is Hermitian), meaning it is something that can be measured. But remember that

$$\sigma_x |\pm\rangle = |\mp\rangle, \quad \sigma_y |\pm\rangle = \pm i |\mp\rangle,$$

so the operator will turn $|+\rangle |+\rangle |+\rangle$ into $|-\rangle |-\rangle |-\rangle$, except with two factors of i from the two σ_ys, meaning it will turn into $-|-\rangle |-\rangle |-\rangle$. Similarly, the $-|-\rangle |-\rangle |-\rangle$ will become $+|+\rangle |+\rangle |+\rangle$, so Φ is actually an **eigenstate of our**

operator:

$$\left(\sigma_x^A \otimes \sigma_y^B \otimes \sigma_y^C\right)|\Phi\rangle = |\Phi\rangle$$

with eigenvalue 1. The same logic works for the other two operators, and thus we've verified the $\vec{x}\vec{y}\vec{y}$ correlation property for this GHZ state.

But now we can try seeing what happens when we measure all three particles along the x-direction:

$$\left(\sigma_x^A \otimes \sigma_x^B \otimes \sigma_x^C\right)|\Phi\rangle = \frac{1}{\sqrt{2}}\left(|-\rangle|-\rangle|-\rangle - |+\rangle|+\rangle|+\rangle\right) = -|\Phi\rangle,$$

so we actually get an eigenvalue of -1! So the answer is exactly opposite from what we see in the classical case, and thus we've already found a way to violate the classical assumptions. And we don't even need to repeat this argument: any one single measurement gives the wrong answer. And one thing to learn here is that

$$(\sigma_x \otimes \sigma_y \otimes \sigma_y) \otimes (\sigma_y \otimes \sigma_x \otimes \sigma_y) \otimes (\sigma_y \otimes \sigma_y \otimes \sigma_x) = (\sigma_x\sigma_y\sigma_y) \otimes (\sigma_y\sigma_x\sigma_y) \otimes (\sigma_y\sigma_y\sigma_x),$$

and the reason this doesn't reduce to $\sigma_x \otimes \sigma_x \otimes \sigma_x$ is that the matrices don't commute in the second term. In fact, we just end up with

$$\sigma_x \otimes (-\sigma_x) \otimes \sigma_x = -(\sigma_x \otimes \sigma_x \otimes \sigma_x),$$

as we've already demonstrated.

37 Addition of Angular Momentum, Part 1

We'll start this new topic by introducing some elements of **perturbation theory**, which is discussed much more in 8.06. The idea is that many of the results of perturbation theory will be important for understanding various examples that come up in this last part of the class. (We won't do any derivations here, just a general primer of results.)

Suppose that we have a Hamiltonian

$$H = H^{(0)} + \delta H,$$

where $H^{(0)}$ is known and δH is some small perturbation. Suppose that our eigenstates of the known Hamiltonian are indexed by k, such that

$$H^{(0)}\left|k^{(0)}\right\rangle = E_k^{(0}\left|k^{(0}\right\rangle.$$

(The (0)s reflect the fact that we're working with the original Hamiltonian.) This means we know the (degenerate or nondegenerate) spectrum of $H^{(0)}$, and we want to understand what the perturbation does to this spectrum.

Each of the nondegenerate states will be perturbed a little, and the degenerate states will typically split apart from each other as well: δH may move the energies up more than others. We'll look at each of these cases now.

In the nondegenerate case, there is a single eigenstate indexed by k, and the state $\left|k^{(0)}\right\rangle$, as well as the energy E_k, will change by a bit:

$$E_k = E_k^{(0)} + \delta E_k + O((\delta H)^2).$$

Here, we're making a **first-order** approximation of the Hamiltonian correction δH. It turns out the formula is of the form

$$\delta E_k = \left\langle k^{(0}\middle|\delta H\middle|k^{(0}\right\rangle.$$

what's striking here is that the correction to the energy doesn't require the exact form of the eigenvectors: we just need to look at the expectation value on the original eigenstate.

On the other hand, when we have degenerate states (meaning they have the same value of E_k), we can understand

what happens to the splitting at first order. Suppose that our energy level is $E_n^{(0)}$, and there are N total degenerate energy eigenstates at that level: we'll label them as $\left|n^{(0)}, \ell\right\rangle$, where we have the additional indexing by the integer $1 \leq \ell \leq N$. Assume that we've also chosen these states to be orthonormal, so that $\left\langle n^{(0)}, \ell \middle| n^{(0)}, k\right\rangle = \delta_{\ell k}$.

To lowest (zeroth) order, all of these states have the same energy, which is the eigenvalue

$$H^{(0)} \left|n^{(0)}, \ell\right\rangle = E_n^{(0)} \left|n^{(0)}, \ell\right\rangle.$$

To understand what happens to the splitting, note that our N states span a vector space V_N: what we need to do is compute the matrix for δH in our space V_N. This means we need the matrix elements

$$(\delta H)_{k\ell} = \left\langle n^{(0)}, k \middle| \delta H \middle| n^{(0)}, \ell \right\rangle :$$

this gives us an $N \times N$ matrix.

And then we get our answer by **diagonalizing that $N \times N$ matrix**. We need to find the eigenvalues and eigenvectors of this (Hermitian by definition) matrix, and if the energies split, some of the eigenvalues will be different. Labeling those N eigenvectors $\left|\psi_I^{(0)}\right\rangle$ (where $1 \leq I \leq N$) and the corresponding N eigenvalues δE_{nI}, we can think of each eigenvector as a column vector, which corresponds to a linear combination of our **original** basis states $\left|n^{(0)}, k\right\rangle$:

$$\left|\psi_I^{(0)}\right\rangle = \sum_k \left|n^{(0)}), k\right\rangle a_{Ik}^{(0)}.$$

These $\left|\psi_I^{(0)}\right\rangle$s are then the (approximate) **new energy eigenstates** for our perturbed Hamiltonian, and the energies are $E_{nI} = E_n^{(0)} + \delta E_{nI} + O(\delta H^2)$. So it takes a bit more time to state what happens, but we just diagonalize the matrix that explains the matrix elements of δH, which allows us to separate the corrections to the energy $E_n^{(0)}$.

Now, we're ready to move on to addition of angular momentum, and we'll start by stating the fundamental result:

Theorem 276

Suppose there are a set of operators $J_i^{(1)}$ on the state space V_1 satisfying the algebra of angular momentum (that is, $[J_i^{(1)}, J_j^{(1)}] = i\hbar\varepsilon_{ijk} J_k^{(1)}$), as well as another set of operators $J_2^{(2)}$ on the state space V_2. Then there is a new angular momentum

$$J_i = J_i^{(1)} \otimes I + I \otimes J_i^{(2)}$$

which satisfies the algebra of angular momentum in the space $V_1 \otimes V_2$.

Note that we needed to state this in terms of the tensor product space, because $J_i^{(1)}$ cannot act on V_2 (and vice versa). But soon we'll just call this operator $J_i^{(1)} + J_i^{(2)}$ to make the notation easier. Note that if we had tried to add **any other linear combination** of these two angular momenta, it wouldn't work!

Proof. We need to verify the angular momentum relation:

$$[J_i, J_j] = \left[J_i^{(1)} \otimes I + I \otimes J_i^{(2)}, J_j^{(1)} \otimes I + I \otimes J_j^{(2)}\right].$$

But now if we look at the cross terms, the commutator will be zero, because (for example)

$$(J_i^{(1)} \otimes I)(I \otimes J_j^{(2)}) = (I \otimes J_j^{(2)})(J_i^{(1)} \otimes I) = J_i^{(1)} \otimes J_j^{(2)}.$$

So operators originally living in different vector spaces will commute, and what we're left with is

$$\left[J_i^{(1)} \otimes I, J_j^{(1)} \otimes I\right] + \left[I \otimes J_i^{(2)}, I \otimes J_j^{(2)}\right]$$

and then the I's don't really do anything: we just get

$$[J_i^{(1)}, J_j^{(1)}] \otimes I + I \otimes [J_i^{(2)}, J_j^{(2)}]$$

by the formulas for angular momentum in the individual vector spaces, and this is exactly what we want: it evaluates to $i\hbar\varepsilon_{ijk}\left(J_k^{(1)} \otimes I + I \otimes J_k^{(2)}\right) = i\hbar\varepsilon_{ijk}J_k$. □

And with a bit more practice, we won't need to use the tensor products when we're working with these objects.

Example 277

Our first example will be **spin-orbit coupling**: we'll have a hydrogen atom, with an additional term $\Delta H = -\vec{\mu}\cdot\vec{B}$.

We didn't have a $\vec{B}$ in the original hydrogen atom, but we'll say that $\vec{\mu}$ is the magnetic dipole moment for the electron:

$$\vec{\mu} = -\frac{e}{m}\vec{S},$$

where $\vec{S}$ is the spin. We're using Gaussian units, we can instead state this as

$$\vec{\mu} = -\frac{ge}{2mc}\vec{S},$$

because this allows us to estimate terms more easily. And the magnetic field $\vec{B}$ comes from **the electron's interaction with the proton**: since the proton is going around the electron (in the electron's frame), we have an "current that generates a magnetic field," and this current is then going to be proportional to the angular momentum $\vec{L}$.

Specifically, let's fix coordinates so that the electron is at the origin at some point in time, moving into the plane with some velocity $\vec{v}$, and the proton is to the left of the electron so that there is an electric field $\vec{E}$ pointing to the right (remember that electric field is not the same as electric force). Relativistically, the electric and magnetic fields that we see in different reference frames are actually different: thus, the magnetic field from the point of view of the electron will be

$$\vec{B}' = -\frac{\vec{v}\times\vec{E}}{c},$$

and this (by the right-hand rule) yields a magnetic field pointing upward: this is consistent with the picture of having a proton going around in circles and creating a current. We'll remove the negative sign by using $\vec{E}\times\vec{v}$ instead, and we can calculate the electric field by looking at the scalar potential

$$V(r) = -\frac{e^2}{r} \implies V'(r) = \frac{e^2}{r^2} \implies \vec{E} = \frac{V'(r)}{e}\frac{\vec{r}}{r},$$

where the last step comes from replacing electric force with electric field and also noting that the electric field points radially outward. And now plugging things in,

$$\vec{B}' = \frac{1}{ec}\frac{1}{r}V'(r)(\vec{r}\times\vec{v}),$$

and borrow a factor of m to write this in terms of the angular momentum:

$$= \frac{1}{ecm}\frac{1}{r}\frac{dv}{dr}\vec{L}.$$

Thus, we can finally calculate the perturbation:

$$\Delta H = -\vec{\mu}\cdot b\vec{B} = \frac{ge}{2mc}\left(\vec{S}\cdot\vec{L}\right)\frac{1}{ecm}\frac{1}{r}\frac{dV}{dr}.$$

Unfortunately, it turns out there's a relativistic error here: **Thomas precession** tells us that we must replace g with $g-1$ (because the interactions of magnetic fields and dipoles change the precession rate when we don't have an inertial system), which means that we basically lose a factor of 2: plugging everything in, we end up with

$$\boxed{\Delta H = \frac{e^2}{2m^2c^2r^3}(\vec{S}\cdot\vec{L})}.$$

To estimate this, recall that we have the Bohr radius $a_0 = \frac{\hbar^2}{me^2}$, and we also have the **fine structure constant**

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}.$$

Since $\vec{S}$ has multiples of $\hbar$ and so does $\vec{L}$, we can estimate the dot product to be on the order of $\hbar$, and we end up with

$$\Delta H \sim \frac{1}{m^2c^2}(\hbar^2)\frac{1}{r}\frac{e^2}{r^2} \approx \frac{1}{m^2c^2}\frac{e^2}{a_0^3}\hbar^2.$$

The ground state energy of the hydrogen atom is $E_{\text{gs}} = \frac{e^2}{2a_0}$, and now

$$\frac{\Delta H}{E_{\text{gs}}} == \frac{\hbar^2}{m^2c^2a_0^2} = \frac{\hbar^2}{m^2c^2\frac{\hbar^4}{m^2e^4}} = \frac{e^4}{\hbar^2c^2} = \alpha^2.$$

This means the ratio of the spin orbit coupling energy with the ground state energy is $\frac{1}{137^2}$, which is pretty small. This is called the **fine structure of the hydrogen atom**: the splitting of energies is therefore going to be pretty small.

Remark 278. *Note that we've been using Gaussian units this whole time: in SI units, we instead have*

$$\Delta H = \frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2r^3}(\vec{S}\cdot\vec{L}),$$

where we've already replaced g with $g-1$ in this expression.

Now that we have the perturbation ΔH, we can work with this a bit more to understand what happens to the hydrogen spectrum. We'll start with the simplest state of angular momentum, the state of $\boxed{\ell = 1, n = 2}$ (recall that $n = \ell + \nu$, so this is the lowest energy state for $\ell = 1$). Remember that this is actually a multiplet of states: $\ell = 1$ has states of $m = -1$, 0, and 1, and our states can also be up or down, so we actually have **$3 \times 2 = 6$ total states** of the form

$$|\ell, m\rangle \otimes |s, m_s\rangle,$$

where we're **fixing** $\ell = 1$ and $s = \frac{1}{2}$, but we can have $m = -1, 0, 1$, and we can have $m_s = \pm\frac{1}{2}$. Remember that $|\ell, m\rangle$ denote the angular part of our wavefunction, though there is also a radial dependence $\psi_1(r)$ which luckily only depends on ℓ (so it basically factors out of any consideration we're doing here). All in all, this means we have six degenerate states, and we'll need to use the perturbation Feynman–Hellmann result carefully: we need to select the correct basis of eigenstates from our 6×6 matrix δH. Theoretically, we could find $\langle i|\Delta H|j\rangle$ for all matrix elements $1 \le i, j \le 6$ and find the eigenvectors as δH goes to 0: basically, we want to find a basis $|1'\rangle, |2'\rangle, \cdots, |6'\rangle$ of this energy level such that the matrix $\Delta H'$ becomes diagonal, so that the changes of energies are just those diagonal entries.

What we'll find is that we can relate the basis of states $|\ell = 1, m\rangle \otimes \left|s = \frac{1}{2}, m_s\right\rangle$ to a basis which tracks **total angular momentum**. To understand this, let's look some more at the $\vec{L}\cdot\vec{S}$ operator: it acts on our tensor product, and it's actually defined as

$$L_1 \otimes S_1 + L_2 \otimes S_2 + L_3 \otimes S_3 = \sum_i L_i \otimes S_i,$$

and we also have the sum of the angular momenta

$$J_i = L_i \otimes I + I \otimes S_i.$$

The idea is to square J:

$$J^2 = \sum_i J_i \cdot J_i$$

(this is not a tensor product – we're applying J_i twice), which can be written as

$$= \sum_i (L_i \otimes I + I \otimes S_i)(L_i \otimes I + I \otimes S_i) = \sum_i (L_i L_i \otimes I + 2L_i \otimes S_i + I \otimes S_i S_i),$$

and now we can rewrite this as

$$\boxed{J^2 = L^2 \otimes I + 2\sum_i L_i \otimes S_i + 1 \otimes S^2}$$

(and when we have more practice, this can basically just be written as $J^2 = L^2 + S^2 + 2\vec{L} \cdot \vec{S}$, though that can be confusing when we think about how it acts on states). Therefore, we have the formula for that term of our Hamiltonian:

$$\vec{L} \cdot \vec{S} = \frac{1}{2}(J^2 - L^2 - S^2).$$

And now L^2 is a diagonal matrix in our original basis, because the eigenstates we're choosing all have $\ell = 1$, and similarly S^2 is a diagonal matrix – both are actually constants times the identity. That means that $\vec{L} \cdot \vec{S}$ is basically just a linear transformation of J^2, and thus the total angular momentum is indeed the important quantity here.

We'll call the original basis states $|1, m\rangle \otimes \left|\frac{1}{2}, m\right\rangle$ **uncoupled states** (there's no entanglement going on), and all of these uncoupled states are eigenvectors of L^2, S^2. But because all of the eigenvalues are actually equal – each one has an eigenvalue of $\hbar^2 \ell(\ell+1) = 2\hbar^2$ for L^2 and $3 \cdot \left(\frac{\hbar}{2}\right)^2 = \frac{3\hbar^2}{4}$ for S^2 – if we take **any** linear combination of our uncoupled states, we will still have eigenvectors of both L^2 and S^2 (with the same eigenvalues). Thus, we just need to select **specific linear combinations** that are also eigenstates of J^2, and then we'll be happy.

Remember that L^2 and S^2 commute with all L_i and S_i, respectively, and Ls and Ss always commute because they act on different state spaces. So L^2 is known as a **Casimir operator** – it commutes with everything that is rotationally invariant constructed with Ls and Ss. So when we consider our matrix elements $\langle i|\Delta H|j\rangle$, remember that we're considering overlaps of the states $|i\rangle$, which have a radial component as well as an angular and spin wavefunction, which we'll call $|\underline{i}\rangle$. Since

$$\Delta H = \beta \frac{1}{r^3}(\vec{L} \cdot \vec{S})$$

for some constant β, the inner product calculation $\langle i|\Delta H|j\rangle$ looks like

$$\beta \int r^2 dr \psi_1^*(r)\psi_1(r) \cdot \frac{1}{r^3} \left\langle \underline{i} \middle| \vec{L} \cdot \vec{S} \middle| \underline{j} \right\rangle.$$

So we just select these $\underline{i}, \underline{j}$ to be eigenstates of $\vec{L} \cdot \vec{S}$, which will give us

$$= \left\langle \frac{1}{r^3} \right\rangle_{\ell=1,n=2} \cdot \left\langle \underline{i} \middle| \vec{L} \cdot \vec{S} \middle| \underline{j} \right\rangle,$$

and the inner product will be diagonal and indicate the relevant energy corections ΔE.

We'll now turn our attention back to our complete set of commuting observables: normally for an unperturbed hydrogen atom, we have H_0, L^2, and L_z (where L tells us about the orbital angular momentum), and we can't add any more operators because L_x and L_y do not commute with L_z. But now adding in the spin term, we can now have

the complete set

$$\{H_0, L^2, L_z, S^2, S_z\},$$

because the original Hamiltonian doesn't actually know about the spin at all. On the other hand, if we have $\vec{L} \cdot \vec{S}$ coupling, we now have a full Hamiltonian H' instead of H_0. We want to check whether L^2 and L_z can be put in our complete set again – we know that L^2 commutes with H_0, and we just need to check whether it commutes with $\vec{L} \cdot \vec{S}$, which is does. But the L_is do not actually commute with $\vec{L} \cdot \vec{S}$, so this time we can't keep L_z anymore. Similarly, S^2 is okay, but S_z is not, and so our new set currently sits at

$$\{H', L^2, S^2\}.$$

But we can actually add something new this time: the total angular momentum in the form of J^2. To check this, note the following:

- J^2 is built with L_is and S_is, which commute with H_0, so J^2 and H_0 commute.
- J^2 commutes with $\vec{L} \cdot \vec{S}$, because we can remember that

  $$[J^2, \vec{L} \cdot \vec{S}] = \left[J^2, \frac{1}{2}(J^2 - L^2 - S^2)\right]$$

  and each term commutes.
- Similarly, J^2 commutes with L^2, S^2.

So we can add J^2 to this, and the natural question is whether we can also add J_i (analogous to adding L_z or S_z). We go through the argument again: $J_i = L_i + S_i$ commutes with H_0 because both L_i and S_i do, J_i commutes with the remaining operators because it commutes with J^2, L^2, S^2. We can't add multiple J_is, so we get our final set of Hermitian commuting observables which we can simultaneously diagonalize:

$$\boxed{H', L^2, S^2, J^2, J_z}.$$

But in our analysis, we won't be finding exact energy eigenstates: we'll use the Feynman-Hellmann method of diagonalizing J^2 instead. Remember that $\vec{L}$ and $\vec{S}$ have eigenvalues proportional to $\hbar$, so we often divide through to get rid of that. We have the very useful formula, which is the action of our lowering and raising operators $J_\pm$:

$$J_\pm |j, m\rangle = \hbar\sqrt{j(j+1) - m(m \pm 1)}\, |j, m \pm 1\rangle .$$

We can write our uncoupled states in the following groups:

$$\begin{aligned}
\frac{J_z}{\hbar} &= \frac{3}{2} : |1,1\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \\
\frac{J_z}{\hbar} &= \frac{1}{2} : |1,0\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle, \quad |1,1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \\
\frac{J_z}{\hbar} &= -\frac{1}{2} : |1,0\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle, \quad |1,-1\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \\
\frac{J_z}{\hbar} &= -\frac{3}{2} : |1,-1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle .
\end{aligned}$$

This is because the value of $\frac{J_z}{\hbar}$ is basically just $m + s_m$, where m is one of $1, 0, -1$ and s_m is either $\frac{1}{2}$ or $-\frac{1}{2}$. So J_z can be diagonalized without forming linear combinations, but we haven't diagonalized J^2 yet: we want to find the eigenstates $|j, m\rangle$ which have eigenvalue from $J_z = \hbar m$ and eigenvalue from $J^2 = \hbar(j(j+1)$.

And now we think about this by thinking about J_z as an abstract angular momentum. We know that J_z is at most

$\frac{3}{2}$ here, and $-j \leq m \leq j$, so we must have an eigenstate of J^2 which has $j = \frac{3}{2}$ we couldn't have something like $j = \frac{5}{2}$, because that would require us to have a state with $J_z = \frac{5}{2}\hbar$ in the multiplet, which we definitely cannot have from our above listing. So there are **four states** here:

$$j = \frac{3}{2} \implies m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}.$$

We must have $m = \frac{3}{2}$ only coming from the top state by our above argument, so

$$\boxed{\left|j = \frac{3}{2}, m = \frac{3}{2}\right\rangle = |1,1\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle}.$$

Similarly, for $m = -\frac{3}{2}$, we can only use the bottom state:

$$\boxed{\left|j = \frac{3}{2}, m = -\frac{3}{2}\right\rangle = |1,-1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle}.$$

But for each of $m = \pm\frac{1}{2}$, we'll need to take some linear combination of the states in each of the rows for $\frac{J_z}{\hbar}$ – it's not so easy to describe them directly right now. And this accounts for four states, and the remaining two states must live in a $j = \frac{1}{2}$ multiplet (it can't be $j = 0$ because all of our m-eigenvalues are $\pm\frac{1}{2}$). Therefore, we can write what we've found as

$$(\ell = 1) \otimes \left(s = \frac{1}{2}\right) = \left(j = \frac{3}{2}\right) \oplus \left(j = \frac{1}{2}\right) :$$

both vector spaces have dimension $3 \times 2 = 4 + 2 = 6$. Before we find the energy splittings, let's try to finish constructing the other four coupled states in our $j = \frac{1}{2}$ and $j = \frac{3}{2}$ multiplets. We'll act with the operator $J_- = L_- + S_-$ on the boxed expression for $\left|j = \frac{3}{2}, m = \frac{3}{2}\right\rangle$: for the left side, we have an equation for how J_- acts on this state, which is

$$\hbar\sqrt{\frac{3}{2}\cdot\frac{5}{2} - \frac{3}{2}\cdot\frac{1}{2}}\left|\frac{3}{2}, \frac{1}{2}\right\rangle = \boxed{\hbar\sqrt{3}\left|\frac{3}{2}, \frac{1}{2}\right\rangle}.$$

To deal with the right hand side, we'll act with the operator $J_- = L_- \otimes I + I \otimes S_-$. This yields

$$J_-\left(|1,1\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle\right) = L_-|1,1\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + |1,1\rangle \otimes S_-\left|\frac{1}{2}, \frac{1}{2}\right\rangle,$$

and now we use the formula for lowering operators again:

$$= \hbar\sqrt{1\cdot 2 - 1\times 0}\,|1,0\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + |1,1\rangle \otimes \hbar\sqrt{\frac{1}{2}\cdot\frac{3}{2} - \frac{1}{2}\cdot -\frac{1}{2}}\left|\frac{1}{2}, -\frac{1}{2}\right\rangle,$$

which evaluates to

$$\boxed{\hbar\sqrt{2}\,|1,0\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + \hbar\,|1,1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle}.$$

So now we can set the two sides equal, and we find that

$$\boxed{\left|j = \frac{3}{2}, m = \frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\,|1,0\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\hbar\,|1,1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle}.$$

We can do a similar thing to find $\left|j = \frac{3}{2}, m = -\frac{1}{2}\right\rangle$ by raising $\left|j = \frac{3}{2}, m = -\frac{3}{2}\right\rangle$ with the J_+ operator: the calculations

are very similar, and we end up with

$$\boxed{\left|j=\frac{3}{2}, m=-\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\hbar\left|1,-1\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle}.$$

Indeed, these ended up being linear combinations of the states where $\frac{J_z}{\hbar}$ are $\pm\frac{1}{2}$, respectively, and the states have ended up normalized as well.

This means we've now constructed the entire $j=\frac{3}{2}$ multiplet: this isn't necessary if we just care about the energy splittings, but it's nice to have a concrete expression.

Now we just need to build the $j=\frac{1}{2}$ multiplet, and we can do that in a few different ways. We want $\left|\frac{1}{2},\frac{1}{2}\right\rangle$ and $\left|\frac{1}{2},-\frac{1}{2}\right\rangle$, which are going to use the same uncoupled states as $\left|\frac{3}{2},\frac{1}{2}\right\rangle$ and $\left|\frac{3}{2},-\frac{1}{2}\right\rangle$, but the key idea is that we're forming an **orthonormal basis** (because eigenstates of Hermitian operators with different eigenvalues are orthogonal). So up to a sign, there's only one possible solution: it's going to be

$$\boxed{\left|j=\frac{1}{2}, m=\frac{1}{2}\right\rangle = -\frac{1}{\sqrt{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\hbar\left|1,1\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle},$$

$$\boxed{\left|j=\frac{1}{2}, m=-\frac{1}{2}\right\rangle = -\frac{1}{\sqrt{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\hbar\left|1,-1\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle}.$$

(The central idea here is that the vector $\begin{bmatrix}a\\b\end{bmatrix}$ is orthogonal to $\begin{bmatrix}-b\\a\end{bmatrix}$, so that's all we need to do to our coefficients.) And we can indeed check that these are states with $j=\frac{1}{2}$ – we've chosen our signs so that having J_- act on $\left|j=\frac{1}{2}, m=\frac{1}{2}\right\rangle$ will yield $\left|j=\frac{1}{2}, m=-\frac{1}{2}\right\rangle$.

And now we can wrap everything up: remember that our energy perturbation looks like

$$\Delta H = \frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2}\frac{1}{r^3}\frac{1}{2}(J^2-L^2-S^2),$$

but because we're looking at the $\ell=1$ case, the eigenvalue of L^2 is always $\hbar^2\cdot 1\cdot 2 = 2\hbar^2$, and similarly the eigenvalue of S^2 is always $3\cdot\frac{\hbar^2}{4}$. Thus,

$$\Delta H = \frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2}\frac{1}{r^3}\frac{\hbar^2}{2}\left(\frac{J^2}{\hbar^2}-2-\frac{3}{4}\right).$$

Since we're working with eigenstates of J^2 in our **coupled basis**, this parenthetical term is just $j(j+1)-\frac{11}{4}$. The matrix ΔH is now a diagonal matrix because our new states are orthogonal and eigenstates of J^2, which is what we were trying to achieve all along – now we can finally write down the perturbation of energy in our new state, which is

$$\Delta E_{j,m} = \frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2}\left(\int_0^\infty r^2 dr \psi_1^*(r)\psi_1(r)\frac{1}{r^3}\right)\cdot\frac{\hbar^2}{2}\left(j(j+1)-\frac{11}{4}\right) = \boxed{\frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2}\left\langle\frac{1}{r^3}\right\rangle_{\ell=1,n=2}\cdot\left(j(j+1)-\frac{11}{4}\right)}.$$

The expectation value of $\frac{1}{r^3}$ is known: in general, it turns out that

$$\left\langle\frac{1}{r^3}\right\rangle_{\ell,n} = \frac{1}{\ell\left(\ell+\frac{1}{2}\right)(\ell+1)}\cdot\frac{1}{n^3}\cdot\frac{1}{a_0^3}.$$

But we'll just set

$$\Delta E_0 = \frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2}\left\langle\frac{1}{r^3}\right\rangle_{\ell=1,n=2},$$

which is some energy which is on the order of α^2 compared to the ground state energy of the hydrogen atom, and

now

$$\Delta E_{j,m} = \Delta E_0 \left(j(j+1) - \frac{11}{4} \right).$$

This means that we started off with six degenerate states at this level $\ell = 1, n = 2$. Four of them have the same energy after splitting: plugging in $j = \frac{3}{2}$, we find that those four states **go up** by ΔE_0. THe other two states have a different energy after splitting: plugging in $j = -\frac{1}{2}$, those two states will **go down** by $2\Delta E_0$. And we've solved an interesting problem without needing to write down the complicated six-by-six matrix! In general, we'll figure out how to figure out the right hand sides of tensor product equations like

$$1 \otimes \frac{1}{2} = \frac{3}{2} + \frac{1}{2},$$

and if we care about energy splittings, that's all we will need to know.

38 April 27, 2020

We'll be spending most of the time in the rest of this class on addition of angular momentum, but today we'll mostly focus on the upcoming test for Wednesday. (As a housekeeping reminder, we have just one more homework assignment – it's due next Friday. The general pace of this class will go down in the last two weeks because of this exam.)

Problems on uncertainty and compatible observables will be the first explicitly covered topic on this exam, and questions up to problem set 7 are fair game (so up to angular momentum). We'll spend this recitation doing some practice problems.

Problem 279

What are the traces of J_x and J^2 for the $j = \frac{3}{2}$ multiplet?

We know that there are four different allowed values of m for this value of j, meaning there are four basis vectors that span the multiplet: they are $\left| j = \frac{3}{2}, m \right\rangle$ for $m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$. Thus, the matrices J_x and J^2 are both 4×4 matrices, meaning the trace of any operator A looks like

$$\text{tr}(A) = \sum_m \left\langle \frac{3}{2}, m \middle| \hat{A} \middle| \frac{3}{2}, m \right\rangle,$$

where we sum over the values of m above.

We know that all states here are eigenvectors of J^2 with eigenvalue $\hbar^2 j(j+1) = \frac{15\hbar^2}{4}$ (so the matrix is diagonal with all diagonal entries $\frac{15\hbar^2}{4}$), so the trace for J^2 will be $4 \cdot \frac{15\hbar^2}{4} = \boxed{15\hbar^2}$. To find the trace for J_x, we can write it as $\frac{J_+ + J_-}{2}$ and find the traces of the raising and lowering operators: since no state is left invariant, both of those traces are zero, so the answer is just $\boxed{0}$ for J_x.

Alternatively, remember that J_z is the operator

$$\begin{bmatrix} \frac{3}{2}\hbar & 0 & 0 & 0 \\ 0 & \frac{\hbar}{2} & 0 & 0 \\ 0 & 0 & -\frac{\hbar}{2} & 0 \\ 0 & 0 & 0 & -\frac{3\hbar}{2} \end{bmatrix}$$

(the eigenvalues of J_z are $\hbar m$, so we have a diagonal matrix). And the trace of this matrix is 0, so we should expect that the trace of J_x is also zero. Indeed, we can write this as a **commutator**, which always has trace zero for

finite-dimensional vector spaces:

$$\operatorname{tr}(J_x) = \operatorname{tr}\left(\frac{1}{i\hbar}[J_y, J_z]\right) = \operatorname{tr}\left(\frac{1}{i\hbar}(J_yJ_z - J_zJ_y)\right) = 0.$$

Indeed, this means that **any** angular momentum operator will always have zero trace.

One thing to keep in mind is that the identity operator

$$I = \frac{1}{i\hbar}[\hat{x}, \hat{p}]$$

does have infinite trace, even though it is written as a commutator. But this is just because we're working with infinite dimensional vector spaces, where we have to be more careful.

Problem 280

Define (for any $\gamma \in \mathbb{R}$)

$$S(\gamma) = \exp\left(-\frac{\gamma}{2}(\hat{a}^\dagger\hat{a}^\dagger - \hat{a}\hat{a}\right).$$

Calculate $f(\gamma) = S^\dagger(\gamma)\hat{a}S(\gamma)$ in terms of $\hat{a}^\dagger$ and $\hat{a}$.

We know that $S(\gamma)$ is a **unitary operator**, because $-\frac{\gamma}{2}(\hat{a}^\dagger\hat{a}^\dagger - \hat{a}\hat{a}$ (the expression inside the exponential) is anti-Hermitian. (One notable thing that we can verify is that $(e^A)^\dagger = e^{(A^\dagger)}$.) That means that one way we can calculate this is to commute the commutator in

$$S^\dagger(\gamma)\hat{a}S(\gamma) = S^\dagger(\gamma)S(\gamma)\hat{a} + S^\dagger(\gamma)[\hat{a}, S(\gamma)],$$

or to use the formula $e^ABe^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \cdots$. But another way is to consider the derivative

$$\frac{d}{d\gamma}f(\gamma) = \frac{dS^\dagger}{d\gamma}\hat{a}S(\gamma) + S^\dagger(\gamma)\hat{a}\frac{dS(\gamma)}{\gamma}:$$

bringing down the terms in the chain rule (by putting them next to the middle term) yield the commutator

$$= S^\dagger(\gamma)\left[-\frac{1}{2}(\hat{a}^\dagger\hat{a}^\dagger - \hat{a}\hat{a}), \hat{a}\right]S(\gamma),$$

and this commutator turns out to be $\hat{a}^\dagger$. And taking a second derivative yields

$$\frac{d^2f}{d\gamma} = S^\dagger(\gamma)\hat{a}S(\gamma) = f,$$

which means that $f = A\cosh\gamma + B\sinh\gamma$ for some A, B. Using the initial conditions yields $\boxed{f = \cosh\gamma\hat{a} - \sinh\gamma\hat{a}^\dagger}$.

Problem 281

What is $\langle\beta|H|\alpha\rangle$, where α, β are coherent states and H is the (one-dimensional) simple harmonic oscillator Hamiltonian?

We can rewrite the Hamiltonian so this expression becomes

$$\left\langle\beta\middle|\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\middle|\alpha\right\rangle.$$

This can then be rewritten as

$$= \hbar\omega\left(\langle\beta|\hat{a}^\dagger\hat{a}|\alpha\rangle + \frac{1}{2}\langle\beta|\alpha\rangle\right),$$

and now remember that $|\alpha\rangle$ is an eigenvector for $\hat{a}$, so we can let the $\hat{a}$ act on the $|\alpha\rangle$ and the $|a\rangle^\dagger$ act on the $\langle\beta|$ (remembering the complex conjugate):

$$\hbar\omega\left(\langle\beta|\beta^*\alpha|\alpha\rangle + \frac{1}{2}\langle\beta|\alpha\rangle\right)$$

And now all that's left is to compute the bra-ket $\langle\beta|\alpha\rangle$, and that's given in our formula sheet: it's

$$e^{-\frac{1}{2}|\alpha-\beta|^2+i\,\mathrm{Im}(\beta^*\alpha)}.$$

Here's one final problem to think about on our own:

Problem 282

Alice and Bob share an entangled pair of particles in the singlet state. Suppose Bob has a cloning machine: how can Alice and Bob use this to communicate a yes-no message without sending any information?

(This gives us a method of instantaneous communication, which is not physically allowed – that's why we have the no cloning theorem.) Basically, just have Alice measure along x if the answer is "Yes" and along z if the answer is "No." Afterward, Bob can clone many copies of his (now edited) state, and try measuring along the x and z-directions: only one of these will always yield the same answer.

39 Addition of Angular Momentum, Part 2

We'll begin discussing addition of angular momentum more generally now, and we'll start with the most important and simplest example:

Example 283

Consider the addition of angular momentum for two spin 1/2 particles.

As always, we label angular momentum states with two labels – we'll use $|s,m\rangle$ here (because we have spin and not orbital angular momentum here), and we have the operator S^2 (analogous to J^2) such that

$$S^2|s,m\rangle = \hbar^2 s(s+1)|s,m\rangle,$$

and also the operator S_z (analogous to J_z)

$$S_z|s,m\rangle = \hbar m|s,m\rangle.$$

So $|s,m\rangle$ are the simultaneous eigenstates for S^2 and S_z for a single particle. When we want to introduce two particles, we'll end up with two vector spaces V_1, V_2 and two sets of spin operators $\vec{S}^{(1)}$ and $\vec{S}^{(2)}$: thus, we need to write things in the tensor product formalism here.

In the case with spin 1/2, the particles' individual states can be written with basis

$$\left|\frac{1}{2},\pm\frac{1}{2}\right\rangle_1, \quad \left|\frac{1}{2},\pm\frac{1}{2}\right\rangle_2.$$

When we take the tensor product, we'll now have four basis states (pick one of the states for particle 1 and one of the states for particle 2), and in this space we'll have the total angular momentum operator

$$\hat{S}_i = \vec{S}_i^{(1)} \otimes I + I \otimes \vec{S}_i^{(2)}.$$

We'll organize our states with respect to this tensor product: we know that

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle_2$$

have both particles spin up,

$$\left|\frac{1}{2},-\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle_2, \quad \left|\frac{1}{2},\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle_2$$

have one particle spin up and one particle spin down, and

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle_2$$

have both particles spin down. We'll want to look at our states in terms of **total angular momentum in the z-direction**, which we find by adding up the angular momentum of the first and second particles: since the z-component for a single particle $|s,m\rangle$ is $\hbar m$, we can just add up the contributions for our four states, and we find that

$$S_z = S_z^{(1)} \otimes I + I \otimes S_z^{(2)}$$

will be $\hbar$ for the first state, 0 for the two middle states, and $-\hbar$ for the last two states.

Our next step is to rearrange this uncoupled basis, much like we did last lecture, so that we can have eigenstates for the **total** angular momentum as well. Since one of our states has $m = 1$, we need an $s = 1$ multiplet here (which gives us $m = 1, 0, -1$), and then we'll also need an $s = 0$ multiplet (which is the only value of s that yields a singlet). So our total space

$$V_1 \otimes V_2 = (s = 1) \oplus (s = 0),$$

which means we can write

$$\boxed{\left(s = \frac{1}{2}\right) \otimes \left(s = \frac{1}{2}\right) = (s = 1) \oplus (s = 0)}.$$

So now let's go ahead and find these new basis states $|s,m\rangle$, where we're now labeling our states by total angular momentum. Remember the formula for our raising and lowering operators for a general angular momentum J:

$$J_\pm |j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\,|j,m\pm 1\rangle\,.$$

For example,

$$J_- \left|\frac{1}{2},\frac{1}{2}\right\rangle = \hbar\sqrt{\frac{1}{2}\cdot\frac{3}{2} - \frac{1}{2}\cdot -\frac{1}{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle,$$

so the lowering operator acts in a simple way on the top state for J_z. We can also find that (now looking at the top state for $j = 1$)

$$J_- |1,1\rangle = \hbar\sqrt{1\cdot 2 - 1\cdot 0}\,|1,0\rangle = \hbar\sqrt{2}\,|1,0\rangle\,.$$

So now we'll specialize to the identification for spin 1/2: we're looking for a multiplet of total spin $s = 1$, and this must contain the top state (the only state with $m = 1$)

$$\boxed{|s = 1, m = 1\rangle = \left|\frac{1}{2},\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle_2}.$$

Similarly, we know that we must have

$$\boxed{|s = 1, m = -1\rangle = \left|\frac{1}{2},-\frac{1}{2}\right\rangle_1 \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle_2},$$

because this is the only state with $m = -1$. So we need to figure out which state corresponds to $|1,0\rangle$ and which corresponds to $|0,0\rangle$, and we just need to use the lowering operator on $|1,1\rangle$:

$$S_- |s=1, m=1\rangle = S_- \left(\left| \frac{1}{2}, \frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle_2 \right),$$

and because the total lowering operator can be written as $S_- = S_-^{(1)} \otimes I + I \otimes S_-^{(2)}$, we have

$$\hbar\sqrt{2}\,|s=1, m=0\rangle = \left| \frac{1}{2}, \frac{1}{2} \right\rangle_1 \otimes S_- \left| \frac{1}{2}, \frac{1}{2} \right\rangle_2 + S_- \left| \frac{1}{2}, \frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle_2,$$

and evaluating the lowering operators on the individual vector spaces with our usual formula yields

$$= \hbar \left(\left| \frac{1}{2}, \frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_2 + \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle_2 \right).$$

So moving the constants around, we find that

$$\boxed{|s=1, m=0\rangle = \frac{1}{\sqrt{2}} \left| \frac{1}{2}, \frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_2 + \frac{1}{\sqrt{2}} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle_2},$$

and now we have the full $s = 1$ multiplet. To finish identifying the $s = 0$ singlet, we need to take some linear combination of the $m = 0$ states which is orthogonal to the $|1,0\rangle$ state (this is because they're eigenstates of a Hermitian operator S^2 with different eigenvalues). We can achieve this by switching the sign of one of the terms above, and we'll take

$$\boxed{|s=0, m=0\rangle = \frac{1}{\sqrt{2}} \left| \frac{1}{2}, \frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_2 - \frac{1}{\sqrt{2}} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_1 \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle_2}$$

to get the **singlet state** (remember that this actually made an appearance when we talked about the Bell inequality!). Indeed, looking at these four basis vectors, notice that they are all already normalized, and for example we can verify that (dropping the $\otimes$ for notational convenience)

$$\langle 0,0|1,0\rangle = \frac{1}{\sqrt{2}} \left(\left\langle \frac{1}{2}, \frac{1}{2} \right|_1 \left\langle \frac{1}{2}, -\frac{1}{2} \right|_2 - \frac{1}{\sqrt{2}} \left\langle \frac{1}{2}, -\frac{1}{2} \right|_1 \left\langle \frac{1}{2}, \frac{1}{2} \right|_2 \right) \frac{1}{\sqrt{2}} \left(\left| \frac{1}{2}, \frac{1}{2} \right\rangle_1 \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_2 + \frac{1}{\sqrt{2}} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle_1 \left| \frac{1}{2}, \frac{1}{2} \right\rangle_2 \right)$$

just simplifies to 0. And there are many other tests we can do on these states: for instance, if we act with the raising operator or lowering operator on $|0,0\rangle$, the state will be killed.

So we have solved our problem, but the notation is a bit complicated. Instead, we'll denote $\left|\frac{1}{2}, \frac{1}{2}\right\rangle = |\uparrow\rangle$ and $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = |\downarrow\rangle$, which will make our states look much cleaner:

$$\boxed{|1,1\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 = |\uparrow\uparrow\rangle},$$

$$\boxed{|1,0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_1 \otimes |\downarrow\rangle_2 + |\downarrow\rangle_1 \otimes |\uparrow\rangle_2 \right) = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right)},$$

$$\boxed{|1,-1\rangle = |\downarrow\rangle_1 \otimes |\downarrow\rangle_2 = |\downarrow\downarrow\rangle},$$

$$\boxed{|0,0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_1 \otimes |\downarrow\rangle_2 - |\downarrow\rangle_1 \otimes |\uparrow\rangle_2 \right) = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)}.$$

(The first arrow will tell us about particle 1, and the second arrow about particle 2 – we've simplified the tensor product notation.) And now we're done with this problem: we've figured out what kind of angular momenta occur when we add two spin 1/2 particles.

Example 284

An application of the problem we just considered is the **hyperfine splitting** in the ground state of the hydrogen atom.

We discussed some of these ideas in the previous lecture as well: physically, this happens because the electron can have a spin up or down, which means that the ground state $|n=1,\ell=0,m=0\rangle$ is actually (double-fold) degenerate. If we also consider the proton's spin as well, our hydrogen atom now has two spin 1/2 particles. It turns out that what's relevant is the **interaction** between the two spins: the proton's magnetic dipole creates a magnetic field for the electron.

We'll see through this calculation that some subtle complications will come up when we try to look at the spin 1/2 addition. First of all, remember that the important quantities are the the proton's magnetic dipole

$$\vec{\mu}_p = g_p \frac{e}{2m_p}\vec{S}_p,$$

as well as the electron's magnetic dipole

$$\vec{\mu}_e = -\frac{e}{m_e}\vec{S}_e.$$

Remember that $g_e = 2$ cancels out with the 2 in the denominator, and this g factor tells us what we need to multiply the classical dipole value by to get the quantum value. Because the proton is composed of different parts, it has a weird g_p constant, which is about 5.59. (Even the neutron, which is supposed to be neutral, has a nonzero g_p because the charge isn't symmetrically distributed between its three quarks.) So now we care about the new perturbed Hamiltonian with respect to the reduced-mass nucleus:

$$\Delta H = -\vec{\mu}_e \cdot \vec{B}_p = \frac{e}{m_e}\vec{S}_e \cdot \vec{B}_p,$$

where $\vec{B}_p$ is the magnetic field due to the proton at the electron's current position. We know that this magnetic field due to a dipole usually has a $\frac{1}{r^3}$ dependence, but one thing we may learn in a (later) electromagnetism class is that we need to add a delta function at $r = 0$. (Intuitively, we can produce a dipole by rotating a sphere of charge and taking that radius to 0.) So the point is that we'll have

$$\vec{B}_p(\vec{r}) = \frac{1}{r^3}[\text{(usual dot product term)}] + \frac{2\mu_0}{3}\mu_p\delta(\vec{x}),$$

where μ_0 is the SI permeability of the vacuum.

Remember from last class that the Feynman-Hellmann theorem (in perturbation theory) tells us to look at the expectation value of this extra term ΔH to see how the energy shifts from the ground state. Because there are four generate states (due to up/down spins of the proton and electron), we'll need to diagonalize the matrix of ΔH matrix elements.

We'll start with the four states

$$\psi_{1,0,0} \otimes \begin{bmatrix} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{bmatrix},$$

where $\psi_{1,0,0}$ is the spatial (radial) wave function for the ground state, and we need to figure out how to find eigenstates of our Hamiltonian that we've introduced. All of our states have the same spatial part, so the spin part is what we need to worry about when we diagonalize.

In principle, we should just evaluate $\langle i|\Delta H|j\rangle$ in all states i, j, and it turns out the first $\frac{1}{r^3}$(dot product) term vanishes whenever $\ell = 0$, so we can ignore it – only the delta function is relevant here. So plugging in our magnetic field, the relevant term that contributes to energy differences is

$$\Delta H = \frac{2e}{m_e}\frac{\mu_0}{3}\frac{g_p e}{2m_p}\vec{S}_e \cdot \vec{S}_p \delta(\vec{x}) = \frac{g_p \mu_0 e^2}{3m_e m_p}\vec{S}_e \cdot \vec{S}_p \delta(\vec{x}).$$

If we try to evaluate this expectation value in any state ψ, we find that because nothing else besides ψ, ψ^*, and our delta function have spatial dependence, we'll end up with

$$\langle \psi|\Delta H|\psi\rangle = \frac{g_0 \mu_0 e^2}{3m_e m_p}|\psi_{1,0,0}(0)|^2 \vec{S}_e \cdot \vec{S}_p$$

(the delta function means we just evaluate ψ^* from the bra and ψ on the ket at zero), and we can further simplify by plugging in the wave function for the ground state of hydrogen: we end up with

$$= \frac{g_p \mu_0 e^2}{3\pi m_e m_p}\frac{1}{a_0^3}\vec{S}_e \cdot \vec{S}_p.$$

Our next task will be to deal with this product of spin operators, and the main identity we care about is

$$\vec{S}_e \cdot \vec{S}_p = \frac{1}{2}(S^2 - S_e^2 - S_p^2).$$

(We should remember that there are secretly tensor products here: for example, $\vec{S}_e \cdot \vec{S}_p$ is really $|sum_i \vec{S}_{ei} \otimes \vec{S}_{pi}.$) And we know the eigenvalues of S_e^2 and S_p^2 (because these are just ordinary spin 1/2 things – we'll have $\hbar^2 \cdot \frac{1}{2} \cdot \frac{3}{2} = \frac{3}{4}\hbar^2$, no matter what state we're in). So again, this issue is the **addition of angular momentum** term S^2. We want to find states that are diagonal for the Hamiltonian contribution ΔH, so we need to find the eigenstates for the total angular momentum operator S^2.

This means that we must turn our attention back to the triplet and singlet state that we found earlier in this lecture. These states will have eigenvalue for $\vec{S}_e \cdot \vec{S}_p$ of (plugging in the values we already know)

$$\frac{1}{2}\hbar^2\left(\frac{S^2}{\hbar^2} - \frac{3}{2}\right).$$

Thus, the states in the triplet, corresponding to $s = 1$, will have eigenvalue for S^2 of $2\hbar^2$ and therefore a total eigenvalue $\frac{\hbar^2}{4}$. Meanwhile, the state in the singlet will have eigenvalue $-\frac{3\hbar^2}{4}$. And **because these are eigenstates** for ΔH, we now know our energy shifts:

$$\Delta H = \Delta E \cdot \frac{\vec{S}_e \cdot \vec{S}_p}{\hbar^2},$$

where ΔE is the **difference in energy between the top and bottom splittings** (because some states go up by $\frac{1}{4}\Delta E$, and the other goes down by $-\frac{3}{4}\Delta E$, so the difference is indeed ΔE). And now we know the answer we're looking for: the triplet with total angular momentum $s = 1$ goes up in energy by $\frac{\Delta E}{4}$, and the singlet goes down in energy by $\frac{3\Delta E}{4}$. We can plug in all of the constants now:

$$\Delta E = \frac{g_p \mu_0 e^2}{3\pi m_e m_p}\frac{\hbar^2}{a_0^3},$$

and we can simplify this by using the fact that $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$ in SI units, as well as $\mu_0\varepsilon_0 = \frac{1}{c^2}$, and everything simplifies to

$$\Delta E = \frac{4 g_p \hbar^4}{3 m_p m_e^2 c^2}\frac{1}{a_0^4}.$$

This is still not easy to understand, and plugging numbers in won't really tell us much. Instead, the point is to introduce the fine structure constant $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ in Gaussian units: then a_0^G (a_0, but in Gaussian units) is just $\frac{\hbar^2}{m_e e^2}$, and we'll

end up with

$$\Delta E = \frac{4}{3} g_p \frac{m_e}{m_p} \alpha^4 (m_e c^2).$$

We already know the units work out: $m_e c^2$ has units of energy (in fact, it is the rest mass of the electron) and everything else is unitless. To understand why this is small, note that

$$\alpha^2 (m_e c^2) \sim \text{Bohr energy}$$

(the 13.6 eV constant), and then multiplying by another $\alpha^2 \approx \frac{1}{20000}$ gives us the spin-orbit coupling energy, which is again much smaller. Then including the ratio of masses makes this ΔE smaller still: now we can plug in all the numbers, and we end up with

$$\Delta E = 5.88 \times 10^{-6} \text{ eV}.$$

To understand the significance of this, suppose that a photon transitions between this splitting of energy levels – we'll get an emitted wavelength of

$$\lambda = \frac{c}{\nu} = \frac{c}{\Delta E / h} = \frac{2\pi \hbar c}{\delta E} \approx \frac{2\pi \cdot 197 \text{ MeV} \cdot \text{ fm}}{5.88 \times 10^{-6} \text{ eV}},$$

where 1 fm is 10^{-13} centimeters, and then simplifying out the units yields an answer around **21.1 centimeters** – this means that measuring the decay from this hyperfine splitting will give us a **hyperfine splitting line** for a wave around 1420 MHz.

But it turns out that the probability of the hydrogen decay is extremely small: the lifetime is about $\frac{1}{3} \times 10^{15}$ seconds, which is about 10 million years. And this phenomenon has useful applications: it helps us measure how fast galaxies are rotating (by looking at how the line moves), and the line is extremely sharp because of the uncertainty arguments we made earlier in the class.

Let's move on: we'll now try to make more general statements about adding angular momentum, and we'll develop a systematic way of discussing this kind of problem. Suppose we consider the vector space of two-state systems containing **all possible** angular momenta: write the individual vector spaces as

$$\mathcal{H}_1 = \bigoplus_{j_1} \mathcal{H}_1^{(j_1)}, \mathcal{H}_2 = \bigoplus_{j_2} \mathcal{H}_2^{(j_2)},$$

and our goal will be to construct tensor products between $\mathcal{H}_1$ and $\mathcal{H}_2$. Remember that each value of j corresponds to a subspace which we can also write as a direct sum (it's some j multiplet):

$$\mathcal{H}_1^{(j_1)} = \bigoplus_{m_1} |j_1, m_1\rangle, \quad \mathcal{H}_2^{(j_2)} = \bigoplus_{m_2} |j_2, m_2\rangle.$$

We know that we already have angular momentum operators $\vec{J}_1, \vec{J}_2$ on the two spaces, and we're going to tensor some states in $\mathcal{H}_1$ and $\mathcal{H}_2$ together. For a **fixed** j_1, j_2, consider the tensor product space

$$V_{j_1 j_2} = \mathcal{H}_1^{(j_1)} \otimes \mathcal{H}_2^{(j_2)},$$

which means we are considering a spin from each vector space. Since j_1, j_2 are fixed here, we can define the "sum of angular momentum" operator. To understand how it acts on the vector space $V_{j_1 j_2}$, we use a basis defined via

$$|j_1, j_2, m_1, m_2\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

(we keep the notation with j_1, j_2 just to remind ourselves what space we're looking at).

Definition 285

The **uncoupled basis** for a vector space V_{j_1,j_2} is the set of vectors $|j_1, j_2, m_1, m_2\rangle$ (where m_1 and m_2 range over all allowed values).

Because there are $2j_1+1$ possible values for m_1 and $2j_2+1$ possible values for m_2, we have that

$$\dim V_{j_1,j_2} = (2j_1+1)(2j_2+1).$$

These uncoupled basis states are relevant because they tell us the eigenvectors of operators for the individual states V_1 and V_2: after all, associated with these uncoupled states, we have a complete set of commuting observables, which includes J_1^2, J_2^2, J_{1z} and J_{2z}. But we want to recognize our states in terms of the total angular momentum instead, so we need to reconstruct our basis in general to have eigenvectors of the total angular momentum operators. Now we'll define our **total angular momentum** operator

$$\vec{J} = \vec{J}_{(1)} \otimes I + I \otimes \vec{J}_{(2)},$$

which acts on V_{j_1,j_2}, and we'll try to construct a new orthonormal basis consisting of eigenvalues of a new set of commuting observables. That set of observables will be

$$\{J_1^2, J_2^2, J^2, J_z\}.$$

We first check that these indeed commute with each other – indeed, J_1^2 commutes with everything in the first vector space, and it doesn't need to interact with anything in the second vector space. Since J^2 and J_z are built from J_1 and J_2s, we indeed show that J_1^2 commutes with everything, and we can continue this logic for the other observables.

Then we can check that we can't add other commuting observables either – for example, J_{1z} won't commute with J^2. But ultimately, what this set of commuting observables allows us to do is to label our **coupled basis states** with the indices

$$|j_1, j_2, j, m\rangle .$$

(Here, j_1 corresponds to the eigenvalue $\hbar^2 j_1(j_1+1)$ of J_1^2, j_2 corresponds to that of J_2^2, and similarly j and m tell us the eigenvalues of J^2 and J_z.) So what we're claiming physically is that the **total angular momentum operator keeps us inside the state space** V_{j_1,j_2}, and we can in fact break up the space into (a direct sum of) subspaces, each of which corresponds to a specific representation of total angular momentum.

But we do need to figure out how to find the possible values of j and m (that is, which ones appear for a given j_1 and j_2), and we also need to understand how we get a given coupled state with some j and m from our uncoupled states (which have some j_1 and m_1). This means we need to understand how to start with the completeness relation

$$\sum_{m_1,m_2} |j_1, j_2; m_1, m_2\rangle \langle j_1, j_2; m_1, m_2| = I$$

(which says that our **uncoupled** basis states span the space) and turn it into a statement about our coupled basis states by multiplying both sides by $|j_1, j_2, j, m\rangle$, which gives us

$$\sum_{m_1,m_2} |j_1, j_2; m_1, m_2\rangle \langle j_1, j_2; m_1, m_2 | j_1, j_2, j, m\rangle = |j_1, j_2, j, m\rangle .$$

But now this bra-ket term is just a number, so figuring out how to evaluate it will tell us how to get the coupled basis states as a linear combination of the uncoupled basis states! That's what we've been doing out explicitly in the past

few examples, and now we want to speak in more generality:

Definition 286

The numbers

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2, j, m \rangle$$

are called the **Clebsch-Gordon coefficients**.

We've already seen a few examples of how to find these coefficients – it involves using raising and lowering operators to get a recursive formula, and there isn't really a simple way of finding the values without going through that computation. So there are actually tables for this, and we'll also get some practice for doing everything out ourselves, but we'll focus now on the question of **when these coefficients are zero** and **which js appear in this addition of angular momentum**.

Proposition 287

Whenever $m \neq m_1 + m_2$,

$$\langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m \rangle = 0.$$

In other words, we only get a contribution from a state if the angular momenta in the z-direction add up properly.

Proof. We know that

$$\langle j_1, j_2, m_1, m_2 | J_z | j_1, j_2, j, m \rangle = \langle j_1, j_2, m_1, m_2 | J_{1z} + J_{2z} | j_1, j_2, j, m \rangle ,$$

and because we know that our states are eigenvalues of the relevant operators we've included in this equation, we can replace everything with its eigenvalue:

$$\langle j_1, j_2, m_1, m_2 | \hbar m | j_1, j_2, j, m \rangle = \langle j_1, j_2, m_1, m_2 | \hbar (m_1 + m_2) | j_1, j_2, j, m \rangle$$

(where we've had the $J_{1z} + J_{2z}$ act on the bra vector and used the fact that all eigenvalues are real). Therefore, we can move everything to one side to get

$$\hbar (m - m_1 - m_2) \langle j_1, j_2, m_1, m_2 | j_1, j_2, j, m \rangle = 0,$$

which is exactly the result we want (at least one of the terms in the product must be zero). □

In other words, the quantum number m is easy to deal with, and now we'll move on to understanding which j values appear.

Proposition 288

The values of j that come in the addition of angular momentum are

$$|j_1 - j_2| \leq j \leq j_1 + j_2,$$

where we go down by 1 each time starting from $j_1 + j_2$.

This can be thought of in a "triangle inequality" way: the largest possible j value we can get is if j_1 and j_2 line up, and the smallest is if they point in opposite directions. Another way to write this is that

$$J_1 \otimes J_2 = (J_1 + J_2) \oplus (J_1 + J_2 - 1) \oplus \cdots \oplus (|J_1 - J_2|).$$

We can check that this is consistent with the simple cases we already have, and also it is nice that the **dimensions actually match up**: the dimension on the left side is $(2j_1+1)(2j_2+1)$, and if we add up the dimensions on the right side, we will also end up with that same constant. We'll check that fact:

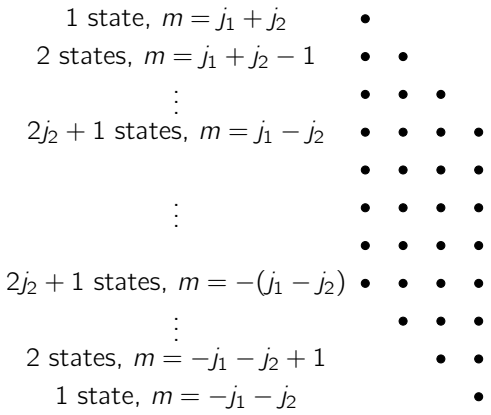
Proposition 289

For half-integers $j_1, j_2 > 0$, we have

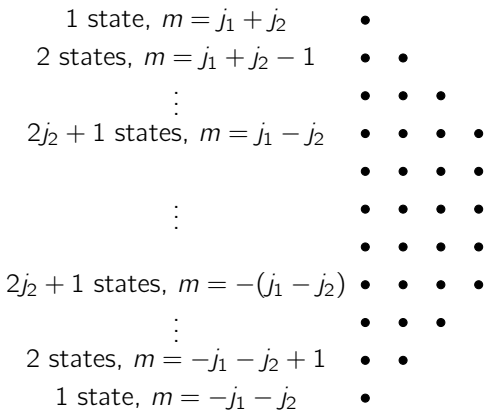
$$(2j_1+1)(2j_2+1) = (2(j_1+j_2)+1) + \cdots + (2(|j_1-j_2|+1).$$

Proof. Without loss of generality assume $j_1 > j_2$ (relabel otherwise). The right side is an arithmetic sequence with average $2j_1+1$ and a total of $2j_2+1$ terms, and that yields the result. □

We'll finish by explaining pictorally how our uncoupled states $|j_1, j_2, m_1, m_2\rangle$ break down into the j-multiplets. First of all, if we take $j_1 > j_2$, we will draw each of the groups with a fixed m_2 in its own column, with vertical height corresponding to the value of $m = m_1 + m_2$. Then there are $2j_2+1$ total columns, each with $2j_1+1$ different values of m_1, and they're arranged in the following kind of pattern:



Notice that the number of states goes up to $2j_2+1$, stays there for a while, and then goes back down. But now we know that j-multiplets are groups of these states from top to bottom, and (for example) the topmost state must be in a multiplet with $j = j_1 + j_2$. Rearrange as shown:



And now the vertical lines correspond exactly to the j-multiplets that we want! The left-most has states ranging from $m = -(j_1+j_2)$ to (j_1+j_2), so $j = j_1+j_2$, and the right-most has states ranging from $m = -(j_1-j_2)$ to (j_1-j_2), so it has $j = j_1 - j_2$. And because we've verified that the dimensions add up, this is indeed the correct set of j-values to use.

40 May 4, 2020

The distribution of grades on the test was pretty broad (average around 70, standard deviation around 20). We're nearing the end of the class now – addition of angular momentum is our final main topic. (We'll still discuss density matrices in the last lecture, which is a new addition to the course – they used to be in 8.06, but they've disappeared from the cUrriculum over the years.) There will be one last assignment for this Friday, and then we will have our final exam.

Fact 290

We don't cover path integrals in 8.05 or 8.06, because they don't help very much in more elementary study and require lots of work to find use in quantum field theory. But we can write our term paper on them when we get to 8.06.

We'll start today by discussing the basics of angular momentum. We can start by thinking about the hydrogen atom

$$H = \frac{\vec{p}^2}{2m} - \frac{e^2}{r},$$

where $a_0 = \frac{\hbar^2}{me^2}$ is the Bohr radius, and $E = -\frac{e^2}{2a_0}\frac{1}{n^2}$ is the ground state energy (where $n = \ell + \nu$ is the principal quantum number). If we let $\hat{L}_i$ be the orbital angular momentum operators, then we have

$$[H, \hat{L}_i] = 0,$$

because the $\hat{L}_i$s "generate rotations," the $\frac{\vec{p}^2}{2m}$ always commutes (it's a vector under rotations), and then the $-\frac{e^2}{r}$ is a **central potential**. Meanwhile, with the new theory we've been discussing

$$[H, \hat{S}_i] = 0,$$

where $\hat{S}_i$s are the electron's spin operators, because the H affects the **spatial component** of the wavefunction, not the spin – therefore, the two operators live in different tensor product spaces. One way we can write this is that $H = \left(\frac{p^2}{2m} - \frac{e^2}{r}\right) \otimes I_{2\times 2}$, but we can also suppress the tensor product symbol itself.

So we want to come up with a complete set of commuting observables (to give us freedom in diagonalizing multiple operators at once). We always want energy eigenstates, so we always want to include H, and we want L^2 and L_z because introducing L_z allows us to label our states with values of m, and introducing L^2 allows us to label with values of ℓ (so that we can get a state $|\ell, m\rangle$). And if we have a spin for the electron, we also need to introduce $\hat{S}^2$ and S_z. It might seem like $\hat{S}^2$ is trivial or that it isn't useful – any spin 1/2 state has eigenvalue $\frac{\hbar^2}{4} + \frac{\hbar^2}{4} + \frac{\hbar^2}{4} = \frac{3\hbar^2}{4}$, but the purpose is to start developing a system for adding together angular momentum, and we don't quite need to label all of our states with a value of s (since it's always $\frac{1}{2}$ in this case). So we just label our states in the hydrogen atom + spin system with

$$|n, \ell, m, m_s\rangle,$$

which fully characterize our new system.

We know that the $\ell = 0$ states start with $n = 1$, the $\ell = 1$ states start with $n = 2$, and so on. But remember that we have multiplets for each (n, ℓ). Whenever $\ell = 0$, there are two states (up and down for the spin). Then whenever $\ell = 1$, we have **six** states (three possibilities for m, two possibilities for m_s), and whenever $\ell = 2$, there are **ten** states. And each of these states can be thought of as eigenstates for our operators, but interpreting what these quantum numbers n, ℓ, m mean also has significance in chemistry.

To analyze this system more, note that we're using **uncoupled basis states** – the spin and orbital angular momentum are not being related to each other, and in fact nothing is really talking to the m_s. But there is in fact a correction we should be making to the Hamiltonian, related to the **fine structure**, which comes up because of relativistic movement: as we saw in lecture, **spin-orbit coupling** means that some of our states in each multiplet (n, ℓ) move up or down in energy and split apart.

To study this more complicated system, we need to be more careful about how which operators actually commute. We now have a new (fine-structure) Hamiltonian

$$H_T = H + H_{f.s.},$$

where we've introduced a $\vec{S} \cdot \vec{L}$ term, and we now care about whether our operators still commute. $[H_T, \vec{L}^2] = 0$ works out, because $\vec{L}^2$ commutes with everything made up of Ss and Ls, and similarly $[H_T, \vec{S}^2] = 0$. But we should remember that there are secretly tensor products everywhere:

$$\vec{S} \cdot \vec{L} = S_x \otimes L_x + S_y \otimes L_y + S_z \otimes L_z,$$

and now we know that we do **not** have $[H_T, \hat{L}_z] = 0$: even though $\hat{L}_z$ commutes with the original Hamiltonian, the different L_i operators don't commute. And similarly $[H_T, \hat{S}_z] \neq 0$, so our list of commuting observables only contains $\{H_T, L^2, S^2\}$ right now – we need to more to properly characterize our states.

So here's where addition of angular momentum comes in: we construct the operator

$$J^2 = (L + S)^2 = L^2 + S^2 + 2\vec{L} \cdot \vec{S}.$$

We can now check whether our new Hamiltonian commutes with $J_i = L_i + S_i$. The original Hamiltonian works with all of these operators, and now we just need to check whether

$$[\vec{L} \cdot \vec{S}, L_i + S_i] \stackrel{?}{=} 0.$$

But we can solve for the dot product: we know that $2\vec{S} \cdot \vec{L} = J^2 - L^2 - S^2$, so it's equivalent to ask whether

$$[J^2 - L^2 - S^2, J_i] = 0.$$

L^2 and S^2 commnute with anything here, and J^2 commutes with J_i by the algebra of angular momentum. So this does indeed work out, and now we can expand our set of commuting operators to

$$[H_T, L^2, S^2, J^2, J_z].$$

And now these five operators mean that we can label our states via

$$|n, \ell, j, m_j\rangle$$

(again we supress $s = \frac{1}{2}$ because it's the same for all states). These are the labels for the observables relevant to our perturbed Hamiltonian, and now we have **coupled basis states**: we keep ℓ, but we replace m, m_s (the individual azimuthal quantum numbers) with j, m_j (the numbers related to the addition of angular momentum). As we have seen in the lectures now, this allows us to make statements like

$$2 \otimes \frac{1}{2} = \frac{5}{2} \oplus \frac{3}{2},$$

where the left side represents (m, m_s) representations and the right side represents (j, m_j) representations. And then

we use the notation (nL_j) to denote these subspaces, using the letters $S, P, D, \cdots$ for $\ell = 0, 1, 2, \cdots$ – for example, the ten states at $n = 3, \ell = 2$ organize themselves into a $3D_{5/2}$ group and a $3D_{3/2}$ group. And we'll learn in 8.06 that the perturbations of energy ΔE are actually just functions of n and j alone.

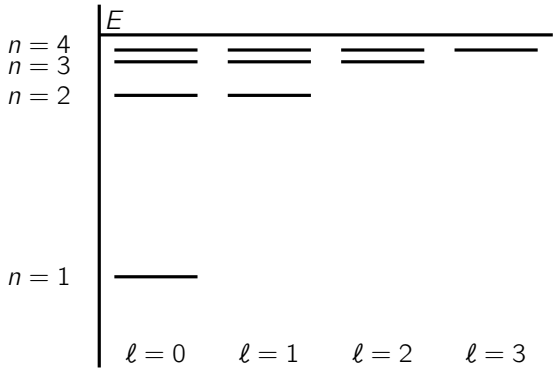
41 Addition of Angular Momentum, Part 3

We'll start with a review of some important ideas: recall that $J_1 \otimes J_2$ means we have some states in an angular momentum in a $J_1 = j_1$ multiplet, and we also have some states in a $J_2 = j_2$ multiplet, and we have these two (commuting) angular momenta act on different particles or different degrees of freedom in a single particle. The key identity to remember is that

$$J_1 \otimes J_2 = (J_1 + J_2) \oplus (J_1 + J_2 - 1) \oplus \cdots \oplus (|J_1 - J_2|),$$

where all representations on the right live in the **tensor product space** and are multiplets of our new angular momentum $\vec{J} = \vec{J_1} + \vec{J_2}$. The basis states on the left form the uncoupled basis, and the basis states on the right form the coupled basis.

Our first goal for this lecture will be to understand the spectrum of the hydrogen atom. Recall that the spectrum when we don't care about spin looks like the following:



Here, the energies at level n are

$$E_n = -\frac{e^2}{2a_0}\frac{1}{n^2},$$

where a_0 is the usual Bohr radius, and for each n we have states for each of $\ell = 0, 1, 2, \cdots, (n-1)$. This means that for each level n, we have a total of n^2 energy states (we can verify this by adding up the states for each ℓ). Our current goal is to understand why we have these n^2 states in this configuration, and we'll need to return to the Runge-Lenz vector to do that.

Recall that the Hamiltonian and Runge-Lenz vector we are working with are

$$H = \frac{\vec{p}^2}{2m} - \frac{e^2}{r}, \quad \vec{R} = \frac{1}{2me^2}(\vec{p} \times \vec{L} - \vec{L} \times \vec{p}) - \frac{\vec{r}}{r}.$$

Here, recall that $\vec{R}$ is a constant, unitless vector which points in a fixed direction – classically, that direction is the major axis of the ellipse of rotation. Remember that the classical operator is just $\frac{1}{me^2}(\vec{p} \times \vec{L})$: the corrections we make above account for the fact that $\vec{L}$ and $\vec{p}$ don't commute as operators, and also to make sure that we have

$$[H, \vec{R}] = 0.$$

There are a few other useful properties for this vector operator as well: note that we have the identity

$$\vec{p} \times \vec{L} = -\vec{L} \times \vec{p} + 2i\hbar\vec{p},$$

and we can plug this into our expression for $\vec{R}$ (in either direction) to find

$$\vec{R} = \frac{1}{me^2}(\vec{p} \times \vec{L} - i\hbar\vec{p}) - \frac{\vec{r}}{r} = \frac{1}{me^2}(-\vec{L} \times \vec{p} + i\hbar\vec{p}) - \frac{\vec{r}}{r}.$$

But we still need to understand this conserved quantity better, and here is where we do something trickier. Since $\vec{R}$ is conserved, so is $\vec{R}^2$, and doing out the computation yields the conserved quantity

$$\vec{R}^2 = 1 + \frac{2H}{me^4}(\vec{L}^2 + \hbar^2).$$

(Indeed, H and $\vec{L}^2$ are both conserved, so everything checks out here.) To make more progress, we'll need to learn a bit more about these operators we're constructing: in order to relate the Runge-Lenz vector to something we already know well, let's try to evaluate $\vec{R} \cdot \vec{L}$. Remember that we already showed earlier in the class that

$$\vec{r} \cdot \vec{L} = \vec{p} \cdot \vec{L} = 0$$

(this was clear classically but required a bit more symbol pushing in the quantum case), which means that most terms in

$$\vec{R} \cdot \vec{L} = \left(\frac{1}{me^2}(\vec{p} \times \vec{L} - i\hbar\vec{p}) - \frac{\vec{r}}{r}\right) \cdot \vec{L}$$

disappear immediately – we're just left with the term that is proportional to $(\vec{p} \times \vec{L}) \cdot \vec{L}$. If there aren't any identities that immediately come to mind, we can just bash this with index notation: we get

$$(\vec{p} \times \vec{L})_i \vec{L}_i = \varepsilon_{ijk} p_j L_k L_i.$$

From here, it's tempting to say that k and i are symmetric in the L operators while ε_{ijk} is antisymmetric, so everything cancels out. The expression is indeed zero, but the explanation is incorrect – remember that L_k and L_i don't commute! So we need to be more careful: we can write this expression as

$$= \varepsilon_{jki} p_j L_k L_i = p_j (\vec{L} \times \vec{L})_j,$$

and now remember that we have the commutation relation $\vec{L} \times \vec{L} = i\hbar\vec{L}$, so this then simplifies to

$$= \vec{p} \cdot (i\hbar\vec{L}) = 0.$$

So all of the terms in the expression $\vec{R} \cdot \vec{L}$ vanish, and we're left with $\boxed{\vec{R} \cdot \vec{L} = 0}$. This doesn't necessarily imply that $\vec{L} \cdot \vec{R} = 0$, but we'll see shortly that this is also true.

To proceed, recall that we have the important defining property for a **vector under rotation**

$$[L_i, v_j] = i\hbar\varepsilon_{ijk} v_k,$$

which can be rewritten in terms of cross products as

$$\boxed{\left(\vec{L} \times \vec{v} + \vec{v} \times \vec{L}\right)_i} = \varepsilon_{ijk}(L_j v_k + v_j L_k) = \varepsilon_{ijk}(L_j v_k - v_k L_j),$$

where we've swapped j and k in the second term at the cost of a negative sign in the ε_{ijk} symbol. But now this is just

a commutator

$$\left(\vec{L}\times\vec{v}+\vec{v}\times\vec{L}\right)_i=\varepsilon_{ijk}[L_j,v_k]=i\hbar\varepsilon_{ijk}\varepsilon_{jk\ell}v_\ell,$$

where we've used the vector under rotations property in the last step. And now we can use the identity when we have two such ε symbols: we first reorder to get

$$=i\hbar\varepsilon_{jki}\varepsilon_{jk\ell}v_\ell=2i\hbar\delta_{i\ell}v_\ell=\boxed{2i\hbar v_i}.$$

Since the relation holds for all indices i, this actually gives us the identity

$$\boxed{\vec{L}\times\vec{v}+\vec{v}\times\vec{L}=2i\hbar\vec{v}}$$

whenever $\vec{v}$ is a vector under rotations. And we can apply this to our Runge-Lenz vector $\vec{R}$ – this is because the cross product of two vectors under rotations is still a vector under rotations, meaning all three terms of $\vec{R}$ are vectors under rotations. So we know that

$$\vec{L}\times\vec{R}+\vec{R}\times\vec{L}=2i\hbar\vec{R},$$

and now this is getting us towards the commutation relations that we want. Writing out the above statement index by index yields

$$[L_i,R_j]=i\hbar\varepsilon_{ijk}R_k,$$

and now we finally know why $\vec{R}\cdot\vec{L}$ and $\vec{L}\cdot\vec{R}$ are actually equal: whenever we plug in $i=j$, we have $[L_i,R_i]=0$, so each pair of operators in the dot product $L_1R_1+L_2R_2+L_3R_3$ commute. So we have indeed checked that $\boxed{\vec{L}\cdot\vec{R}=0}$.

But now we'll turn our attention to the last set of commutators we haven't considered, which is $[R_i,R_j]$. Doing this by brute force is difficult – there are lots of terms, and remember that operators like $\frac{1}{r}$ don't commute with $\vec{p}$. So what we'll do is make an argument to show what the answer can be, and then we'll be left with an easier calculation (which we can verify on our own). Essentially, our goal is to compute

$$\vec{R}\times\vec{R}.$$

Here there's no real reason that we should expect $\vec{R}$ to be an angular momentum – the expression is more complicated than that for $\vec{L}$.

Proposition 291

We know that $\vec{R}\times\vec{R}$ is a vector, and in fact the components $[R_i,R_j]$ should be **proportional to a conserved quantity**.

This line of reasoning is interesting: if S_1 and S_2 are symmetries, meaning that $[S_1,H]=[S_2,H]=0$, then $[S_1,S_2]$ is also a symmetry – that is, $[[S_1,S_2],H]=0$. This follows from the **Jacobi identity**

$$[A,[B,C]]+[B,[C,A]]+[C,[A,B]]=0$$

for operators A,B,C (where we plug in S_1,S_2, and H). So we can keep taking commutators to get new conserved quantities, and sometimes (when we're lucky) we get all of the conserved quantities in our system.

So in this system, the conserved vectors are $\vec{L},\vec{R}$, and $\vec{L}\times\vec{R}$, but it's possible that $\vec{R}\times\vec{R}$ is proportional to some linear combination of these. Here we'll use a trick by Schwinger (who also invented the trick for the two-dimensional harmonic oscillator): if we do a **parity transformation** and replace $\vec{r}$ with $-\vec{r}$, then the momentum $\vec{p}$ also changes sign (because it is related to the rate of change of $\vec{r}$), and $\vec{L}=\vec{r}\times\vec{p}$ stays fixed. This means that $\vec{R}$ changes sign, because one operator in each term of the definition changes sign, so $\vec{R}$ changes sign as well.

But now notice that $\vec{R} \times \vec{R}$ will not change sign (both $\vec{R}$s pick up a negative sign), so out of the operators that could potentially be our conserved quantities, only $\vec{L}$ is left! So

$$\vec{R} \times \vec{R} \sim \vec{L},$$

and we can derive the constants to find that our identity is

$$\boxed{\vec{R} \times \vec{R} = i\hbar \left(-\frac{2H}{me^4} \right) \vec{L}}.$$

So now we know all of the relations between L and R, including the commutators and products, and now we want to apply this to our hydrogen atom problem. The idea is that we're going to **come up with two sets of angular momenta**, even though $\vec{R}$ is not an angular momentum.

Proposition 292

We'll start by restricting our problem to a **specific subspace of degenerate energy**: this subspace can have one, two, or more states, but we'll analyze this problem at some fixed energy.

The reason this is a valuable approach is that the operator $\vec{R}^2$ has an H term, and because H commutes with all of our operators here, we can always treat H as a constant (the energy eigenvalue that we're working with in our degenerate subspace), and that will make our calculations easier. So from here on, we'll consider the fixed energy

$$H = -\frac{me^4}{2\hbar^2} \frac{1}{\nu^2},$$

where ν is some arbitrary real number. (We write the energy in this specific way because we know that ν will end up being an integer, and this will make our algebra easier later on.) So now we have that

$$-\frac{2H}{me^4} = \frac{1}{\hbar^2 \nu^2},$$

which means we have the simpler-looking formulas

$$\boxed{\vec{R} \times \vec{R} = \frac{i}{\hbar \nu^2} \vec{L}, \quad \vec{R}^2 = 1 - \frac{1}{\hbar \nu^2} (\vec{L}^2 + \hbar^2)}.$$

To make this look even nicer, we can put an $\hbar\nu$ next to each $\vec{R}$, which yields

$$(\hbar\nu\vec{R}) \times (\hbar\nu\vec{R}) = i\hbar\vec{L}, \quad \hbar^2\nu^2\vec{R}^2 = \hbar^2(\nu^2 - 1) - L^2.$$

Writing this in terms of indices and commutators, this also means that we have

$$[\hbar\nu R_i, \hbar\nu R_j] = i\hbar\varepsilon_{ijk} L_k,$$

and we can notice that we can derive these formulas in the same way that we derived the identity $\vec{L} \times \vec{L} = i\hbar\vec{L}$.

And now we're ready to introduce our two angular momenta: we want to take $\hbar\nu\vec{R}$, which has the right units, and add it to something else to get an angular momentum.

Definition 293

Define the angular momenta

$$J_1 = \frac{1}{2}(\vec{L} + \hbar\nu\vec{R}), \quad J_2 = \frac{1}{2}(\vec{L} - \hbar\nu\vec{R}).$$

We don't actually know that these are angular momenta yet, but the units match up and we have some hope. (We can recover $\vec{L}$ by adding J_1 and J_2, and we can recover $\hbar\nu\vec{R}$ by subtracting them.)

First of all, note that J_1 and J_2 **commute with each other**:

$$[J_{1i}, J_{2j}] = \frac{1}{4}[L_i + \hbar\nu R_i, L_j - \hbar\nu R_j],$$

and now we can expand out the commutator and use the commutators we already know to get

$$= \frac{1}{4}\left(i\hbar\varepsilon_{ijk}L_k - \hbar\nu[L_i, R_j] + \hbar\nu[R_i, L_j] - i\hbar\varepsilon_{ijk}L_k\right).$$

The first and last term cancel, and the middle two terms also cancel out (because $[L_i, R_j] - [R_i, L_j] = [L_i, R_j] + [L_j, R_i]$, and now both of these commutators are R_k but with opposite signs in the ε_{ijk} symbol). So we have verified that the commutator of J_{1i} and J_{2j} is zero, meaning they commute for all i, j.

Now we need to show that J_1 and J_2 are indeed angular momenta by showing that they form the appropriate algebra. It suffices to calculate $J_1 \times J_1$ and $J_2 \times J_2$: this yields

$$\frac{1}{4}(\vec{L} \pm \hbar\nu\vec{R}) \times (\vec{L} \pm \hbar\nu\vec{R}),$$

and now this isn't too bad to work with, because we already have all of our formulas for products of $\vec{L}$ and $\vec{R}$. Plugging in the expressions we've derived for each of the terms here, we end up with

$$\frac{1}{4}\left(i\hbar\vec{L} \pm (\vec{L} \times \hbar\nu\vec{R} + \hbar\nu\vec{R} \times \vec{L}) + i\hbar\vec{L}\right) = \frac{1}{4}\left(2i\hbar\vec{L} \pm 2i\hbar \cdot \hbar\nu\vec{R}\right).$$

And indeed, this simplifies to

$$= i\hbar\frac{1}{2}(\vec{L} + \hbar\nu\vec{R}),$$

which is either J_1 or J_2 based on the sign we chose at the beginning. So we've indeed shown that we have **two independent angular momenta in the hydrogen atom!**

And now we're almost done. We know how to write $\vec{L}$ and $\vec{R}$ in terms of our angular momenta, so

$$\vec{L} \cdot \hbar\nu\vec{R} = 0 \implies (\vec{J_1} + \vec{J_2}) \cdot (\vec{J_1} - \vec{J_2}) = 0.$$

Because $\vec{J_1}$ and $\vec{J_2}$ commute, the cross terms will cancel, and this yields

$$\vec{J_1}^2 - \vec{J_2}^2 = 0 \implies \boxed{\vec{J_1}^2 = \vec{J_2}^2}.$$

The squares being equal is interesting, and if we square the definition of J_1, we get

$$\vec{J_1}^2 = \frac{1}{4}(\vec{L}^2 + \hbar\nu\vec{R}^2)$$

(again the cross terms cancel because $\vec{L} \cdot \vec{R} = 0$), and now we can use our expression for $\hbar\nu\vec{R}^2$ to find that this is

$$= \frac{1}{4}(\vec{L}^2 + \hbar^2(\nu^2 - 1) - \vec{L}^2) = \boxed{\frac{1}{4}\hbar^2(\nu^2 - 1)}.$$

And now we've actually solved our problem! We've been working with a degenerate energy subspace in which we have two angular momenta with equal squares: in such a system, we have angular momentum eigenstates with eigenvalues for J_1^2 and J_2^2 being $\hbar^2 j(j+1)$ (where j is a half-integer). Therefore,

$$J_1^2 = J_2^2 = \frac{1}{4}\hbar^2(\nu^2 - 1) = \hbar^2 j(j+1),$$

and solving for ν yields

$$\nu^2 = 1 + 4j(j+1) = (2j+1)^2.$$

This means that because j takes on one of the values $0, \frac{1}{2}, 1, \cdots$, ν must take on one of the values $1, 2, 3, \cdots$, respectively! (This means we can write it with the **principal quantum number** n we've been using in the hydrogen atom.) And because n characterized the allowed energies of our hydrogen atom, we have indeed ended up with the correct allowed energies, which are $-\frac{me^4}{2\hbar^2}\frac{1}{n^2}$ for integer n. Notice that in this problem, we are **not using a spin for the proton or electron**: the angular momenta have just popped out of the representations of our eigenstates. And now we can even recover the structure in the picture above for our spectrum: we've invented the degenerate subspace consisting of vectors

$$|j, m_1\rangle \otimes |j, m_2\rangle ,$$

where we use the same j for both operators J_1 and J_2 because their squares are equal. So this is just the tensor product of a j-multiplet with another j-multiplet, and we know how those play out:

$$j \otimes j = (2j) \oplus (2j-1) \oplus \cdots \oplus 0.$$

And the subspaces on the right are of the **total angular momentum** $J_1 + J_2$, which is exactly that of our ordinary angular momentum $\vec{L}$! So everything falls into place: we have that $n = 2j+1$, and the energy eigenspace at energy level n has states with $\ell = 0$ up to $2j = n-1$, which is exactly what we want.

42 May 6, 2020

We've now seen how we can use the Runge-Lenz vector to construct angular momenta, which helps us predict the structure of every level of the hydrogen atom. Remember that for each principal quantum level n, we have states that run from $\ell = 0$ to $\ell = n-1$, and the Runge-Lenz vector actually helps us move across the various ℓ-multiplets.

Remember that this solution is only valid for the original hydrogen Hamiltonian – the degeneracy is broken once we add the fine structure from the spin-orbit coupling. When we add this extra term to the Hamiltonian, all of the energy levels adjust according to the total angular momentum.

We'll have a lecture about density matrices for next week, which we should read. It's still part of our course, but we won't have any homework problems on it, so we'll only get conceptual questions about it on the final. (The final will not be completely cumulative – it will focus on the later part of the course.)

Today, we'll start with a conceptual discussion related to one of the problem set problems:

Example 294

Suppose we have a particle X, in the rest frame of the lab, which decays into two particles A and B (for instance, a pion π^0 decaying into two photons 2γ).

We can consider the angular momenta of our particles before and after the decay. Even though X is at rest, it may have some spin S_X, and similarly particles A and B have some spin S_A, S_B. We expect that the total angular momentum might be conserved: we can define the quantity

$$\vec{J} = \begin{cases} \vec{S}_X & t < 0 \\ \vec{S}_A + \vec{S}_B + \vec{L} & t \geq 0. \end{cases}$$

Basically, because our particle X is sitting at the center of our frame of reference, there is no orbital angular momentum

at first. But after the decay, it's possible the two particles also have some orbital angular momentum (like with the hydrogen proton and electron) in addition to the spin. But we can put that into a single quantity $\vec{L}$, much like we did with the spin-orbit coupling problem. (And the main thing to keep in mind is that orbital angular momentum isn't always conserved – only the total angular momentum!)

Let's suppose that we are in some initial eigenstate

$$|S_X, m_{S_X}\rangle,$$

so that J^2 has eigenvalue $\hbar^2 S_X(S_X+1)$ and J_z has eigenvalue $\hbar m_{S_X}$. Then these eigenvalues must be the same **after** the decay as well.

Problem 295

Suppose someone claims a neutron decays into a proton and an electron.

The first thing we can check is energy conservation – it is indeed possible, because the neutron is slightly heavier than the proton. Momentum conservation also looks possible – we just need to pick the velocities of our particles accordingly. And charge conservation holds too, so everything here looks like it is consistent so far.

But it turns out this can't actually happen: we know that the neutron, proton, and electron are all spin 1/2 particles, meaning they can be in the states $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ or $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$. So the total angular momentum after the decay, $\vec{S}_p + \vec{S}_{e^-} + \vec{L}$, must be the same as the total angular momentum before the decay. A typical state of the decay product will look like

$$\left|\frac{1}{2}, m_p\right\rangle \otimes \left|\frac{1}{2}, m_e\right\rangle \otimes |\ell, m\rangle$$

where m_p, m_e are the azimuthal quantum numbers for the proton and electron, respectively, and ℓ, m characterize the orbital angular momentum. More abstractly, our states live in the tensor product space

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \ell.$$

We can simplify this product: **the tensor product is associative**, so we can look at $\frac{1}{2} \otimes \frac{1}{2}$ first – it evaluates to $1 \oplus 0$ – so we end up with

$$= (1 \oplus 0) \otimes \ell = (1 \otimes \ell) \oplus (0 \otimes \ell)$$

(where we've now used **distributivity**), and this finally evaluates to

$$= (\ell + 1) \oplus (\ell - 1) \oplus \ell.$$

But we need to get a state of total angular momentum $\frac{1}{2}$, and no matter what the value of ℓ is, the angular momenta will always be integers after the decay! So conservation of angular momentum doesn't work, and this is not possible.

Fact 296

Physicists initially thought that such a decay was observed, but we can add a particle called an **antineutrino** to the products, and now the decay works: our tensor product space becomes

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \ell,$$

which does have fractional angular momenta.

Remark 297. *We may hear about "highly forbidden processes," which can only happen from the action of a highly*

oppressed operator. In those cases, the process may still occur very rarely, but in this case we're saying this particular process will never happen.

Problem 298

Suppose we have three spin 1/2 particles in the Hamiltonian

$$H = \frac{\Delta}{\hbar^2}\left(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1\right).$$

What are the explicit energy eigenstates?

First of all, we know the dimensionality of our state space is $2 \times 2 \times 2 = 8$. To get the highest contribution to this Hamiltonian, we should have all of our spins point in the same direction, meaning that $|+++\rangle$ and $|---\rangle$ should have the highest energy eigenvalue. We can see, for example, that the operator $\vec{S}_1 \cdot \vec{S}_2$ acting on $|+++\rangle$ yields

$$\vec{S}_1 \cdot \vec{S}_2 |+++\rangle = \left(\frac{1}{2}S_{1+}S_{2-} + \frac{1}{2}S_{1-}S_{2+} + S_{1z}S_{2z}\right)|+++\rangle,$$

but now the first two terms both kill the state (because we can't raise the $|+\rangle$ state, so only the last term contributes and gives us something proportional to $|+++\rangle$. (And the same thing occur with $|---\rangle$ – the product of $S_{1z}S_{2z}$ still yields a positive eigenvalue).

In order to understand the energy levels of this 8-dimensional vector space, we can define a total angular momentum $\vec{S}_T = \vec{S}_1 + \vec{S}_2 + \vec{S}_3$ and rewrite the Hamiltonian as

$$H = \frac{\Delta}{\hbar^2} \cdot \frac{1}{2}\left(S_T^2 - S_1^2 - S_2^2 - S_3^2\right).$$

(Note that we can do this because the S_1, S_2, S_3's x, y, z operators commute with each other.) But now the eigenvalues for S_1^2, S_2^2, S_3^2 are each always $\frac{3\hbar^2}{4}$, so the only thing that the system's energy level depends on is the total spin angular momentum s: in particular, our energy eigenvalue is

$$E = \frac{\Delta}{2\hbar^2}\left(\hbar^2 s(s+1) - 3 \cdot \frac{3}{4}\hbar^2\right) = \frac{\Delta}{2}\left(s(s+1) - \frac{9}{4}\right).$$

To understand the possible values of s, we just do the calculation

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = (1 \oplus 0) \otimes \frac{1}{2} = 1 \otimes \frac{1}{2} \oplus 0 \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2} \oplus \frac{1}{2},$$

which means the representations can be at spin $\frac{3}{2}$ (4 states) or $\frac{1}{2}$ (another $2+2=4$ states), corresponding to energies of $\frac{3}{4}\Delta$ and $-\frac{3}{4}\Delta$, respectively.

43 Density Matrices

In this last set of lectures, we'll discuss **ensembles and mixed states**, and we'll be able to appreciate again that probability plays a role in quantum mechanics. Remember that classical mechanics, probability just comes up due to a lack of knowledge – if we roll dice, we can theoretically always predict the result if we have enough information. But this is not true in quantum mechanics anymore: even with perfect knowledge of our state $|\psi\rangle$, we will still need probability every time we measure any observable.

One way we can measure this probability is to make many copies of our state $|\psi\rangle$, measure our observable many times, and form a probability distribution with enough testing. But now, we are introducing a new source of randomness

in our system.

Definition 299

Let V be a vector space of states. A **pure state** is just some $|\psi\rangle \in V$, while a **mixed state** introduces some extra randomness which we will describe now.

For a concrete example, consider the following:

Example 300

Suppose we have an oven which spits out silver atoms towards a Stern-Gerlach machine which causes deflections of those atoms.

In such a system, every atom behaves like a spin 1/2 particle: we eventually find that they are either in the $|\vec{n};+\rangle$ or $|\vec{n};-\rangle$ state, but before going in the machine, they are polarized in **all possible directions** $\vec{n}$ (distributed randomly). It's natural to ask whether this randomness is already accounted for – that is, can we write down a state $|\psi\rangle$ whose **intrinsic randomness** describes the particles coming out of our atom before they hit the Stern-Gerlach machine?

We do know that any spin 1/2 state is in a superposition of the up and down states:

$$|\psi\rangle = a_+ |+\rangle + a_- |-\rangle, \quad a_+, a_- \in \mathbb{C}.$$

But we know that specifying these coefficients tells us the angles ϕ, θ for the normal vector $\vec{n}$, so this fixes the direction of the spin state, rather than picking it from a distribution! So we do need some additional randomness.

So we'll first consider the simple case where the atoms aren't completely uniformly distributed: instead, each particle has a 50 percent chance of being spin up and a 50 percent chance of being spin down, always in the z-direction. We'll describe this with an ordered pair

$$(p_a, |\psi_a\rangle),$$

which means that the particle comes out with the state $|\psi_a\rangle$ with probability p_a. So this oven that we've just described can be written as

$$E_z = \left\{ \left(\frac{1}{2}, |+\rangle\right), \left(\frac{1}{2}, |-\rangle\right) \right\}.$$

This is now an example of a **mixed state**: not all of our particles come out with the same wavefunction even before they hit the Stern-Gerlach machine, which means they are not in the same quantum state. In other words, we may have an **ensemble** where we take 2000 copies of this state, where 1000 copies are in the $|+\rangle$ state and the other 1000 are in the $|-\rangle$. Then when we test a measurement, we work with this enesemble instead. Let's make this definition more generally:

Definition 301

An **ensemble** E is defined by

$$\{(p_1, |\psi_1\rangle), \cdots, (p_n, |\psi_n\rangle)\}$$

where the probabilities p_i are all positive and sum to 1, which dictate the likelihood of the corresponding **normalized** (but not necessarily orthonormal) states $|\psi_i\rangle$.

Note that the dimension $\dim V$ of the vector space has nothing to do with the number of states n we have in our ensemble: we're not trying to form a basis or anything like that. Then $n = 1$ yields a pure state (the ensemble collapses to a single known state $|\psi_1\rangle = (1, |\psi_1\rangle)$, so all particles are in this state), and $n \geq 2$ yields a mixed state.

So now suppose that we have some Hermitian operator $\hat{Q}$, and we want to measure the expectation value of $\hat{Q}$. Then we can let

$$\langle \hat{Q} \rangle_E = \sum_i p_i \langle \psi_i | \hat{Q} | \psi_i \rangle ,$$

since we should take the weighted average of the expectation values for each of the possible states we can have in our ensemble.

Example 302

In the example ensemble E_z above, the expectation value is

$$\langle \hat{Q} \rangle_{E_z} = \frac{1}{2} \langle + | \hat{Q} | + \rangle + \frac{1}{2} \langle - | \hat{Q} | - \rangle .$$

To make this interesting, suppose that we have another ensemble

$$E_x = \left\{ \left(\frac{1}{2}, |x; + \rangle \right), \left(\frac{1}{2}, |x; - \rangle \right) \right\}.$$

(Half of our particles start off pointing in the $+x$-direction, and the other half in the $-x$-direction.) Similarly, we'll have

$$\langle \hat{Q} \rangle_{E_x} = \frac{1}{2} \langle x; + | \hat{Q} | x; + \rangle + \frac{1}{2} \langle x; - | \hat{Q} | x; - \rangle .$$

But now we can write the expectation value in the states $|x; \pm\rangle$ in terms of the expectation in the states $|\pm\rangle$ via

$$|x; \pm\rangle = \frac{1}{\sqrt{2}} (|+\rangle \pm |-\rangle),$$

and now we can plug in to find

$$\langle \hat{Q} \rangle_{E_x} = \frac{1}{2} \cdot \frac{1}{2} (\langle + | + \langle - |) \hat{Q} (|+\rangle + |-\rangle) + \frac{1}{2} \cdot \frac{1}{2} (\langle + | - \langle - |) \hat{Q} (|+\rangle - |-\rangle).$$

Now the $\langle + | \hat{Q} | + \rangle$ and $\langle - | \hat{Q} | - \rangle$ terms will combine, but the cross terms will cancel out, and we're left with

$$= \frac{1}{2} \langle + | \hat{Q} | + \rangle + \frac{1}{2} \langle - | \hat{Q} | - \rangle = \langle \hat{Q} \rangle_{E_z}.$$

So the expectation value for **any Hermitian operator** $\hat{Q}$ always looks the same in both ensembles, even though the ensembles are different! So if we try to measure anything at all, there's no way to get a different answer between these two ensembles E_z and E_x, and thus these are actually indistinguishable from each other quantum mechanically.

We can also consider an **unpolarized ensemble**, where the spins all point in various directions. Then we will need an infinite (in fact uncountable) list to describe the whole system, but we can still describe this as

$$E_{\text{unp}} = \bigcup_{d\Omega} \frac{d\Omega}{4\pi} |\vec{n}(\Omega); + \rangle ,$$

where we're adding over all solid angles, and the total solid angle is 4π. Similarly, we can consider the ensemble

$$E_{\vec{n}} = \left\{ \left(\frac{1}{2}, |\vec{n}; + \rangle \right), \left(\frac{1}{2}, |\vec{n}; - \rangle \right) \right\}.$$

for some fixed vector $\vec{n}$. This is analogous to the ensembles E_z and E_x that we've defined earlier, and we can check with a similar argument that **both the unpolarized ensemble and $E_{\vec{n}}$ will be indistinguishable** from E_x and E_z as well. In other words, we can always describe an unpolarized ensemble by choosing the particles to point half-and-half in some fixed direction.

From here, let's see another instance where mixed states come up:

Example 303

Suppose we have an entangled state of two particles belonging to Alice and Bob, with state

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|+\rangle_A|-\rangle_B - |-\rangle_A|+\rangle_B).$$

This is the usual spin singlet state (which has total spin angular momentum 0, so it's rotationally invariant). We know that if both Alice and Bob have full knowledge and measure along the z-axis, they will measure their particles to be in opposite directions. But now suppose that Bob **does not know** what Alice's measurement is: then Bob's particle is operationally in a mixed state

$$E_{\text{Bob}} = \left\{\left(\frac{1}{2}, |+\rangle\right), \left(\frac{1}{2}, |-\rangle\right)\right\}$$

(because if we have many copies of our entangled state, Alice will measure $+$ half the time and $-$ the other half of the time). In fact, if Alice measures in an arbitrary direction $\vec{n}$, we can use rotational invariance to rewrite our entangled state as

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|\vec{n};+\rangle_A|\vec{n};-\rangle_B - |\vec{n};-\rangle_A|\vec{n};+\rangle_B),$$

and now if Alice measures along the $\vec{n}$-direction and Bob doesn't know what the result is, Bob ends up in the state

$$E_{\text{Bob}} = \left\{\left(\frac{1}{2}, |\vec{n};+\rangle\right), \left(\frac{1}{2}, |\vec{n};-\rangle\right)\right\},$$

which we know is physically the same ensemble as the ensemble we initially had. In other words, Alice's measurement axis does not affect the ensemble for Bob, even though it does affect the particles! (And this is the more satisfactory explanation for why we don't have instantaneous communication.)

And we can confirm that there is no way to avoid using mixed states here: suppose that we have some pure state $|\psi_A\rangle$ that describes Alice's particle when it is entangled (if we only care about Alice's particle and not Bob's). Then we would know that the expectation of an operator is given by

$$\langle\psi_A|\hat{Q}|\psi_A\rangle = \langle\psi_{AB}|\hat{Q}\otimes I|\psi_{AB}\rangle$$

(since we don't really do anything to Bob's particle). So now if we look at the case where our operator $\hat{Q}$ is σ_x, we know that we flip $|+\rangle$ and $|-\rangle$ to each other, so we have that

$$\langle\psi_{AB}|\sigma_x\otimes I|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}(\langle+|_A\langle-|_B - \langle-|_A\langle+|_B)(|-\rangle_A|-\rangle_B - |+\rangle_A|+\rangle_B),$$

and now there is **no overlap** because there is no $|+\rangle|+\rangle$ or $|-\rangle|-\rangle$ in the original singlet state. Similarly, we can calculate in the cases where $\hat{Q} = \sigma_y$ and $\hat{Q} = \sigma_z$ that the expectation is also zero, so any pure state that describes Alice's particle in the singlet state must satisfy

$$\langle\psi_A|\sigma_x|\psi_A\rangle = \langle\psi_A|\sigma_y|\psi_A\rangle = \langle\psi_A|\sigma_z|\psi_A\rangle = 0.$$

And this isn't possible, because any pure spin state points in some direction, so there is some $\vec{n}$ such that

$$\langle\psi_A|\vec{n}\cdot\vec{\sigma}|\psi_A\rangle \neq 0.$$

But then $\vec{n}\cdot\vec{\sigma}$ is a linear combination of the σ_is, so if each of the individual σ_is has expectation value zero, so must

$\vec{n} \cdot \vec{\sigma}$, and this is a contradiction. So **no pure state represents one particle of an entangled state**, and we will now need ensembles to describe something like the singlet state – the point now is to introduce a tool that helps us describes such systems nicely. One of the ideas is that we want to avoid the issue where different-looking ensembles actually correspond to the same situation.

Recall that an ensemble $E = \{(p_1, |\psi_1\rangle), \cdots, (p_n, |\psi_n\rangle)\}$ corresponds to an expectation value

$$\langle \hat{Q} \rangle_E = \sum_{i=1}^{n} p_a \langle \psi_a | \hat{Q} | \psi_a \rangle = \sum_{i=1}^{n} p_a \text{tr} \left(\hat{Q} |\psi_a\rangle \langle \psi_a | \right).$$

Here, we use the fact that $\text{tr}(|u\rangle \langle v|) = \langle v | u \rangle$ (this is a manipulation we did in the past), and we can also use the fact that the sum of traces is the trace of the sum for a set of matrices to rewrite this as

$$= \text{tr} \left(\hat{Q} \sum_a p_a |\psi_a\rangle \langle \psi_a | \right).$$

So we have $\hat{Q}$, and then we have some operator which is only dependent on our ensemble E. That's the operator we're about to introduce in the general case:

Definition 304

A **density matrix** is a linear operator $\rho_E \in \mathcal{L}(V)$ associated to an ensemble E via

$$p_E = \sum_{a=1}^{n} p_a |\psi_a\rangle \langle \psi_a |.$$

In other words, we're describing our states with matrices instead of vectors, and we get the helpful fact that

$$\langle \hat{Q} \rangle_E = \text{tr}(\hat{Q} \rho_E).$$

We can use this to look at our previous ensembles now: our ensemble E_z can now be represented with the operator

$$p_{E_z} = \frac{1}{2} |+\rangle \langle + | + \frac{1}{2} |-\rangle \langle - | = \frac{1}{2} I,$$

because in general summing over an orthonormal basis yields the identity $\sum_i |i\rangle \langle i| = I$. So we also have

$$p_{E_x} = \frac{1}{2} |x;+\rangle \langle x;+| + \frac{1}{2} |x;-\rangle \langle x;-| = \frac{1}{2} I,$$

because $|x;+\rangle$ and $|x;-\rangle$ form an orthonormal basis as well. We find that $\rho_{E_{\text{unp}}}$ is also described by this matrix, and now we can see that the density matrix is describing our states more powerfully than just using the ensemble – we can easily tell when two ensembles are indistinguishable.

We can now check a few properties:

- ρ is a Hermitian operator, because each term in the sum $\sum_a p_a |\psi_a\rangle \langle \psi_a|$ is a Hermitian operator. (Remember that the adjoint of $|u\rangle \langle v|$ is $|v\rangle \langle u|$.) Therefore, it can be diagonalized, and it will have real eigenvalues.
- ρ_E is known as a **positive semidefinite matrix**, which means that all of its eigenvalues are nonnegative. In mathematicians' language, a matrix M is positive semidefinite if $\langle v, Mv \rangle \geq 0$ for all $v \in V$. Therefore, if we take an eigenvector v of unit length, $(v, Mv) = (v, \lambda v) = \lambda \geq 0$. (As an exercise, we can show that any positive semidefinite matrix must be Hermitian.) And this means that for any state ψ in our state space V,

$$\langle \psi | \rho_E | \psi \rangle \geq 0.$$

This is because we can rewrite the above expression as

$$= \sum_{a=1}^{n} p_a \langle\psi|\psi_a\rangle \langle\psi_a|\psi\rangle = \sum_{a=1}^{n} p_a |\langle\psi|\psi_a\rangle|^2,$$

and because the lengths are nonnegative and p_a are probabilities, this expression has all terms at least 0.

- The trace of ρ_E is 1 for any density matrix. This is because

$$\text{tr}(\rho_E) = \text{tr}\left(\sum_a p_a |\psi_a\rangle \langle\psi_a|\right) = \sum_a p_a \text{tr}(|\psi_a\rangle \langle\psi_a|) = \sum_a p_a \langle\psi_a|\psi_a\rangle = \sum_a p_a = 1,$$

because the ψ_as are defined to be of unit length.

- As already mentioned, the density matrix removes redundancy in ensembles: no matter what combination of states we choose in a state space of dimension n, we always end up with a Hermitian $n \times n$ matrix, which is always specified by n^2 real constants (minus one if we fix the trace to be 1).
- Phases in the definitions of our states $|\psi_a\rangle$ do not affect ρ_E, because replacing $|\psi_a\rangle$ with $e^{i\phi_a}|\psi_a\rangle$ will make the ket-bra look like

$$e^{i\phi_a}|\psi_a\rangle e^{-i\phi_a}\langle\psi_a| = |\psi_a\rangle\langle\psi_a|,$$

which is identical to what we start with.

In general, the density matrix is the best way to describe mixed states, and we often call it the **state** of our system or **state operator**.

Example 305

To help us study this object a bit more, let's consider the case where we have a pure state.

This means we have an ensemble

$$E = \{(1, |\psi\rangle)\},$$

and plugging in the definition, we just have

$$\boxed{\rho_E = |\psi\rangle\langle\psi|}.$$

Because our state ψ is normalized, this actually gives us a rank-1 **orthogonal projector** (of trace 1) into the space spanned by the vector $|\psi\rangle$: we can check that $\rho^2 = \rho$ and $\rho^\dagger = \rho$. In other words, **for a pure state**, we have the property that

$$\text{tr}(\rho^2) = \text{tr}(\rho) = 1.$$

But in general, the trace of ρ^2 won't always be 1 when we have a mixed state:

Theorem 306

For any density matrix ρ, we have $\text{tr}(\rho^2) \leq 1$, and saturation of this inequality only occurs when we have a pure state.

Proof. We know that

$$\text{tr}(\rho^2) = \text{tr}\left(\sum_a p_a |\psi_a\rangle\langle\psi_a| \sum_b p_b |\psi_b\rangle\langle\psi_b|\right) = \sum_{a,b} p_a p_b \langle\psi_a|\psi_b\rangle \text{tr}(|\psi_a\rangle\langle\psi_b|)$$

by pulling out all of the constants from our trace matrix and using linearity. But now the trace of $|\psi_a\rangle\langle\psi_b|$ is $\langle\psi_b|\psi_a\rangle$, which is the complex conjugagte of $\langle\psi_a|\psi_b\rangle$. Thus, substituting this back in yields

$$= \sum_{a,b} p_a p_b |\langle\psi_a|\psi_b\rangle|^2.$$

Schwarz's inequality now tells us that

$$|\langle\psi_a|\psi_b\rangle|^2 \leq \langle\psi_a|\psi_a\rangle\langle\psi_b|\psi_b\rangle = 1,$$

and thus our sum simplifies to

$$\leq \sum_{a,b} p_a p_b = \sum_a p_a \sum_b p_b = 1,$$

with saturation only if ψ_a and ψ_b are always pointing in the same direction for **all overlaps**, which only occurs if all $|\langle\psi_a|\psi_b\rangle| = 1$. Since our states are normalized, this means our states only differ by a phase which we can ignore. Thus, at equality, we can combine all terms and we just have a pure state, as desired. □

Definition 307

For any density matrix ρ, define the **purity** of the state to be

$$\zeta(\rho) = \text{tr}(\rho^2).$$

A minimally mixed (or pure) state will then have highest possible purity (1), and a **maximally mixed state** will be one with minimum purity. It turns out this minimum purity is helpful in dealing with unitary time-evolution, since it stays constant even though ρ may not.

Proposition 308

The maximally mixed state ρ is

$$\rho = \frac{1}{\dim V} I,$$

which has a purity of $\frac{1}{\dim V}$.

This should remind us with the characteristic examples from the beginning of this lecture.

Proof. Because the density matrix ρ is Hermitian, we can diagonalize it, and we'll work with a basis in which ρ only has diagonal entries

$$\rho = \text{diag}(p_1, \cdots, p_n),$$

where $n = \dim V$. We know that the p_i are nonnegative and sum to 1 (because the trace of ρ is 1). Then

$$\rho^2 = \text{diag}(p_1^2, \cdots, p_n^2) \implies \text{tr}(\rho^2) = \sum_{i=1}^n p_i^2,$$

and now we can minimize this by being clever and using Cauchy-Schwarz. Alternatively, we can consider the function

$$L(p_1, \cdots, p_n, \lambda) = \sum_{i=1}^N p_i^2 - \lambda(-1 + \sum_i p_i),$$

where λ is a free parameter, and now taking the derivative with respect to λ yields our constraint $\sum p_i = 1$. So now

we can find a minimum by taking the derivative with respect to any p_i:

$$\frac{\partial L}{\partial p_i} = 2p_i - \lambda,$$

and since this holds for all p_i, all p_i must be equal at the minimum, meaning that each p_i is equal to $\frac{1}{n}$. So the density matrix of lowest purity is the diagonal matrix with entries $\frac{1}{n}$, which is just $\frac{1}{\dim V} I$, as desired. And indeed the trace of ρ^2, which is a diagonal matrix with entries $\frac{1}{n^2}$, is $n \cdot \frac{1}{n^2} = \frac{1}{n} = \frac{1}{\dim V}$. □

In conclusion, ensembles determine density matrices, which are linear operators with certain useful properties. Our next step will be to consider certain spin 1/2 density matrices and then understand more properties of the theory.

44 May 11, 2020

Our final exam will be next Wednesday – there should be enough time to review, and it's recommended that we go over everything that we're uncomfortable with in the course.

Last time, we discussed the Hamiltonian of a system of three spin 1/2 particles – we did half of the work, and we'll finish the discussion of that problem today.

Problem 309

As a reminder, we were working with the equation

$$H = \frac{\Delta}{\hbar^2}\left(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1\right).$$

In this class, we aren't dealing with issues of distinguishability: all particles are distinguishable.

The main trick here is to use the total angular momentum $\vec{S}_T = \vec{S}_1 + \vec{S}_2 + \vec{S}_3$ (where the secret meaning of the right side is a tensor product $\vec{S}_1 \otimes I \otimes I + I \otimes \vec{S}_2 I + I \otimes \vec{S}_3 \otimes I$). Then we can expand out

$$S_T^2 = S_1^2 + S_2^2 + S_3^2 + 2\left(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1\right) \implies H = \frac{\Delta}{2\hbar^2}\left(S_T^2 - S_1^2 - S_2^2 - S_3^2\right).$$

From here, the idea is to work with basis states that are eigenstates $|s, m\rangle$ of the total angular momentum S_T instead of our uncoupled states, meaning that we have

$$S_T^2 |s, m\rangle = \hbar^2 s(s+1) |s, m\rangle, \quad S_T^z |s, m\rangle = \hbar m |s, m\rangle.$$

An important point to keep in mind here is that in a spin 1/2 system, we have equations like

$$S_x^2 = \left(\frac{\hbar}{2}\right)^2 \sigma_x^2 = \frac{\hbar^2}{4} I,$$

and we get the same result for S_y and S_z, so the squared operators S_1^2, S_2^2, S_3^2 can all be treated as numbers in this Hamiltonian. And in general, when we have an angular momentum operator L^2 acting on an ℓ multiplet, we know that $L^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle$, so the operator L^2 can be treated as a number $\hbar^2 \ell(\ell+1)$ (times the identity matrix). But this does not mean L_x^2, L_y^2, L_z^2 are necessarily proportional to the identity – that's something special to the spin 1/2 particle.

So if we're doing an angular momentum problem where we combine states $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$, all such states (for a fixed j_1, j_2) are eigenstates of both J_1^2 and J_2^2. So when we rearrange them in terms of total angular momentum, so the operators that we care about are now J_T^2 and J_{zT}, **all states will be eigenstates of J_1^2 and J_2^2 as well.** And

now if we look back at our original three-state problem, but we imagine that we're combining states of the form $|s_1, m_1\rangle \otimes |s_2, m_2\rangle \otimes |s_3, m_3\rangle$ where s_1, s_2, s_3 are **definite**, S_1^2, S_2^2, and S_3^2 can still be treated as just numbers.

As another example of this, we can describe states of the hydrogen atom as either (n, ℓ, m, s, m_s) or (n, ℓ, j, s, m_j): the fact that ℓ and s are being kept here is noting the fact that L^2 and S^2 can be thought of as numbers in both the coupled and the uncoupled basis.

So returning to the problem, we did a calculation last time to show that

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{3}{2} \oplus \frac{1}{2} \oplus \frac{1}{2}$$

(where we have a $2^3 = 4 + 2 + 2 = 8$ dimensional vector space). Then the total energy of our coupled eigenstates was calculated last time: it's $\frac{A}{2}\left(S_T(S_T+1) - \frac{9}{4}\right)$, since the operators S_1^2, S_2^2, S_3^2 are each $\frac{3\hbar^2}{4}$ times the identity, so four states go up by $\frac{3}{4}\Delta$ and the other four go down by $\frac{3}{4}\Delta$.

Problem 310

What are the states of the $\frac{3}{2}$ multiplet for total angular momentum (in terms of the spin 1/2 states)?

We can condense notation by writing

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \to |+--\rangle\,.$$

We know that $|+++\rangle$ and $|---\rangle$ both have a total z-component of angular momentum that is larger than $\frac{1}{2}$, so both of them must be included in the multiplet (they are the states $|j, m\rangle = \left|\frac{3}{2}, \frac{3}{2}\right\rangle$ and $\left|\frac{3}{2}, -\frac{3}{2}\right\rangle$, respectively). To find the others, we can apply the lowering operator $J_- = J_{1-} + J_{2-} + J_{3-}$ on $|+++\rangle$, noting that $|+\rangle$ becomes $\hbar|-\rangle$ under a lowering operator to find

$$J_-|+++\rangle = \hbar|-++\rangle + \hbar|+-+\rangle + \hbar|++-\rangle\,,$$

but also

$$J_-|+++\rangle = J_-\left|\frac{3}{2}, \frac{3}{2}\right\rangle = \hbar\sqrt{3}\left|\frac{3}{2}, \frac{1}{2}\right\rangle.$$

Setting these equal yields

$$\left|\frac{3}{2}, \frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left(|-++\rangle + |+-+\rangle + |++-\rangle\right)$$

(and notice that we also didn't need to actually keep track of the constants, since we know that $|-++\rangle, |+-+\rangle, |++-\rangle$ have equal contribution). Similarly, we can raise the $|---\rangle$ state to find that

$$\left|\frac{3}{2}, -\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left(|+--\rangle + |-+-\rangle + |--+\rangle\right).$$

Remark 311. *One important thing to keep in mind is that directly acting with the operators $J_\pm$ don't produce normalized states, because*

$$J_\pm|j, m\rangle = \hbar\sqrt{j(j+1) - m(m\pm1)}\,|j, m\pm1\rangle$$

and we have an extra $\hbar$ and other constant here.

Problem 312

From here, a natural extension is to find the states in each of the $j = \frac{1}{2}$ multiplets.

Note here that because both j multiplets have equal j, there is **not a unique answer**. We can start each multiplet by finding a state $\left|\frac{1}{2},\frac{1}{2}\right\rangle_1$ (the top state of one of the multiplets) which is orthogonal to $\left|\frac{3}{2},\frac{1}{2}\right\rangle$. Such a state is of the form $\alpha\left|--+\right\rangle+\beta\left|+-+\right\rangle+\gamma\left|++-\right\rangle$, where $\alpha+\beta+\gamma=0$ is the orthogonality condition: for example, we can use

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle_1=\frac{1}{\sqrt{2}}\left(\left|--+\right\rangle-\left|+-+\right\rangle\right),$$

and then lowering this state yields $\left|\frac{1}{2},-\frac{1}{2}\right\rangle_1$. Finally, we can find the last $m=\frac{1}{2}$ state orthogonal to the first two, which is a more complicated calculation: for instance, we can use

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle_2=\frac{1}{\sqrt{6}}\left(\left|--+\right\rangle+\left|+-+\right\rangle-2\left|++-\right\rangle\right),$$

and then lower again to finish the multiplet with $\left|\frac{1}{2},-\frac{1}{2}\right\rangle_2$.

Fact 313

These last two lectures are not part of the 8.051 class for this semester due to COVID-19, but the notes are still included below. (There is also more content in each of these last two lectures.)

45 Density Matrices: Decoherence

Now that we've described density matrices generally, we'll do an example to help us discuss some more properties of these objects.

Example 314

Suppose we have a density matrix for a pure state of a spin 1/2 particle.

We know that this density matrix must be a projector operator to some state $|\vec{n};+\rangle$, so it takes the form

$$\left|\vec{n}\right\rangle\left\langle\vec{n}\right|.$$

If we want to write this as a (Hermitian) matrix, we can write it as a superposition of the four basis Hermitian matrices: we'll say it takes the form

$$=\frac{1}{2}a_0 I+\frac{1}{2}\sum_{i=1}^{3}a_i\sigma_i,$$

where the $\frac{1}{2}$ is to make the normalization a bit nicer. Taking the trace of both expressions, we find that

$$\boxed{1}=\frac{1}{2}a_0\cdot 2+\frac{1}{2}\sum_{i=1}^{3}a_i\cdot 0=\boxed{a_0},$$

because the Pauli matrices are traceless. In order to find the other coefficients, we can multiply both sides by σ_k and then take the trace:

$$\mathrm{tr}(\sigma_k\left|\vec{n}\right\rangle\left\langle\vec{n}\right|)=\mathrm{tr}\left(\frac{1}{2}\sigma_k+\frac{1}{2}\sum_i a_{ii}\sigma_i\sigma_k\right).$$

Again, Pauli matrices are traceless, and because $\sigma_i\sigma_k=\delta_{ik}I+(\text{Pauli matrix})$, the only contribution to the trace comes from $i=k$, meaning

$$\boxed{\mathrm{tr}(\sigma_k\left|\vec{n}\right\rangle\left\langle\vec{n}\right|)}=\frac{1}{2}\mathrm{tr}a_k I=\frac{a_k}{2}\cdot 2=\boxed{a_k}.$$

In other words, we can write the coefficients a_k in terms of an expectation value: the trace of $|a\rangle\langle b|$ is just $\langle a|b\rangle$, so plugging in $a = \sigma_k \vec{n}$ and $b = \langle \vec{n}|$,

$$\boxed{a_k = \langle \vec{n}|\sigma_k|\vec{n}\rangle}.$$

And now we can calculate this using the general formula for the spin state pointing in the direction (θ, ϕ): we end up with n_k, the kth component of the normal vector $\vec{n}$. So now we know how to write down the density matrix of a general pure state:

$$\boxed{|\vec{n}\rangle\langle\vec{n}| = \frac{1}{2}(I + \vec{n}\cdot\vec{\sigma})}.$$

To figure out the density matrix for a general mixed state, we can use this result, but first we should make sure we understand how to build such a mixed state. We know that we can go from an ensemble to a Hermitian, positive semidefinite matrix with trace 1: it turns out a kind of converse is also true.

Theorem 315

Given a Hermitian, unit trace, positive semidefinite matrix M, we can always view it as a density matrix for some associated ensemble E_M, such that $M = \rho_{E_M}$.

In other words, we just need to check a few properties to see if an operator is indeed a valid density matrix.

Proof. Since M is Hermitian and positive semidefinite, it can be diagonalized, and it will have eigenvalues $\lambda_1, \cdots, \lambda_N \geq 0$, such that $\lambda_1 + \cdots + \lambda_N = 1$. Let $|e_i\rangle$ be the eigenvector with eigenvalue λ_i, so $M|e_i\rangle = \lambda|e_i\rangle$. So we can write

$$M = \lambda_i |e_i\rangle\langle e_i|$$

as the diagonal matrix with entries λ_i in the (i, i) spot, and now this is the exact form of the density matrix for the ensemble

$$E_M = \{(p_1, |\psi_1\rangle), \cdots, (p_n, |\psi_n\rangle)\},$$

where $p_i = \lambda_i$ and $|\psi_i\rangle = |e_i\rangle$. (Indeed, the probabilities add to 1 and are nonnegative.) □

This is nice, because it gives us a clean way to describe a general density matrix in any system.

Example 316

Now we're ready to construct density matrices for mixed states of a spin 1/2 particle.

A general mixed state is still supposed to be a Hermitian operator acting on the two-dimensional vector space, so we can still write it as

$$\rho = \frac{1}{2}a_0 I + \frac{1}{2}\sum_{i=1}^{3} a_i \sigma_i.$$

We can still take the trace of both sides, and because $\text{tr}(\rho) = 1$, we still have $a_0 = 1$ by the same argument as above, meaning

$$\rho = \frac{1}{2}(I + \vec{a}\cdot\vec{\sigma})$$

for some unknown components of $\vec{a}$. In order to ensure that this is a valid density matrix, we just need to check the last property now, which is that its eigenvalues are all nonnegative. The eigenvalues of $\vec{a}\cdot\vec{\sigma}$ are $\pm|\vec{a}|$ (because the eigenvalues of $\vec{n}\cdot\vec{\sigma}$ are ± 1 for a unit vector $\vec{n}$), which means the eigenvalues of $I + \vec{a}\cdot\vec{\sigma}$ are just $1 \pm |\vec{a}|$. (This is because any vector is an eigenvector of the identity matrix I, so in particular the eigenvectors of $\vec{a}\cdot\vec{\sigma}$ will work.) Therefore,

the eigenvalues of ρ are

$$\lambda_\pm = \frac{1}{2}\left(1 \pm |\vec{a}|\right),$$

meaning the necessary condition on our coefficients (for eigenvalues to be nonnegative) is $\boxed{|\vec{a}| \leq 1}$. And now we've guaranteed positive semidefiniteness, and therefore any Hermitian matrix with this condition will be a valid density matrix: the most general mixed state looks like

$$\boxed{\rho = \frac{1}{2}(I + \vec{a}\cdot\vec{\sigma}), \quad |\vec{a}| \leq 1}.$$

In other words, $\vec{a} = (a_1, a_2, a_3)$ must live inside the closed sphere $a_1^2 + a_2^2 + a_3^2 \leq 1$. Notably, when we're on the boundary $|\vec{a}| = 1$, the density matrix becomes a pure state (as above), and when we take the zero vector for $\vec{a}$, we get the maximally mixed state: indeed, we end up with $\frac{1}{2}I$, which is exactly the state with lowest purity that we derived last time.

From here, we'll move on and talk about the **effect of measurements on density matrices**.

Example 317

Suppose that we make a measurement along an orthonormal basis $\{|1\rangle, \cdots |n\rangle\}$.

Remember that if we start with a single state $|\psi\rangle$, then the probability that we end up in the basis state $|i\rangle$ is

$$\mathbb{P}(i) = |\langle i|\psi\rangle|^2.$$

So now suppose we have a mixed state of an ensemble $E = \{(p_1, |\psi_1\rangle), \cdots, (p_m, |\psi_m\rangle)\}$. Since we can be in various states with different probabilities, we now have to take a weighted average:

$$\mathbb{P}(i) = \sum_a p_a |\langle i|\psi_a\rangle|^2.$$

We should be able to write this as a quantity that only depends on the density matrix, and that's what we'll work towards. Rewriting this expression more explicitly, we have that

$$\mathbb{P}(i) = \sum_a p_a \langle i|\psi_a\rangle \langle\psi_a|i\rangle.$$

Since the is have nothing to do with the sum, we can pull them out of the sum and rewrite as

$$= \langle i| \sum_a p_a |\psi_a\rangle \langle\psi_a| |i\rangle.$$

And now the middle term is just the definition of the density matrix, and we have a nice result:

$$\boxed{\mathbb{P}(i) = \langle i|\rho|i\rangle}.$$

But if we want to ask about the density matrix after measurement, notice that we'll end up in one of the states $|i\rangle$ with some probability. So our measurement is some operator which sends density matrices to other density matrices! Specifically, we know that ending up in the state $|i\rangle$ corresponds to the density matrix $E_i = |i\rangle\langle i|$, and this is nice to work with because $E_i^\dagger = E_i$ and $E_i E_i = E_i$ (so we have an orthogonal projector), and $\sum_i E_i = I$. So doing a general measurement (where we don't focus on what state we actually end up in) will give us a **mixed state**

$$\tilde{E} = \{(\mathbb{P}(1), |1\rangle), (\mathbb{P}(n), |n\rangle)\},$$

meaning that we get a post-measurement density matrix

$$\tilde{\rho} = \sum_{i=1}^{n} \mathbb{P}(i) \left|i\right\rangle \left\langle i\right| = \sum_{i=1}^{n} \left|i\right\rangle \mathbb{P}(i) \left\langle i\right| = \sum_{i=1}^{n} \left|i\right\rangle \left\langle i|\rho|i\right\rangle \left\langle i\right| ,$$

which we can write in terms of our orthogonal projectors as

$$\boxed{\tilde{\rho} = \sum_{i=1}^{n} E_i \rho E_i}.$$

With this, we're now ready to examine the **dynamics** of the density matrix:

Example 318

Our initial focus will be on unitary time-evolution (similar to the dynamics that we discussed earlier in this class).

In order to describe this time-evolved $\rho(t)$, we'll again think about the density matrix in terms of a corresponding ensemble. We can start with the Schrodinger equation

$$\frac{\partial}{\partial t} \left|\psi\right\rangle = -\frac{i}{\hbar} H \left|\psi\right\rangle ,$$

and then taking the adjoint of both sides yields

$$\frac{\partial}{\partial t} \left\langle\psi\right| = \frac{i}{\hbar} \left\langle\psi\right| H$$

(where nothing happens to H because it is Hermitian). So we can already see what time-evolution looks like for a pure state density matrix: by the product rule,

$$\frac{\partial}{\partial t} \left(\left|\psi\right\rangle \left\langle\psi\right|\right) = -\frac{i}{\hbar} H \left|\psi\right\rangle \left\langle\psi\right| + \left|\psi\right\rangle \frac{i}{\hbar} \left\langle\psi\right| H = -\frac{i}{\hbar} [H, \left|\psi\right\rangle \left\langle\psi\right|].$$

In other words, the time-evolution can be written in terms of the commutator, and this may look familiar (it looks sort of like the Heisenberg equation of motion). But now we can generalize to a mixed state:

$$\boxed{\frac{\partial \rho}{\partial t}} = \frac{\partial}{\partial t} \sum_a p_a \left|\psi_a\right\rangle \left\langle\psi_a\right| ,$$

and now applying the formula we derived for a pure state to each of the terms here yields

$$= \boxed{-\frac{i}{\hbar} \sum_a p_a [H, \left|\psi_a\right\rangle \left\langle\psi_a\right|]}.$$

Rearranging and bringing the sum inside the commutator, we can now write everything in terms of the density matrix itself:

$$\boxed{i\hbar \frac{\partial \rho}{\partial t}} = \left[H, \sum_a p_a \left|\psi_a\right\rangle \left\langle\psi_a\right|\right] = \boxed{[H, \rho]}.$$

This is a clean differential equation, but it will turn out that not all density matrices evolve in this unitary manner (for instance, if we just look at a subsystem that is in contact with the rest of the system). We can say a few more things about this unitary time evolution, though: in the Schrodinger picture, we know that our wavefunction evolves via

$$\left|\psi, t\right\rangle = U(t) \left|\psi, 0\right\rangle ,$$

and now if we think of $\rho(t=0) = \sum p_a |\psi_a, 0\rangle \langle \psi_a, 0|$, we can apply the unitary operator to find

$$\rho(t) = \sum_a p_a |\psi_a, t\rangle \langle \psi_a, t| = \sum_a p_a U(t) |\psi_a, 0\rangle \langle \psi_a, 0| U^\dagger(t).$$

Since $U(t)$ and $U^\dagger(t)$ are in every term of the sum, this tells us that

$$\boxed{\rho(t)} = U(t) \sum_a p_a |\psi_a, 0\rangle \langle \psi_a, 0| U^\dagger(t) = \boxed{U(t)\rho(t=0)U^\dagger(t)}.$$

So just like the discussion we had earlier in the class, we can get both a differential equation for time evolution and an explicit formula in terms of the unitary operator $U(t)$: since our density matrix has a ket and a bra, we hit it with a U from the left (for the ket) and a $U^\dagger$ from the right (for the bra). As a consequence of this, ρ will remain Hermitian, unit trace, and positive semidefinite at all times if it starts off Hermitian, unit trace, and positive semidefinite, respectively (all of these can be easily seen by examining the expression for $\rho(t)$ that we've just derived).

And we can even take a look at how the purity of our state evolves in time: since $\zeta = \text{tr}(\rho^2)$, we know that (trace commutes with the derivative)

$$\frac{d\zeta}{dt} = \text{tr}\left(\rho \frac{d\rho}{dt} + \frac{d\rho}{dt}\rho\right) = \text{tr}\left(\rho \frac{d\rho}{dt} + \rho \frac{d\rho}{dt}\right) = 2\,\text{tr}\left(\rho \frac{d\rho}{dt}\right)$$

by cyclicity of trace, and now we can substitute in the expression we have above for the time-evolution of ρ to find that this is

$$= \frac{2}{i\hbar}\,\text{tr}(\rho[H,\rho]) = \frac{2}{i\hbar}\text{tr}(\rho H\rho - \rho^2 H),$$

and again by cyclicity of trace we can turn this into

$$= \frac{2}{i\hbar}\text{tr}(\rho H\rho - \rho H\rho) = 0.$$

In other words, the purity of a state does not change in time – in fact, this argument generalizes to tell us that $\text{tr}(\rho^3), \text{tr}(\rho^4)$, and so on are all time-independent as well.

Example 319

We'll now turn our attention to the case where we have a density matrices for a subsystem.

Here is where the density matrix becomes more interesting: we'll be considering **bipartite systems**, where a system can be broken up into two parts A and B. Basically, these two subsystems make up an isolated system (so the joint system evolves unitarily), but A and B can interact with each other.

We saw an example of this earlier with two entangled particles A and B, and we found that we couldn't describe one particle with a single pure state. That idea will be generalized now: basically, we can describe A and B with density matrices, and these matrices will satisfy all of the fundamental properties, though the time-evolution will not be as simple because we don't have isolated subsystems.

Let the d_A-dimensional Hilbert space for system A be $\mathcal{H}_A$, and suppose there are orthonormal basis states $e_1^A, \cdots e_{d_A}^A$. Similarly, let the d_B-dimensional Hilbert space for system B be $\mathcal{H}_B$, and suppose there are orthonormal basis states $e_1^B, \cdots, e_{d_B}^B$. Then the joint system AB is **bipartite**, where A and B are **generically entangled** (so there isn't a pure state description for the subsystem A). It's possible AB is in a pure state, or it's possible that AB was prepared in such a way that it can only be represented as an ensemble or density matrix. **Either way, we're claiming that we have a density matrix description for our subsystem**, and here's how we'll phrase this point:

Proposition 320

Suppose we have a density matrix $\rho_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$. Then

$$\rho_A = \mathrm{tr}_B(\rho_{AB}) = \sum_k \left\langle e_k^B \middle| \rho_{AB} \middle| e_k^B \right\rangle$$

is a valid density matrix that describes the subsystem A.

(We'll denote the trace of the whole system AB to be tr, the trace of the subsystem A to be tr_A, and the trace of the subsystem B to be tr_B.)

Proof. We need to check if this density matrix is an operator on the subsystem A and satisfies the characteristic properties. For the calculations, a useful fact to recall is that

$$\mathrm{tr} = \mathrm{tr}_A \,\mathrm{tr}_B = \mathrm{tr}_B \,\mathrm{tr}_A$$

(as an important property of the tensor product space), so

$$\boxed{\mathrm{tr}_A \,\rho_A} = \mathrm{tr}_A \,\mathrm{tr}_B \,\rho_{AB} = \mathrm{tr}\,\rho_{AB} = \boxed{1}$$

since ρ_{AB} is a valid density matrix. Similarly, we can see that A is positive semidefinite and Hermitian, and now we turn our attention to the main question: why does A need to be a density matrix for the subsystem?

To answer this, recall the example we had with our entangled particles last lecture: if we have an operator O_A acting on the space $\mathcal{H}_A$, then its extension to the tensor product space AB should be $O_A \otimes I_B$. In other words, we need to check that

$$\boxed{\mathrm{tr}_A(\rho_A O_A) \overset{?}{=} \mathrm{tr}(\rho_{AB} O_A \otimes I_B)}$$

for any operator O_A, which would tell us that whenever we want to compute an observable O_A for the subsystem A (right side of the equation), we can indeed use the density matrix ρ_A (left side of the equation).

To prove this, we can do an explicit calculation: we write down the most general form for our density matrix ρ_{AB}, which is

$$\rho_{AB} = \sum_{I,J} \tilde{\rho}_{I,J} \left| e_I \right\rangle \left\langle e_J \right|$$

where $\tilde{\rho}_{I,J}$ are matrix elements, and we sum over all indices I, J of the tensor product space $\mathcal{H}_A \otimes \mathcal{H}_B$. So each one should really correspond to two indices: letting I run over (i, ℓ) and J run over (j, m), we have

$$\rho_{AB} = \sum_{i,j,\ell,m} \tilde{\rho}_{i\ell,jm} \left| e_i^A \right\rangle \otimes \left| e_\ell^B \right\rangle \left\langle e_j^A \right| \otimes \left\langle e_m^B \right| .$$

Reorganizing the notation a bit, this can also be written as

$$= \sum_{i,j,\ell,m} \tilde{\rho}_{ij,\ell m} \left| e_i^A \right\rangle \left\langle e_j^A \right| \otimes \left| e_\ell^B \right\rangle \left\langle e_m^B \right| ,$$

where the tensor product separates out the action of the linear operator on the A and B Hilbert spaces. We've now written down the most general density matrix for ρ_{AB}, and now let's try to verify the property we want for ρ_A: by definition,

$$\rho_A = \mathrm{tr}_B \,\rho_{AB},$$

and now tr_B acts only on the B-side of our above expression and moves the ket from one side to the other:

$$\rho_A = \sum_{i,j,\ell,m} \tilde{\rho}_{ij,\ell m} \left|e_i^A\right\rangle \left\langle e_j^A\right| \otimes \left\langle e_m^B\right| \left|e_\ell^B\right\rangle = \sum_{i,j,m} \tilde{\rho}_{ij,mm} \left|e_i^A\right\rangle \left\langle e_j^A\right|$$

because our basis vectors e^B are orthonormal. And now this is indeed an operator on the subsystem A, satisfying

$$\mathrm{tr}(\rho_A O_A) = \sum_{i,j,m} \tilde{\rho}_{ij,mm} \left\langle e_j^A\right| O_A \left|e_i^A\right\rangle$$

by the same computation of the trace we've seen before (we move the ket to the right of the bra). So now we have the left hand side of the boxed equation we're trying to derive, and now we can compute the right hand side: plugging in the definition of our general density matrix yields

$$\mathrm{tr}(\rho_{AB} O_A \otimes I_B) = \mathrm{tr} \sum_{i,j,\ell,m} \tilde{\rho}_{ij,\ell m} \left|e_i^A\right\rangle \left\langle e_j^A\right| O_A \otimes \left|e_\ell^B\right\rangle \left\langle e_m^B\right| I.$$

Since trace is linear, we bring it inside and take the trace for each of A and B, yielding

$$= \sum_{i,j,\ell,m} \tilde{\rho}_{i,j,\ell,m} \left\langle e_j^A\right| O_A \left|e_i^A\right\rangle \delta_{\ell m}.$$

And now setting $\ell = m$ to get rid of the Kronecker delta indeed makes this reduce to the same expression, as desired. □

So the density matrix ρ_A for our subsystem behaves consistently with how we think observables should act, and in some sense it just "erases" the information associated with the other system B.

Example 321

We'll return to the entangled particles for Alice and Bob

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}(|+\rangle_A |-\rangle_B - |-\rangle_A |+\rangle_B).$$

What is the density matrix ρ_B that Bob sees?

Because ρ_{AB} is a pure state of the bipartite system, we know that

$$\rho_{AB} = |\psi_{AB}\rangle \langle\psi_{AB}| = \frac{1}{\sqrt{2}}(|+\rangle_A |-\rangle_B - |-\rangle_A |+\rangle_B) \cdot \frac{1}{\sqrt{2}}(\langle+|_A \langle-|_B - \langle-|_A \langle+|_B).$$

We can expand and find the four terms, writing the A and B parts next to each other: this yields

$$\rho_{AB} = \frac{1}{2}(|+\rangle_A \langle+|_A) \otimes (|-\rangle_B \langle-|_B) + \frac{1}{2}(|-\rangle_A \langle-|_A) \otimes (|+\rangle_B \langle+|_B)$$

$$-\frac{1}{2}(|+\rangle_A \langle-|_A) \otimes (|-\rangle_B \langle+|_B) - \frac{1}{2}(|-\rangle_A \langle+|_A) \otimes (|+\rangle_B \langle-|_B).$$

Our goal is to find

$$\rho_B = \mathrm{tr}_A \rho_{AB},$$

but the A-trace of the first two terms are 1 each, while the A-trace of the last two are 0 each, so we just end up with

$$\boxed{\rho_B = \frac{1}{2}|-\rangle_B \langle-|_B + \frac{1}{2}|+\rangle_B \langle+|_B}.$$

In other words, B is **maximally mixed** when we take the "maximally entangled" state of AB and assume that Alice

does nothing. But notice that even when Alice does make a measurement along any axis (and we don't know what the result is), Bob will **also** end up with a density matrix corresponding exactly to the one we've just found! So the description of B looks the same when Alice measures or does nothing, and we'll understand this a bit more in the coming discussion.

Problem 322

Our next point of discussion is how to write down a nice description of a **pure bipartite state** $|\psi_{AB}\rangle$ in terms of the density matrices ρ_A and ρ_B, known as the **Schmidt decomposition** (this is the same mathematician as the Gram-Schmidt decomposition).

We know that $|\psi_{AB}\rangle$ lives in the tensor product space $\mathcal{H}_A \otimes \mathcal{H}_B$, so we can write it in terms of an orthonormal basis for each of $\mathcal{H}_A$ and $\mathcal{H}_B$ – call them $\{|k_A\rangle\}$ and $\{|k_B\rangle\}$, respectively (where k ranges from 1 to d_A or d_B, respectively). Specifically, **pick the bases** such that ρ_A and ρ_B, the Hermitian density matrices of the subsystems, are **diagonal** (so pick the eigenvectors of ρ_A and ρ_B).

This allows us to write $|\psi_{AB}\rangle$ nicely as follows: we know that its density matrix is

$$\rho_{AB} = |\psi_{AB}\rangle \langle\psi_{AB}|$$

because we have a pure state, and we know that

$$\rho_A = \mathrm{tr}_B \, \rho_{AB}$$

is a $d_A \times d_A$ Hermitian matrix with some eigenvectors $|k_A\rangle$ and eigenvalues p_k – in fact, with our choice of basis, ρ_A will be diagonal, since

$$\boxed{\rho_A = \sum_k p_k \, |k_A\rangle \langle k_A|}.$$

Remark 323. *Note, however, that we don't always actually have d_A different terms in this sum – many of them may turn out to be 0. So we're going to assume that we* **order the eigenvalues** *such that all of the zero p_ks occur at the end.*

And for this reason, we can say that we sum from 1 to r for some $r \leq d_A$ in the above expression. (Without loss of generality, we can assume $d_A \leq d_B$ for now.) And we'll use this to write down an ansatz for $|\psi_{AB}\rangle$: it's some linear combination of the basis states in our tensor product space, so we can write

$$|\psi_{AB}\rangle = \sum_{k=1}^{?} |k_A\rangle \otimes \left|\psi_k^B\right\rangle$$

for some states $\psi_k^B \in \mathcal{H}_B$ indexed by k as well. And now remember that we should get ρ_A when we take the B-trace of this expression, but the resulting density matrix only has ks appearing for $1 \leq k \leq r$. **So we should only sum up to r in this expression**, and to make more progress we should use this ansatz to compute the density matrix ρ_{AB}: this yields

$$\rho_{AB} = |\psi_{AB}\rangle \langle\psi_{AB}| = \sum_{k,\tilde{k}=1}^{r} |k_A\rangle \left|\psi_k^B\right\rangle \left\langle \tilde{k}_A\right| \left\langle\psi_{\tilde{k}}^B\right|.$$

Plugging this into the definition of ρ_A, we find that (again sliding the B-kets to the right of the B-bras)

$$\rho_A = \mathrm{tr}_B \, \rho_{AB} = \sum_{k,\tilde{k}=1}^{r} |k_A\rangle \left\langle \tilde{k}_A\right| \left\langle\psi_{\tilde{k}}^B|\psi_k^B\right\rangle.$$

And now in order for this to be consistent with the boxed expression above, we must have the **same matrix elements**, meaning that

$$\left\langle \psi_{\tilde{k}}^B \middle| \psi_k^B \right\rangle = p_k \delta_{k\tilde{k}}.$$

(so that the diagonal entries are p_k and all off-diagonal entries are zero). So the different $\left|\psi^B\right\rangle$s that show up in the expression for our pure bipartite state must be orthogonal.

With this notation, we can now define

$$\left|\psi_k^B\right\rangle = \sqrt{p_k}\left|k_B\right\rangle,$$

so that we have an orthonormal set of states $|k_B\rangle$ (where $1' \leq k \leq r$). And now we get the result we've been working towards:

Proposition 324 (Schmidt decomposition)
A pure bipartite state can be written as

$$|\psi_{AB}\rangle = \sum_{k=1}^{r} \sqrt{p_k}\,|k_A\rangle \otimes |k_B\rangle,$$

where we have $r \leq \min(d_A, d_B)$, $\sum p_k = 1$, and orthonormal bases $\left\langle k_A \middle| k_A' \right\rangle = \left\langle k_B \middle| k_B' \right\rangle = \delta_{kk'}$, so that

$$\rho_A = \sum_{k=1}^{r} p_k\,|k_A\rangle\langle k_A|, \quad \rho_B = \sum_{k=1}^{r} p_k\,|k_B\rangle\langle k_B|.$$

(And the Gram-Schmidt procedure tells us that even when $r < d_A$ and $r < d_B$, we can still finish constructing an orthonormal basis for the entire state spaces $\mathcal{H}_A$ and $\mathcal{H}_B$.) In words, if we diagonalize the density matrices ρ_A and ρ_B, that lets us write down the pure state $|\psi_{AB}\rangle$ nicely as well.

There are a few things we can observe about this representation:

- Because the coefficients p_k are the same for the density matrices of A and B, those density matrices ρ_A, ρ_B have the **same set of nonzero eigenvalues**. (It's possible that the spaces are of different dimension, so we might have a higher multiplicity of 0 in one case than the other.)
- The integer r is known as the **Schmidt number** of the decomposition: this is the number of terms in the density matrices, as well as the number of terms in the representation of the pure state $|\psi_{AB}\rangle$ itself. Here, r can range from 1 to $\min(d_A, d_B)$: when $r = 1$, we have pure (that is, not entangled) states in the subsystems A and B, and otherwise we have entangled particles, meaning we can't factor into a state of A and a state of B because the density matrices ρ_A, ρ_B are mixed states.
- The purity of ρ_A and ρ_B are the same: both of them are just

$$\zeta = \operatorname{tr}(\rho^2) = \sum_{k=1}^{r} p_k^2.$$

So now let's return to our canonical example of Alice and Bob sharing an entangled pair of particles: recall that the density matrix for Bob is unaffected under a measurement by Alice, unless we know the exact value of Alice's measurement. (In both cases, we get the same maximally mixed state.) We'll make this result more general, and this is what is known as the **no signaling** or **no communication** result.

As discussed above, our density matrix evolves after a measurement via

$$\rho \mapsto \tilde{\rho} = \sum_i E_i \rho E_i$$

when we're measuring along n orthonormal basis $\{|i\rangle\}$ and we define $E_i = |i\rangle\langle i|$. We've discussed this in the context of a single system (not entangled), but now we want to extend this to a bipartite system.

More specifically, suppose we have a system AB, and suppose Alice measures along an orthonormal basis $\{|i\rangle_A\}$. Then we have orthonormal projectors $E_i^A = |i\rangle_A \langle i|_A$ which satisfy the usual properties $(E_i^A)^\dagger = E_i^A, E_i^A E_i^A$, and $\sum_I e_i^A = I_A$, and now (in a completely analogous way as before) we have

$$\rho_{AB} \mapsto \tilde{\rho}_{AB} = \sum_i (E_i^A \otimes I_B)\rho_{AB}(E_i^A \otimes I_B).$$

(We can check this as an exercise.)

Proposition 325 (No signaling)
Under the above transformation, the density matrix $\tilde{\rho}_B = \mathrm{tr}_A \tilde{\rho}_{AB}$ is invariant (it is equal to ρ_B).

So the density matrix of the composite system will change, but Bob's will not.

Proof. First, write our density matrix as a general sum

$$\rho_{AB} = \sum_j O_j^A \otimes O_j^B,$$

where O_j^A and O_j^B are some general operators in the $\mathcal{H}_A$ and $\mathcal{H}_B$ spaces. (This is possible because the tensor product space is spanned by vectors $|i\rangle_A \otimes |j\rangle_B$.) Then

$$\tilde{\rho}_B = \mathrm{tr}_A \tilde{\rho}_{AB} = \mathrm{tr}_A \sum_{i,j} (E_i^A \otimes I_B)(O_j^A \otimes O_j^B)(E_i^A \otimes I_B)$$

which can be simplified by taking the product of operators as

$$= \mathrm{tr}_A \sum_{i,j} E_i^A O_j^A E_i^A \otimes O_j^B.$$

But now if we take the trace term by term, we end up with the operator in the $\mathcal{H}_B$ space

$$= \sum_{i,j} \mathrm{tr}(E_i^A O_j^A E_i^A) O_j^B.$$

But now cyclicity of trace and the property of the projection operator tells us that

$$\sum_i \mathrm{tr}(E_i^A O_j^A E_i^A) = \sum_i \mathrm{tr}(E_i^A E_j^A O_i^A) = \sum_i \mathrm{tr}(E_i O_j^A),$$

and now we can bring the sum inside the trace:

$$= \mathrm{tr}\left(\sum_i E_i O_j^A\right) = \mathrm{tr}(O_j^A).$$

So the introduction of the E_is has not contributed to the trace: bringing it back to the original expression, we're left

with

$$\tilde{\rho}_B = \sum_j \text{tr}(O_j^A) O_j^B,$$

which is indeed what we obtain if we take tr_A of the original density matrix ρ_{AB}. □

Problem 326

We're now ready to return to the question of time evolution, now that we have an "open" system (or subsystem of the whole world).

We're still focusing on bipartite systems here, but we'll call our system AE this time (where A is what we care about, and E is the outside **environment**). E is often larger than A (for example, when we have a thermal ensemble), but because AE is still a quantum system, it still evolves unitarily. A is known here as an **open system**.

The whole system can be described with a density matrix ρ_{AE}, and what we care about is our subsystem

$$\rho_A = \text{tr}_E \, \rho_{AE}.$$

We want to know about ρ_A's evolution in time, and we'll first show that it's not necessarily unitary. To understand this, consider a bipartite system of two **unentangled** spins in a pure state at time $t = 0$: in other words, both A and B have pure state descriptions at first.

But it's possible that interactions between A and B can cause the two particles to become entangled, meaning that A's description is now only possible with a mixed state. This transition from a pure state to a (nontrivial) density matrix is called **decoherence**, and it's only possible when we **don't** have unitary time evolution (because the purity has changed, which isn't allowed in unitary time evolution).

So in general, we can't actually say very much about the evolution of ρ_A, other than that the environment's behavior can lead to decoherence. (Typically, we go from a pure to a mixed state and stay mixed forever if the environment is large enough.) But we can say that

$$\rho_A(t) = \text{tr}_E \, \rho_{AE}(t),$$

and because AE evolves unitarily, this is

$$\text{tr}_E \left(U(t) \rho_{AE}(0) U^\dagger(t) \right)$$

for some unitary operator U. And that's about as much as we can say – since we're taking the partial trace over E, not the whole matrix, we **can't use cyclicity of trace**.

So suppose we have a pure state at time $t = 0$, where the system A and environment E are in pure (unentangled) states $|\phi_A\rangle$ and $|E\rangle$, respectively. Then the density matrix for the whole system takes on a simple form

$$\rho_{AE}(t) = |\phi_A\rangle \langle \phi_A| \otimes |E\rangle \langle E|,$$

and we can plug this into the formula above, assuming we know the Hamiltonian of our combined system. But there's still a possibility of decoherence even in this case, and that's best illustrated with an example.

Example 327

Suppose a box has two spins, and we have a Hamiltonian of

$$H = -\hbar\omega\sigma_z^{(1)}\sigma_z^{(2)}.$$

Also, suppose we start with an initial condition

$$|\psi_{12}(0)\rangle = |x;+\rangle_1 \otimes |x;+\rangle_2 .$$

In this case, the energy is minimized if the two spins point in the same z-direction (so there is indeed an interaction between the two particles). We know that we have an initial pure state of two particles that are not entangled, and our question is basically "what can we say about the density matrix of particle 1?".

To approach this question, we know that

$$\rho_{12}(0) = |\psi_{12}(0)\rangle \langle\psi_{12}(0)|$$

because we have a pure (total) state, which means that

$$\rho_{12}(t) = e^{-iHt/\hbar}\rho_{12}(0)e^{iHt/\hbar}$$

because we have a time-independent Hamiltonian. And from here, we find that

$$\rho_1(t) = \mathrm{tr}_2\, \rho_{12}(t),$$

and now we just need to go through all of the calculations to figure out how the density matrix evolves in time. We'll skip to the answer for now (we can try doing out the math ourselves) – the result is that

$$\boxed{\rho_1(t) = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| + \frac{1}{2}\cos(2\omega t)\left(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\right)}.$$

At time $t = 0$, we have four equally weighted terms, so the density matrix looks like $\begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}$ – another way to phrase this is that if we measured the two particles along the z-direction, we'd get a probability of $\frac{1}{4}$ of any result $\{++, +-, -+, --\}$ (because particles along the x-direction have equal chance to be $+z$ or $-z$ when we measure, and the two particles in our system started off independent). Notably, this is a pure state, and it's only a pure state because of the nonzero off-diagonal terms.

But a little later (at time $t = \frac{\pi}{4\omega}$), the $\cos(2\omega t)$ term disappears, and then our matrix will look like $\begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$, and now we have a maximally mixed state for A! And we can check that as a function of time,

$$\zeta = \mathrm{tr}(\rho_1^2) = 1 - \frac{1}{2}\sin^2(\omega t).$$

So the purity oscillates between 1 (a pure state) and $\frac{1}{2}$ (a maximally mixed state) for all time. This is a toy model where we can see decoherence happening – it's too simple to understand something like decoherence in quantum computers – but it does illustrate that pure states do not need to stay pure for subsystems.

So now we can return to the unitary time evolution equation

$$i\hbar\frac{\partial\rho}{\partial t} = [H, \rho] \implies \frac{\partial\rho}{\partial t}\frac{1}{i\hbar}[H, \rho].$$

This does not suffice for describing subsystems that do not evolve with a unitary operator, but the last topic of today is generalizing this equation to something called the **Lindblad equation**. It's not completely general, but it is able to modify the above equation in a way that preserves the Hermiticity, unit trace, and semi-definiteness of ρ, while removing the assumption of unitary time evolution.

We've just noticed that going from a pure to a mixed state is not always easy to do, and our approach here will be to construct a **phenomenological equation** – that is, it is not derived from first principles, but it is consistent with our observations. Basically, we'll make the argument that a small open system can have its coherence and information "dissipated" into a large environment without disrupting that environment very much.

Proposition 328 (Lindblad equation)

In certain systems, we have the governing equation

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}[H, \rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \right),$$

where L_k are the **Lindblad operators** and k depends on the system.

(Recall that $\{A, B\}$ is the **anticommutator** $AB + BA$). Here, the right hand side is constructed so that it is Hermitian – the L_ks do not talk to each other, and indeed every term that we see here is Hermitian because it's equal to its dagger.

Understanding the other parts of this equation, such as why we have a $-\frac{1}{2}$ constant in this equation, will come about when we verify that this matrix has a constant unit trace: **we wish to show** that

$$\frac{d}{dt}\operatorname{tr}(\rho) = \operatorname{tr}\left(\frac{\partial \rho}{\partial t}\right) = \operatorname{tr}\left(\frac{1}{i\hbar}[H, \rho] + \sum_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \right)\right).$$

is equal to zero. But trace of a commutator vanishes by cyclicity, so the first term goes away. Then we just need to check that the contribution from each L_k is zero: indeed,

$$\operatorname{tr}\left(L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\} \right) = \operatorname{tr}\left(L_k \rho L_k^\dagger - \frac{1}{2} L_k^\dagger L_k \rho - \frac{1}{2}\rho L_k^\dagger L_k \right)$$

and now all of these three terms are just cyclic shifts of each other, so we can reorder and get $\operatorname{tr}(0) = 0$. So **we have verified that the trace is constant in time**.

Showing positive semidefiniteness is also not too difficult: we show that in a time dt, a positive semidefinite matrix will stay positive semidefinite through this evolution. And this is left as an exercise for us.

Example 329

A classic case of decoherence we've already started studying earlier in the class is **nuclear magnetic resonance**.

Remember that in this system, we have a spin, and we have a magnetic field in the z-direction. We then introduce an additional signal which makes this spin state rotate, and that's the rotation that is picked up by detectors in practical applications. But it turns out the lattice of surrounding atoms interacts with the spin in question, which will cause decoherence of the circular motion, known as **transverse relaxation**.

The constant T_2 measures how long it takes for this to occur: once this happens, the spin behavior is destroyed (and the particle basically stops spinning). We also have a related constant T_1, which is the **longitudinal relaxation** time. What we discover there is that the spin stops rotating and starts being described by a probability of being spin up or down – due to thermal effects from the surroundings, we will eventually get some proportion of the states pointing

up versus down (based on the Boltzmann distribution from statistical physics), and T_1 controls how long it takes for this to happen.

Often $T_2 < T_1$ in most materials, and these are the times that we can detect for different materials with a physical machine. So studying this example more carefully is important both practically and for our current understanding. Suppose that our state points in the x-direction at some time: then our wavefunction looks like

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle),$$

which corresponds to a density matrix of

$$\rho = \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\right) \to \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}.$$

(This is a pure state.) In such a matrix, the off-diagonal $\frac{1}{2}$ terms are called **coherences** – after all, if those two terms were zero, we would have a maximally mixed state, which has no coherence at all. So transverse relaxation affecting this rotation means that by the time our coherences are suppressed, we have **complete decoherence** (the diagonal density matrix corresponds to a particle that has a $\frac{1}{2}$ chance to be in $+z$ and a $\frac{1}{2}$ chance to be in the $-z$). It's also possible that the probabilities at the end of the day are not quite $50-50$: it's possible that he diagonal terms are 0.52 and 0.48 or something, due to the magnetic field. (And this is where T_1 comes into play.)

So now let's talk about this in more generality – suppose our initial matrix looks like

$$\rho(t=0) = \begin{bmatrix} \rho_{++}(0) & \rho_{+-}(0) \\ \rho_{-+}(0) & \rho_{--}(0) \end{bmatrix}.$$

Intuitively, what we should expect to happen is that the transverse relaxation eventually kills the off-diagonal terms, so we are always going to go into a mixed state (eventually corresponding to a near-diagonal matrix). And T_1 should adjust the diagonal terms according to the Boltzmann distribution, and we want to know **what kind of Lindblad equation can model this** to get us the correct form that we want. (One way to phrase this is that Lindblad operators **drive** our time evolution.)

It turns out that we'll use three Lindblad operators: we'll make the simplification that we have **no magnetic field**, so $B = 0$ and we'll eventually end up with a maximally mixed state $\begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$. Define

$$\boxed{L_1 = \alpha\,|+\rangle\langle-|\,, \quad L_2 = \alpha\,|-\rangle\langle+|},$$

so L_1 and L_2 basically swap $+$ and $-$, meaning they mostly affect the longitudinal relaxation – they change the population of our eventual $+$ and $-$ states. We say that α is some real number – since we always have L and $L^\dagger$ appearing at the same time, we just end up with a contribution of $|\alpha|^2$ anyway. And we'll also need

$$\boxed{L_3 = \beta\sigma_z}:$$

the purpose of this operator is that

$$L_3\rho L_3 =\sim \sigma_z\rho\sigma_z$$

changes the signs of the off-diagonal term, so in our Lindblad equation we are driving the off-diagonal terms to zero (because this $L_3\rho L_3$ is a term that affects $\frac{\partial\rho}{\partial t}$). So now our matrix in general will look like

$$\rho(t) = \begin{bmatrix} \rho_{++}(t) & \rho_{+-}(t) \\ \rho_{-+}(t) & \rho_{--}(t) \end{bmatrix},$$

and we now need to plug everything in to the Lindblad equation by calculating matrix products: what we end up with is that

$$\begin{bmatrix} \dot{\rho}_{++}(t) & \dot{\rho}_{+-}(t) \\ \dot{\rho}_{-+}(t) & \dot{\rho}_{--}(t) \end{bmatrix} = \begin{bmatrix} -\alpha^2(\rho_{++} - \rho_{--}) & -(\alpha^2 + 2\beta^2)\rho_{+-} \\ -(\alpha^2 + 2\beta^2)\rho_{-+} & -\alpha^2(\rho_{--} - \rho_{++}) \end{bmatrix}$$

(the left side is the partial derivative of the density matrix, and we're computing the right side explicitly, skipping the calculations).

Looking at this equation, we can already see some of the physics: α should affect longitudinal relaxation, and indeed the diagonal terms will be driven towards $(\frac{1}{2}, \frac{1}{2})$, because a larger ρ_{++} than ρ_{--} drives the top left expression down and the bottom right expression up. (In the case where $B = 0$, this means equilibrium occurs when the terms of ρ_{++} and ρ_{--} are the same.)

But also β (along with some help from α) give us a simple exponential decay of the off-diagonal terms, because the time-derivative of each term is just proportional to its value! We'll find that the **off-diagonal terms** evolve via

$$\rho_{+-}(t) = \rho_{+-}(0)e^{-t/T_2}, \quad \rho_{-+}(t) = \rho_{-+}(0)e^{-t/T_2}, \quad T_2 = \frac{1}{\alpha^2 + 2\beta^2}$$

(this is a short time if we make β very large, but we can also consider the case where $\beta = 0$ and the constant of decay for longitudinal and transverse relaxation is of the same order). Similarly, the **diagonal terms** evolve via

$$\rho_{++}(t) = \frac{1}{2} + e^{-t/T_1}\left(\rho_{++}(0) - \frac{1}{2}\right), \quad \rho_{--}(t) = \frac{1}{2} + e^{-t/T_1}\left(\rho_{--}(0) - \frac{1}{2}\right)$$

(as t gets large, the extra terms decay exponentially), and $T_1 = \frac{1}{2\alpha^2}$. (And now we see that a large β is indeed necessary for us to have a physically correct model).

In summary, we've now concluded the study of a simple open system (nuclear magnetic resonance for $B = 0$) using the Lindblad operators. Basically, this is a nice way of approaching a problem without needing to understand all of the dynamics of the whole quantum mechanical system.

46 Density Matrices: Measurement

Now that we've discussed some interesting ideas of density matrices, we'll now reexamine the problem of measurement in quantum mechanics. There's lots of questions that come up at the foundational level – so far, we've been following the **Copenhagen interpretation** of quantum mechanics, developed from 1925–1927. Here are the main points of that interpretation:

- States evolve unitarily via the Schrodinger equation.
- Measurements can be described mathematically in a simple way: states are projected (non-unitarily) by measurements into invariant spaces of observables (Hermitian operators), such as eigenspaces.
- The possible values of a measurement are the eigenvalues of the corresponding operator, with probabilities given by the **Born rule**.

(There is no uncertainty once we make a measurement, and we're taking all of these as axioms of the theory.) We've discussed measurement in various ways – measuring along a basis, looking at a partial space or subspace of the Hilbert space, and so on. But the interesting point is that of measurement being non-unitary: what is this specific measurement apparatus doing which is different from a normal evolution?

Despite lots of work and many debates, not very much insight has been obtained here, but it's still worth considering these questions to get a better understanding. One way in which this happens is in the reading of Bohr and Heisenberg's

original papers, trying to understand how they understood these concepts.

Fact 330

The **orthodox reading** of the Copenhagen interpretation is that our measuring devices are classical: this means that the fundamental laws don't actually apply to them in some way.

Often, this type of reading is associated with a **Heisenberg cut** between the quantum and classical domains: the idea is that at the microscopic level, quantum mechanics takes effect, but we need classical mechanics to make sense of all of the measurements.

Fact 331

But the **modern reading** is that the Heisenberg cut doesn't really make sense: in fact, we can now build very large quantum systems, where we have a billion charge carriers in a superposition of two different states.

In other words, classical physics is now essentially thought of as "what quantum physics looks like at large scales:" there aren't fundamental differences in the two domains.

So there are a few proposals for how to interpret measurement in this framework, and we'll discuss one that has to do with **decoherence**, as well as one centered around the **many-worlds interpretation**.

We'll start with a more accessible question: **what does it mean for the wavelength to collapse?** It should be possible to look inside of our measurement apparatus and see when this non-unitary transformation occurs, and perhaps that will give us a clearer picture.

Example 332

Suppose we are trying to detect a photon by using a photomultiplier tube.

Basically, a photon can go into a box, and there is a cathode (electrically charged) near the entrance. The photon will hit the cathode, which will release an electron because of the photoelectric effect, and this electron will hit another plate along the box, which ejects more electrons. This process continues to the anode, and by this point there are many, many electrons – we will have a macroscopic current. So then our photomultiplier tube will be able to detect a photon when we measure a nonzero current.

The direction of the incoming photon beam is not completely certain here – if we have a few different boxes next to each other, then there is a superposition of different states that this photon could be in (based on which detector it entered). But only one of these detectors will actually go off, and when that happens, we will have collapsed the wavefunction.

Example 333

Suppose we have a calcite crystal (in which the index of refraction depends on the angle and polarization of the incoming beam).

Then when a photon enters this crystal, it can exit in one of two possible basis states: $|H\rangle$, corresponding to the exit angle from a horizontal polarization, or $|V\rangle$, corresponding to the exit angle from a vertical polarization. Then when we send a photon in, it can be in an arbitrary superposition of a $|H\rangle$ and $|V\rangle$ state, and when it comes out, it doesn't actually need to be in one of those two basis states. In fact, the wavefunction will still be spread out over the possible angles (it still lives in some superposition, and this is known as **pre-measurement**), but **once we put a**

photon detector along the $|H\rangle$ and $|V\rangle$ directions, exactly one of the two detectors will go off, and the position is known. So having this measurement apparatus forces the wavefunction to collapse, and the act of measuring with our detectors is what we usually mean when we say that we "measure along a basis."

Example 334

Suppose we want to measure the momentum of a charged particle.

We can send in the particle through a small slit in a wall: at that point, it can be in a superposition of many momentum states. If we put a uniform magnetic field, then the Lorentz force is proportional to the particle's velocity, so it will bend into a circular orbit. But again, the act of interacting with the magnetic field does not constitute a measurement – our particle is put into a superposition of orbits, and it isn't until the particle curves back and hits a detector in the wall that we know the velocity, and that's when the wavefunction collapses.

These three examples are all a bit different from the measurements we've been talking about earlier in this class, though, where we end up in an eigenstate and will get the same result if we measure again and again. In the examples above, the particle is actually destroyed or irreparably changed, which is why some other experiments, known as **quantum non-demolition measurements**, have also been considered.

So we've now thought about how measurements can be done in a few experimental setups, and now we'll think about how these measurements can be established quantum mechanically. The ideas here are due to von Neumann – it doesn't really remove the mystery of measurement, but it does explicitly suggest how certain systems actually behave.

Example 335

Suppose we have a system S and an apparatus A, where S and A interact with each other. A is a quantum system with **pointer states** (for example, in a Stern-Gerlach system, they could point to $+z$ or $-z$).

Even if the apparatus may be macroscopic, we'll still think of it as a quantum system. Say that our system S has an observable O_S and eigenvectors $|s_i\rangle$ for it, such that we have a finite number of possible states:

$$O_S |s_i\rangle = s_i |s_i\rangle , \quad 1 \leq i \leq n.$$

In other words, we wish to "measure" with O_S to see which of the n possible states we're living in. So now we can say that our apparatus A has an observable O_A and pointer states $|a_j\rangle$, such that

$$O_a |a_j\rangle = a_j |a_j\rangle , \quad 1 \leq j \leq m, \quad m \geq n.$$

Basically, we want each pointer state to correspond to a configuration $|s_i\rangle$ of our system, so we must have at least as many pointer states as we have O_S eigenstates.

At time $t = 0$, we must be in some state $|\psi(0)\rangle$ for our system, and this is in some superposition of the basis states:

$$|\psi(0)\rangle_S = \sum_{i=1}^{n} c_i |s_i\rangle .$$

But because our system is connected to an apparatus, we should really be thinking about this in terms of the composite system: then we have the apparatus in some initial state, meaning we can write

$$|\psi(0)\rangle_{SA} = \left(\sum_i c_i |s_i\rangle \right) \otimes |\psi(0)\rangle_A .$$

But we want to design the apparatus in a way so that there is an interaction between S and A, so there is also an interaction Hamiltonian H_{SA}.

Proposition 336

We can pick a Hamiltonian such that at some later time τ, $|\psi(\tau)\rangle$ has **achieved pre-measurement**, meaning that we are in an entangled state

$$|\psi(\tau)\rangle = \sum_i c_i e^{ip_i} |s_i\rangle \otimes |a_i\rangle ,$$

where p_i is an arbitrary phase.

What we're saying is that we've essentially **coupled the system with the measurement apparatus**: if the state of the system is $|s_i\rangle$, then our apparatus is in the $|a_i\rangle$ state. And this is really as far as we can go – we can create this correlation, and then the apparatus allows us to measure things at a classical level, but it doesn't solve the mystery of the non-unitary transformation.

Instead of proving in general that we can go from $|\psi(0)\rangle$ to $|\psi(\tau)\rangle$ by picking some appropriate Hamiltonian or unitary time-evolution U, we'll do an interesting example:

Example 337

Suppose S and A both have Hilbert space $V = \mathbb{C}^2$ (that is, the spin 1/2 vector space), where the operators are $O_S = \sigma_z^S$, $O_A = \sigma_z^A$.

We claim that the Hamiltonian

$$H_{SA} = \frac{1}{2}\hbar\omega(1 + \sigma_z^S) \otimes \sigma_x^A$$

will be able to establish the desired interaction between S and A. Let's start with the wavefunction

$$|\psi(0)\rangle_{SA} = (c_+ |+\rangle_S + c_- |-\rangle_S) \otimes |-\rangle_A$$

(so we start off in a single state of the apparatus, just like in the discussion above). Then we need to figure out the unitary time-evolution of this state, so that the $|+\rangle$s and $|-\rangle$s line up in the system and apparatus. Since we have a σ_x^A in the Hamiltonian, it's convenient to rewrite

$$|-\rangle_A = \frac{1}{\sqrt{2}}(|x;+\rangle_A - |x;-\rangle_A),$$

and then plugging this back in, we can rewrite our initial state as

$$\boxed{|\psi(0)\rangle_{SA} = \frac{1}{\sqrt{2}}(c_+ |+\rangle_S |x;+\rangle_A - c_+ |+\rangle_S |x;-\rangle_A) + c_- |-\rangle_S |-\rangle_A}.$$

Let's now see how the Hamiltonian given evolves our composite system: the unitary time-evolution operator is

$$U(t) = e^{iH_{SA}t/\hbar} = \exp\left(-\frac{i}{2}\omega t(1 + \sigma_z^S) \otimes \sigma_x^A\right),$$

which means that our state at a later time is

$$|\psi(t)\rangle_{SA} = U(t) |\psi(0)\rangle_{SA} .$$

Note that in the last term of the boxed expression above, because the system is in the $-$ state (and therefore has an eigenvalue of -1 for σ_z^S), the exponential term will collapse, and therefore **the last term is left invariant**. Since this

last term is of the desired "coupled" form that we are looking for, we've chosen a good Hamiltonian, and now we just need to apply the unitary operator on the first two terms. Notice that because our states are already eigenstates of the unitary operator, we have

$$U(t)\left|+\right\rangle_S\left|x;\pm\right\rangle = e^{-\frac{1}{2}i\omega t(1+1)\cdot\pm 1}\left|+\right\rangle_S\left|x;\pm\right\rangle = e^{\mp i\omega t},$$

so

$$\boxed{\left|\psi(t)\right\rangle_{SA} = \frac{1}{\sqrt{2}}e^{-i\omega t}c_+\left|+\right\rangle_S\left|x;+\right\rangle_A - \frac{1}{\sqrt{2}}e^{i\omega t}c_+\left|+\right\rangle_S\left|x;-\right\rangle_A + c_-\left|-\right\rangle_S\left|-\right\rangle_A}.$$

And now we just rewrite everything in terms of the z-eigenstates: rewriting $\left|x;\pm\right\rangle$ as $\frac{1}{\sqrt{2}}(\left|+\right\rangle \pm \left|-\right\rangle)$, we find that

$$\left|\psi(t)\right\rangle_{SA} = \frac{1}{2}c_+(e^{-i\omega t} - e^{i\omega t})\left|+\right\rangle_S\left|+\right\rangle_A + \frac{1}{2}c_+(e^{-i\omega t} + e^{i\omega t})\left|+\right\rangle_S\left|-\right\rangle_A + c_-\left|-\right\rangle_S\left|-\right\rangle_A,$$

which we can rewrite as

$$\left|\psi(t)\right\rangle_{SA} = -i\sin(\omega t)c_+\left|+\right\rangle_S\left|+\right\rangle_A + \cos(\omega t)c_+\left|+\right\rangle_S\left|-\right\rangle_A + c_-\left|-\right\rangle_S\left|-\right\rangle_A$$

The $\left|+\right\rangle\left|-\right\rangle$ is the bad term that we're trying to remove through time evolution, and indeed after some time $t^* = \frac{\pi}{2\omega}$, the cross term goes away, and we'll have

$$\boxed{\left|\psi(t^*)\right\rangle_{SA} = -ic_+\left|+\right\rangle_S\left|+\right\rangle_A + c_-\left|-\right\rangle_S\left|-\right\rangle_A}.$$

This means that after a time of t^* spent evolving unitarily, our states in the system and apparatus have been entangled perfectly (up to some changes in phase, but not amplitude). And now if we measure our apparatus to be in the $\left|+\right\rangle$ state, we will also find the system in the $\left|+\right\rangle$ state, and same with $\left|-\right\rangle$.

At the end of the day, though, our system still hasn't actually found a way to collapse into one of the two states: we've reached pre-measurement, but we haven't solved the mystery of how the measurement is actually made. So our focus now will be on the modern viewpoint of this issue and the crux of this measurement problem at hand.

Fact 338

Here is where decoherence really comes in to play: remember that an open system does not evolve unitarily, so we can try to claim that the non-unitary nature of projectors comes from the non-unitary evolution of an open system.

To expand on this idea, suppose that our SA composite system is now connected to an environment E. Then

$$\left|\psi(t^*)\right\rangle_{SA} = \sum_i c_i\left|s_i\right\rangle \otimes \left|a_i\right\rangle$$

is in the pre-measurement state, but when we introduce the environment, we can now write the states as

$$\left|\psi(t^*)\right\rangle_{SAE} = \sum_i c_i\left|s_i\right\rangle \otimes \left|a_i\right\rangle \otimes \left|e_i\right\rangle.$$

The $\left|e_i\right\rangle$ states can be very different from each other, but what we have is still a pure state for SAE. To introduce something interesting (and get the decoherence in the picture), let's **look at the density matrix of** SA, which is

$$\rho_{SA} = \mathrm{tr}_E\,\rho_{SAE} = \mathrm{tr}_E\sum_{i,j} c_i c_j^*\left|s_i\right\rangle\left|a_i\right\rangle\left|e_i\right\rangle\left\langle s_j\right|\left\langle a_j\right|\left\langle e_j\right|.$$

This then simplifies (with the usual rule) to

$$\sum_{i,j} c_i c_j^* \left|s_i\right\rangle \left|[\right\rangle a_i] \left\langle s_j\right| \left\langle a_j\right| \left\langle e_j|e_i\right\rangle .$$

Because there are many degrees of freedom in the environment, we can approximate $\langle e_j|e_i\rangle$ as δ_{ij} (one possible explanation is that pointer states could couple to different orthogonal environment states, and another is that the total overlap ends up being small), and thus this expression becomes

$$= \sum_i |c_i|^2 \left|s_i\right\rangle \left|a_i\right\rangle \left\langle s_i\right| \left\langle a_i\right| ,$$

and given the normalization of our states, we must have $\sum |c_i|^2 = 1$. So this is indeed a valid density matrix, corresponding to an ensemble

$$E = \{(|c_1|^2, |s_1\rangle |a_1\rangle), \cdots, (|c_n|^2, |s_n\rangle |a_n\rangle)\}.$$

In words, this means that when we measure if we don't know about the environment, our SA composite system has a probability $|c_i|^2$ of being in the state $|s_i\rangle \otimes |a_i\rangle$. (So density matrices indeed give a motivation for why we have the familiar-looking probabilities!)

Example 339

One instance in which we might have seen a system like this is Schrodinger's cat.

In such a system, it may seem plausible to start with a superposition

$$\frac{1}{\sqrt{2}}(|☺\rangle + |☹\rangle) \otimes |E_0\rangle$$

where the cat is either alive or dead (Schrodinger describes a contraption which puts the cat in this state), and there's definitely an environment around the cat. But it doesn't actually make sense to have the same $|E_0\rangle$ environment state attached to both the live and dead cat: the live cat (for example) needs to breathe, so it interacts with the environment in a different way from the dead cat. Therefore, we will eventually end up (after basically any instant in time) in the state

$$\frac{1}{\sqrt{2}}(|☺\rangle |E_1\rangle + |☹\rangle |E_2\rangle).$$

So now if we assume that E_1 and E_2 are orthogonal, the density matrix of the cat should be

$$\rho_{\text{cat}} = \frac{1}{2} \left|☺\right\rangle \left\langle ☺\right| + \frac{1}{2} \left|☹\right\rangle \left\langle ☹\right| ,$$

and now it seems to makes sense that decoherence can lead us to a mixed state.

Unfortunately, what we've been discussing with decoherence actually raises more questions than it answers: **introducing the environment still yields some issues with measurement**. It's not clear that the environment states $|e_i\rangle$ need to couple to the SA states in the way that they do – instead, it's possible that they couple to linear combinations of the SA states, in which case we have a different-looking density matrix. In addition, we know that different-looking ensembles can give the same density matrix – that is, the resulting ensemble E can be ambiguous.

So now we'll turn our attention to the other idea, which is the **many-worlds interpretation**, proposed by Everett. In this theory, the wavefunction doesn't collapse in the same way that it does in our previous discussion. Instead, upon measurement, the universe splits (based on the result of that measurement).

Example 340

Suppose Alice has a spin 1/2 particle in the state

$$|\psi\rangle = c_+ |+\rangle + c_- |-\rangle .$$

As always, $|c_+|^2 + |c_-|^2 = 1$, so the Copenhagen interpretation tells us that we have a $|c_+|^2$ probability of ending up in the $|+\rangle$ state and a $|c_-|^2$ probability of ending up in the $|-\rangle$ state after a measurement along the z-axis.

The many-worlds interpretation accounts for this by requiring us to include the measurement apparatus (and in particular Alice) in the wavefunction, so that we have

$$|+\rangle = (c_+ |+\rangle + c_- |-\rangle) \otimes |\text{Alice}\rangle .$$

Then when Alice does a measurement, we claim that the state factors into

$$\Longrightarrow \; c_+ |+\rangle |\text{Alice sees } +\rangle + c_- |\text{Alice sees } -\rangle .$$

So Alice is "acting like a pointer state" like in the von Neumann argument above, and from here the idea is that there are two independent branches of the universe: in one of them, Alice sees $+$ and the state is in $|+\rangle$, and in the other, Alice sees $-$ and the state is in $|-\rangle$. Those two branches then never interact with each other, so further experiments in each branch will just keep splitting our universe into different paths.

So if everything happens in some path of the universe, we need another interpretation of probability: one argument is that before Alice observes the measurement, she has some **self-location probability** of ending up in the different branches, dictated by the coefficients $c_\pm$. But this idea is a big conceptual departure from what we've been discussing so far – we don't really know what we're talking about when we write down a ket like $|\text{Alice sees } +\rangle$, and we need more evidence to make this a valuable theory. (If we read the literature and compare the ideas, we can think through these thoughts ourselves as well.)

To finish off the class, we'll discuss the topic of **quantum computation**, an area of ongoing research. Basically, quantum computers are able to do computations in a different way from normal computers, exploiting the properties of superposition and interference, which often makes computations go faster.

Definition 341

A **bit** is the basic unit of information: it is an object with two possible states, 0 and 1. A **qubit** is a quantum object with two possible **basis** states, $|0\rangle$ and $|1\rangle$.

As we've mentioned before, there are infinitely many possible states that a qubit can be in (corresponding to the different linear superpositions of $|0\rangle$ and $|1\rangle$), but only finitely many states that a bit can be in. A qubit can be created in many physical manifestations – a spin 1/2 particle, a particle in a potential with two energy levels, and so on – but the point is that we'll be using qubits to do calculations faster than bits.

Fact 342

In 2019, Google did a computation with a 53-qubit computer that took 200 seconds, which a normal computer takes a few days to do.

One concept stronger than just "being faster" is **quantum supremacy**, which is the idea that a quantum computer can solve problems that normal computers cannot. The idea of having a "programmable computer" (made precise by

Turing, so they're called Turing machines) is connected to the **Church-Turing thesis**, which says that any algorithm we can do with a computer can be done with a Turing machine (the simplest possible programmable computer). This result is widely believed, but there's a stronger version of the thesis which claims that any algorithm on any computer can be recreated **efficiently** on that Turing machine.

In other words, if we have a problem of (for example) input size N, an **efficient** algorithm takes a polynomial number of operations in N. (A non-efficient algorithm would be, for example, one that takes exponential time.) So the stronger Church-Turing thesis basically says that we can be equally efficient with a computer and a Turing machine, and the question here is **whether this is true for quantum computers as well**. At the moment, it does seem like quantum computation may be able to do calculations (like prime factorization) efficiently, while classical computers can not. But a quantum computer has limitations due to decoherence, and at some level this is unavoidable (so we need to build in error correction). That means that quantum computation algorithms are more complicated, and thus we don't actually know how much that error correction will affect the efficiency of our algorithm.

What we'll spend time on here is to understand **theoretically** how a quantum computer takes advantage of superposition, and one main idea is that we can simulate many quantum particles (which is very difficult in a classical computer).

Let's start with the qubits themselves. By convention, the notation we often use here is

$$|0\rangle = |z;+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = |z;-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

(These are sometimes called the **computational basis states**.) Then a general arbitrary state of the qubit is

$$|\psi\rangle = a_0 |0\rangle + a_1 |1\rangle = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix},$$

where $a_0, a_1 \in \mathbb{C}$ and $|a_0|^2 + |a_1|^2 = 1$, as usual. We can measure the value of the qubit along a basis, which corresponds to "reading the bit and seeing if it is 0 or 1:" if we measure along the computational basis states, we get $|0\rangle$, corresponding to the bit 0, or $|1\rangle$, corresponding to the bit 1.

So now, suppose we have two qubits instead of one: we can describe a general state as

$$|\psi\rangle = a_{00} |0\rangle \otimes |0\rangle + a_{01} |0\rangle \otimes |1\rangle + a_{10} |1\rangle \otimes |0\rangle + a_{11} |1\rangle \otimes |1\rangle,$$

where $a_{ij} \in \mathbb{C}$ and $\sum_{i,j} |a_{ij}|^2 = 1$. To make the notation a little nicer, we'll just rewrite this as

$$|\psi\rangle = a_{00} |00\rangle + a_{01} |01\rangle + a_{10} |10\rangle + a_{11} |11\rangle,$$

and now we have four computational basis states (corresponding to the tensor product of the basis states of the individual qubits). And again, measuring along this basis means that we can read the two bits as $00, 01, 10$, or 11.

One useful rule to keep in mind here is that we can identify states with binary numbers, so that

$$|00\rangle \to 0, \quad |01\rangle \to 1, \quad |10\rangle \to 2, \quad |11\rangle \to 3$$

in this case. And we can generalize this to a **system of n qubits**, which corresponds to a tensor product space of dimension $N = 2^n$: we write the computational basis states here as

$$|x_1\rangle \otimes \cdots \otimes |x_n\rangle = |x_1 \cdots x_n\rangle, \quad x_i \in \{0, 1\},$$

And then a sequence $x_1 \cdots x_n$ represents a binary number, which then corresponds to a nonnegative integer:

$$|x_1 \cdots x_n\rangle = \overline{x_1 \cdots x_n}_2 \in [0, 2^n - 1].$$

A typical state of this state space is then

$$\psi = a_{0\cdots0} |0\cdots0\rangle + a_{0\cdots1} |0\cdots1\rangle + \cdots + a_{1\cdots1} |1\cdots1\rangle,$$

where there are $N = 2^n$ total coefficients that need to be stored.

So here we can see the drastic difference already: if we consider a 53-bit quantum computer like Google used, the state space has dimension 2^{53}, which is on the order of 10^{16}. So specifying a state of a 53-bit classical computer requires us to write down a list of 53 numbers, each of which is 0 or 1, while specifying a state of a 53-qubit classical computer requires us to write down a list of 2^{53} numbers, each of which is some complex number! So the memory needed to store the state of a quantum computer grows exponentially.

Remark 343. *If we store each coefficient using 8 bytes (a byte is 8 bits), we'll need $2^{53} \cdot 2^3 = 2^{56}$ bytes just to specify a single state. This is 64 petabytes, which is about a quarter of IBM's largest supercomputer's storage. So working with this state is very difficult – just going from 53 qubits to 60 qubits means that our supercomputers can't deal with this anymore, especially when we need to time-evolve the state forward as well.*

So now we want to do **operations** on our qubits: these are the calculations that make normal computation possible, and they're interesting to study in the quantum case as well.

Definition 344

A (quantum) **gate** is a unitary operator on qubits.

Example 345

The simplest gates act on a single qubit, meaning that they are unitary operators on a 2-dimensional vector space.

Remember that the Pauli matrices are Hermitian and square to the identity matrix I, so they are also unitary: thus, we have the matrices

$$X = \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

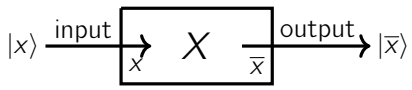
Notice, for example, that

$$X |0\rangle = |1\rangle, \quad X |1\rangle = |0\rangle$$

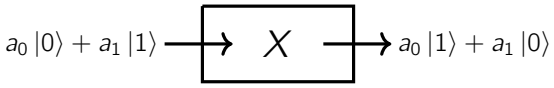
(don't forget that we're zero-indexing), so this can be described as the **NOT gate**, which **reverses** a bit. Another way to write this is that the output of the NOT gate is

$$\overline{x} = \text{NOT}(x) = x \oplus 1,$$

where the $\oplus$ symbol means addition mod 2. We like to represent these gates with diagrams: here's a representation of the NOT gate.



(In one sentence, the X gate takes $|x\rangle$ into $|\overline{x}\rangle = |x \oplus 1\rangle$.) In the classical case, we can only have an input of 0 or 1, but in the quantum case, we can also send in some superposition and find its NOT value:



(Basically, linearity means that it's easy to write down the result of any superposition of $|0\rangle$ and $|1\rangle$.) We can also write down the action of the Y and Z gates, but there's another gate which is more interesting, known as the **Hadamard gate** H:

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

Then we can calculate

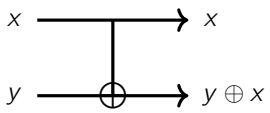
$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle),$$

and we will see soon why this is useful.

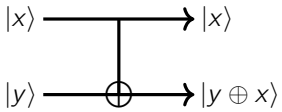
Example 346

Now let's look at unitary operators on two qubits, which means we now need unitary matrices acting on a 4-dimensional vector space.

Here, it is still possible to visualize the 4×4 matrices, but we'll need to describe them with clear language. One well-known gate is the **controlled NOT** or **cNOT** gate, and in the classical case, it looks like this:



Here, x is known as the "control bit," while y is known as the "target bit" – the control bit remains unchanged, but y is changed based on the value of x. To transfer this into the quantum case, we will need a control and target qubit, and we'll transform on the basis states in the exact same way:



This is called a "controlled NOT" gate, because it acts like a NOT whenever the control bit x is $|1\rangle$, but it does nothing when the control bit x is $|0\rangle$. And remember that the quantum gate only acts like this on **computational states**: we get the rest by linearity.

Since the two qubits live in a tensor product space, another way to describe the action here is that

$$|x\rangle \otimes |y\rangle \overset{\text{c-NOT}}{\to} |x\rangle \otimes |y \oplus x\rangle.$$

We can ask **whether the cNOT gate is unitary**, and the way to check this is to look at the matrix representation of the gate: choose basis vectors in the tensor product space to be

$$|00\rangle, |01\rangle, |10\rangle, |11\rangle$$

in that order (so that the numbers are ascending in binary), and notice that the basis elements are sent to

$$|00\rangle, |01\rangle, |11\rangle, |10\rangle$$

respectively. So the **matrix corresponding to cNOT** is

$$U_{\text{cNOT}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

which is $\begin{bmatrix} 1 & 0 \\ 0 & X \end{bmatrix}$ in block form. And this block matrix form is a nice way of thinking about the cNOT gate intuitively – the action depends on the state of the first bit – and now this matrix is indeed unitary because it is Hermitian and squares to the identity matrix I (by block multiplication).

Example 347

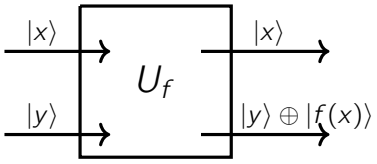
Our next step is to try to construct a function using these types of unitary gates.

For example, we may want to take one of the four (classical) functions $f(x) : \{0, 1\} \to \{0, 1\}$, which sends each bit to some bit, and write it in terms of our quantum gates. In other words, **does there exist a gate** G such that

$$G|x\rangle = |f(x)\rangle?$$

Somewhat surprisingly, it's not always possible to do this! One function that we **can** construct is the identity function (where $f(0) = 0, f(1) = 1$), since we can just act with the identity matrix, which is certainly a unitary operator. Similarly, we **can** construct the function such that $f(0) = 1, f(1) = 0$ by using the NOT gate that we described above. But the other two functions are constant functions (which send either bit to 0 or to 1), and that's not a unitary transformation (since it's not invertible), so we **can't** find a gate G that does the job here. That means that not all functions f can be "unitarily implemented" like this for even this simple domain and range, and thus we should not expect to be able to represent functions f in general: after all, **unitary operators are always injective**.

So if we want to be able to use gates to implement a function f and do general computation, **all such computations must be reversible**. One trick to address this issue is to enlarge the state space: even when our function f only acts on a single qubit, we can use a gate U_f that takes in two inputs and also spits out two outputs:



In other words, this is the unitary operator

$$U_f|x\rangle \otimes |y\rangle = |x\rangle \otimes |y \oplus f(x)\rangle\,,$$

and now $|x\rangle$ serves as a kind of "control bit" for the function because it's unchanged, but it is also the bit that is being evaluated by f. A slightly cleaner way of writing the above equation is

$$U_f|x, y\rangle = |x, y \oplus f(x)\rangle\,,$$

and we'll choose to use this kind of notation from here. (Notice that when $y = 0$, we have $U_f|x, 0\rangle = |x, f(x)\rangle$, so plugging in $y = 0$ will give us back the function reading $f(x)$ on the bottom bit.)

Indeed, this function is reversible – in fact, applying it twice yields

$$\boxed{U_f U_f |x, y\rangle} = U_f |x, y \oplus f(x)\rangle = |x, y \oplus f(x) \oplus f(x)\rangle$$

but $f(x) + f(x)$ is always 0 mod 2 (whether $f(x) = 0$ or 1), so this is just $\boxed{|x, y\rangle}$ back again. So this gate squares to itself (meaning it is its own inverse), and we want to make sure it's Hermitian as well. We can do this by constructing the matrix representation again, but let's try something different this time: note that we can write U_f in terms of "matrix elements" by considering the operator

$$U_f = \sum_{(x,y)\in\{0,1\}^2} |x, y \oplus f(x)\rangle \langle x, y| .$$

(We can check that this has the correct action on each of the computational basis states, because they are are orthonormal.) Then the Hermitian conjugate flips the kets and the bras, so we now have

$$U_f^\dagger = \sum_{(x,y)\in\{0,1\}^2} |x, y\rangle \langle x, y \oplus f(x)| .$$

To show that $U_f^\dagger = U_f$, we do a change of variables: let $x' = x, y' = y \oplus f(x)$ (we can check that this is a reversible change of variables, because it is injective). Then $y = y' \oplus f(x)$ as well (because everything is taken mod 2), meaning we can rewrite the above expression:

$$= \sum_{(x',y')\in\{0,1\}^2} |x', y' \oplus f(x')\rangle \langle x', y'| ,$$

which is the same expression as U_f with different dummy variables. Thus U_f is indeed Hermitian (so combined with the above information, it's unitary), and we've now found a way to describe our function f using a unitary gate, just by using a larger state space.

So now we have seen how to represent a **classical** function f with one input, using a two-qubit quantum gate.

Fact 348

It turns out that if we have a function f with an n-bit domain and a 1-bit range

$$f(x_1, \cdots, x_n) \in \{0, 1\}^n$$

(which is clearly not going to be injective in general because we have 2^n possible inputs and 2 possible outputs), we can always construct a quantum U_f with $(n + 1)$ inputs $|x_1\rangle, \cdots, |x_n\rangle, |x_{n+1}\rangle$, such that

$$(|x_1\rangle, \cdots, |x_n\rangle, |y\rangle) \to (|x_1\rangle, \cdots, |x_n\rangle, |y \oplus f(x_1, \cdots, x_n)\rangle).$$

In other words, the first n inputs are the inputs to our function – the gate won't change them – and the last input will "carry the answer" – it will change based on the value of our function. (It is rather striking that we can fix all of the non-injectivity issues with just a single additional bit as input!)

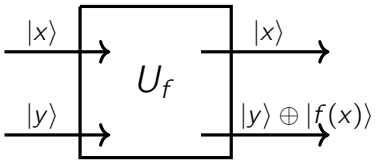
Example 349

So now we're ready to see a simple quantum algorithm, known as **Deutsch's algorithm**, in action.

We'll suppose that we have access to an **oracle**, which can tell us the value of a function given any input. If we want to know about a function f with a one-bit input and output, we need to make two calls to the oracle (asking for

the values of $f(0)$ and $f(1)$) in an ordinary computer. But now suppose that we care about the value of $f(0) \oplus f(1)$ (mod 2): in the classical setting, we will need to make the two calls for $f(0)$ and $f(1)$ separately, but there is actually a way to get around that in the quantum case – **we will only need one call of the oracle!**

We'll need to use the quantum gate that we constructed above:



Applying U_f is our oracle here (because that's what tells us the value of the function f), and we claim here that we will only need to apply U_f once to get $f(0) \oplus f(1)$. And this makes some sense when we think about U_f as a linear operator: consider the action of U_f on the state

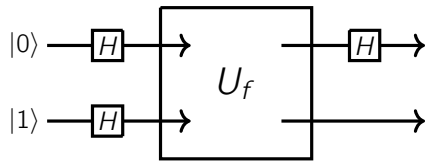
$$|\psi\rangle = H|0\rangle \otimes |0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle .$$

Since our first input $|x\rangle$ is a superposition of $|0\rangle$ and $|1\rangle$, it almost seems like we're evaluating x simultaneously at both of those values here. By linearity, we have that

$$U_f|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|f(0)\rangle + |1\rangle|f(1)\rangle\right),$$

and we now have entanglement of the two qubits (between the argument and the function), meaning that we've extracted the information of $f(0)$ and $f(1)$ simultaneously. But notice that we cannot actually extract both of those pieces of information at once, because measuring the value of the first bit will collapse us into either $|0\rangle|f(0)\rangle$ or $|1\rangle|f(1)\rangle$, and the other information is destroyed.

Nevertheless, we **can** get composite information like $f(0) \oplus f(1)$, and here's the quantum computer that does the job:



Proposition 350
The output of this computer will give us a state where we can read off the value of $f(0) \oplus f(1)$.

Proof. Call the initial state $|\psi_0\rangle$, the state after the first two Hadamard operators $|\psi_1\rangle$, the state after the U_f "oracle query" $|\psi_2\rangle$, and the state after the final Hadamard operator $|\psi_{\text{out}}\rangle$. We know that

$$|\psi_0\rangle = |0\rangle \otimes |1\rangle ,$$

which means that

$$|\psi_1\rangle = H|0\rangle \otimes H|1\rangle = \frac{1}{2}(|0\rangle + |1\rangle) \otimes (|0\rangle - |1\rangle) = \frac{1}{2}|0\rangle \otimes (|0\rangle - |1\rangle) + \frac{1}{2}|1\rangle \otimes (|0\rangle - |1\rangle).$$

(Expanding out in this way will become useful soon.) We now want to act on this function with U_f: we have

$$|\psi_2\rangle = U_f|\psi_1\rangle = \frac{1}{2}|0\rangle \otimes (|f(0)\rangle - |1 \oplus f(0)\rangle) + \frac{1}{2}|1\rangle \otimes (|f(1)\rangle - |1 \oplus f(1)\rangle),$$

because U_f leaves the first bit invariant. Finally, acting with H on the first output yields

$$|\psi_{\text{out}}\rangle = \frac{1}{2}H|0\rangle \otimes (|f(0)\rangle - |1 \oplus f(0)\rangle) + \frac{1}{2}H|1\rangle \otimes (|f(1)\rangle - |1 \oplus f(1)\rangle),$$

and expanding this out yields

$$= \boxed{\frac{1}{2\sqrt{2}}|0\rangle \otimes (|f(0)\rangle - |1 \oplus f(0)\rangle + |f(1)\rangle - |1 \oplus f(1)\rangle) + \frac{1}{2\sqrt{2}}|1\rangle \otimes (|f(0)\rangle - |1 \oplus f(0)\rangle - |f(1)\rangle + |1 \oplus f(1)\rangle)}.$$

We're trying to find the value of $f(0) \oplus f(1)$, but it doesn't seem to pop out obviously from our calculations – we'll need to be a bit more careful. Notice that whenever $f(0) = f(1)$, we have $f(0) \oplus f(1) = 0$, and otherwise we have $f(0) \oplus f(1) = 1$. And now let's consider each of these two cases: if $f(0)$ and $f(1)$ are **equal**, then **everything in the second group** cancels out in the above boxed expression, and whenever $f(0)$ and $f(1)$ are **different**, **everything in the first group** cancels out. So in both cases, the amplitude of one of our two terms will disappear – more specifically, the expression for our final state simplifies to

$$|\psi_{\text{out}}\rangle = \begin{cases} |0\rangle \otimes \frac{1}{\sqrt{2}}(|f(0)\rangle - |1 \oplus f(0)\rangle) & \text{when } f(0) = f(1) \implies f(0) \oplus f(1) = 0, \\ |1\rangle \otimes \frac{1}{\sqrt{2}}(|f(0)\rangle - |1 \oplus f(0)\rangle) & \text{when } f(0) \neq f(1) \implies f(0) \oplus f(1) = 1. \end{cases}$$

(Notice that $f(0)$ and $1 \oplus f(0)$ always take on different values, so neither case has a wavefunction that is just zero.) So now we just need to **measure along the computational basis states** of the first qubit: whatever answer we end up with must be the value of $f(0) \oplus f(1)$, and we're done. (And we end up with a $\pm(|0\rangle - |1\rangle)$ no matter what the value of $f(0)$ is, so we cannot extract any more information beyond what we have described.) □

We have now seen a bit of the power of quantum computation, but now we'll do another example that is a bit more interesting:

Example 351

Grover's algorithm helps us solve a search problem of the sort where we are (figuratively) trying to find a black marble in a bag otherwise containing white marbles.

Normally, we have to examine the marbles one by one, so in a large bag of N marbles, it will take about $\frac{N}{2}$ tries to find the marble on average. But it turns out that we're only going to need about $\sqrt{N}$ calls in the quantum case! (There are even more drastic improvements that we can make with quantum computation, such as with Shor's algorithm, but this example here is illustrative enough.)

So let's describe this problem more formally: suppose we have a set of size $N = 2^n$ (where $n \geq 1$ is some usually large positive integer). We can correspond the elements of the set $X = \{0, 1, \cdots, N-1\}$, and we can then correspond those with the binary strings of length n, $\{x_1 \cdots x_n\}$.

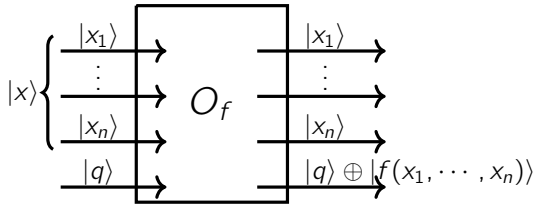
We now have a function

$$\underline{f(x)} = f(x_1, x_2, \cdots, x_n) \in \{0, 1\}$$

which can be thought of as the **oracle** in this problem: for each integer x from 0 to $N-1$, we have either $f(x) = 0$ or 1. Then the problem we're facing is to **identify some element with** $f(x) = 1$: suppose we're told that there M such values of x (so there are $(N - M)$ non-solutions where $f(x) = 0$), and we're going to assume $M \ll N$ here (because that's when the problem is "hardest"). Again, we need about $\frac{N}{2}$ queries of the oracle for $M = 1$, but it turns out a quantum computer will only take about $\frac{\pi}{4}\sqrt{N}$ steps.

Remark 352. *When we say that we have an oracle, the idea is that the formula or method of finding $f(x)$ is not transparent to us (so we can't just solve the equation $f(x) = 1$ ourselves): all we're told is the final value.*

The idea is that when we feed in a label $|x\rangle$ (which is a set of n qubits), we're getting a reading of the oracle as follows:



As usual, the first n qubits are inputs and stay unchanged, and the last input is changed by the value of f. So the operator O_f takes the state $|x\rangle |q\rangle$ into the state $|x\rangle |q \oplus f(x)\rangle$, where we're (again) using the condensed notation that $x = (x_1, \cdots, x_n)$. And this time, the idea is that we're going to pick a particularly nice starting state $|q\rangle$ so that our computation turns out nicer: we'll use

$$|q\rangle = H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$$

Then the action of O_f on our input will look like

$$O_f(|x\rangle \otimes H|1\rangle) = |x\rangle \otimes \frac{1}{\sqrt{2}}(|f(x)\rangle - |1 \oplus f(x)\rangle)$$

by linearity, and now we want to exploit that this last expression only depends up to a sign $f(x)$ (we'll either have $|f(0)\rangle - |f(1)\rangle$ or $|f(1)\rangle - |f(0)\rangle$). Specifically, the second term of the tensor product is $H|1\rangle$ if $f(x) = 0$ and $-H|1\rangle$ if $f(x) = 1$: another way to write this is that our final state is very similar to our initial state:

$$\boxed{O_f(|x\rangle \otimes H|1\rangle)} = |x\rangle \otimes (-1)^{f(x)} H|1\rangle = \boxed{(-1)^{f(x)}(|x\rangle \otimes H|1\rangle)}.$$

So now we now have information about our function in a "sign" or "phase," rather than the ket itself, and that's nice when we're trying to do things with interference. And since this last qubit $|q\rangle = H|1\rangle$ is unaffected by our transformation O_f, **we will omit it from the notation from now on** (we'll just write things like $O_f|x\rangle = (-1)^{f(x)}|x\rangle$).

The next idea is to choose an input $|x\rangle$ which works well with our operator, and the idea here is that the Hadamard gate is very useful when combining information together. We will start with an initial state

$$|\psi_0\rangle = (H|0\rangle)^{\otimes n} = H|0\rangle \otimes H|0\rangle \otimes \cdots \otimes H|0\rangle$$

(n terms in total), and if we write out the definition of $H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, this initial state turns out to be

$$= \frac{1}{\sqrt{2^n}}(|0\rangle + |1\rangle)^n = \frac{1}{\sqrt{N}}(|0\rangle + |1\rangle) \otimes \cdots \otimes (|0\rangle + |1\rangle).$$

So each of the n terms in this final tensor product corresponds to one of the qubits, and thus if we expand all of the products, we will find an equal contribution from **each** of the N computational basis states (each of the n-digit binary numbers from 0 to $N-1$):

$$= \frac{1}{\sqrt{N}}(|0\cdots0\rangle + |0\cdots1\rangle + \cdots + |1\cdots1\rangle) = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle .$$

Because this initial state "represents all of the states at the same time," having the oracle act on this will give us "information about all of the states" (though we can't disentangle that information easily, which is why the problem is

difficult). To prepare for the action of O_f, we can rewrite this state in a slightly different way, splitting based on the value of f:

$$= \frac{1}{\sqrt{N}} \sum_{x:f(x)=0} |x\rangle + \frac{1}{\sqrt{N}} \sum_{x:f(x)=1} |x\rangle .$$

We now want to "normalize each of these components separately:" since there are $(N-M)$ states in the first sum and M states in the second sum, we can rewrite this as

$$|\psi_0\rangle = \sqrt{\frac{N-M}{N}} \frac{1}{\sqrt{N-M}} \sum_{x:f(x)=0} |x\rangle + \sqrt{\frac{M}{N}} \frac{1}{\sqrt{M}} \sum_{x:f(x)=1} |x\rangle ,$$

so that we have a superposition of two normalized states: let's call them $|\alpha\rangle$ and $|\beta\rangle$ respectively, so that

$$|\psi_0\rangle = \sqrt{\frac{N-M}{N}} |\alpha\rangle + \sqrt{\frac{M}{N}} |\beta\rangle .$$

By construction, we know that $\langle\alpha|\alpha\rangle = \langle\beta|\beta\rangle = 1$, and also $\langle\alpha|\beta\rangle = 0$ because the (computational basis) kets that appear in the definition of $|\alpha\rangle$ are disjoint from those that appear in $|\beta\rangle$. And now we're going to work in the vector space

$$\mathbb{R}^2 = \text{span}(|\alpha\rangle , |\beta\rangle)$$

(note that we have a **real** vector space because our coefficients are all going to be real in this case), which is nice because we can visualize $|\alpha\rangle$ and $|\beta\rangle$ as the orthonormal basis vectors along the x- and y-axis of an ordinary regular xy-plane (where $|\alpha\rangle$ represents the "non-solutions" and $|\beta\rangle$ represents the "solutions" that we're trying to find). $|\psi_0\rangle$ is then a normalized vector pointing "mostly" in the $|\alpha\rangle$ direction, because $M \ll N$: this means we can write it as a **unit vector**

$$|\psi_0\rangle = \cos\theta_0 |\alpha\rangle + \sin\theta_0 |\beta\rangle$$

for some small angle $\theta_0 = \sin^{-1}\sqrt{\frac{M}{N}}$. Intuitively, our quantum circuit is going to slowly move this unit vector towards the $|\beta\rangle$-axis (at which point we can just measure the state to get a solution) and that's what we'll describe now.

Notice that O_f takes $|\alpha\rangle$ (a superposition of non-solutions) to itself (because $(-1)^{f(x)} = (-1)^0 = 1$ for every term in $|\alpha\rangle$), but it takes $|\beta\rangle$ to $-|\beta\rangle$ (because $(-1)^{f(x)} = (-1)^1 = -1$ for every term). Therefore, applying O_f preserves the $|\alpha\rangle$-component and flips the $|\beta\rangle$-component, meaning that

$$O_f |\psi_0\rangle = O_f(\cos\theta_0 |\alpha\rangle + \sin\theta_0 |\beta\rangle) = \cos\theta_0 |\alpha\rangle - \sin\theta_0 |\beta\rangle .$$

But now $|\psi_0\rangle$ and $O_f |\psi_0\rangle$ are reflections across the $|\alpha\rangle$ or x-axis, so they are separated by an angle of $2\theta_0$. This means that we'd be in good shape if we figured out how to **reflect about our initial state** $|\psi_0\rangle$: the result would have a larger angle to the horizontal, moving us towards the $|\beta\rangle$-axis. And it turns out the operator that we want is

$$\boxed{R_0 = 2 |\psi_0\rangle \langle\psi_0| - I}.$$

To check that this is indeed what we want, we can rewrite the identity term as $|\psi_0\rangle \langle\psi_0| + |\psi_0^\perp\rangle \langle\psi_0^\perp|$ (for some vector $|\psi_0^\perp\rangle$ perpendicular in the plane to our original state), and then we have

$$R_0 = 2 |\psi_0\rangle \langle\psi_0| - (|\psi_0\rangle \langle\psi_0| + |\psi_0^\perp\rangle \langle\psi_0^\perp|) = |\psi_0\rangle \langle\psi_0| - |\psi_0^\perp\rangle \langle\psi_0^\perp| ,$$

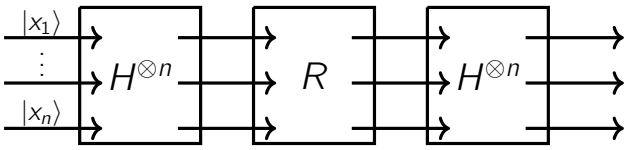
which is an operator that preserves the $|\psi_0\rangle$ component and flips the $|\psi_0^\perp\rangle$ component, so it is indeed a reflection of the desired type (and is also unitary, so it's a valid operator to use here). Because we started with the state

$$|\psi_0\rangle = (H|0\rangle)^{\otimes n} = H^{\otimes n} |0\rangle ,$$

(in this last equality we changed from using qubits 0 to the actual n-digit binary string 0), we can also rewrite our reflection operator as

$$R_0 = H^{\otimes n}(2\,|0\rangle\langle 0| - I)H^{\otimes n}.$$

(We can check that this is valid, because the $H^{\otimes n}$ on the left acts on the ket, the $H^{\otimes n}$ on the right acts on the bra, and the two do nothing to the identity because $H^2 = I$.) So our quantum computer realizes the reflection R_0 by using a series of three gates:



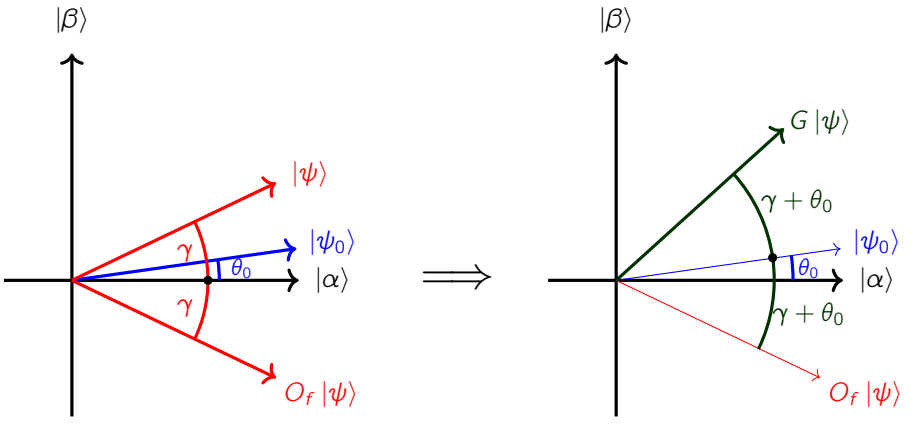
The first and third of the gates are just qubit-wise Hadamard gates, and we need to figure out the second gate. That middle gate $\boxed{R}$ is the same expression at R_0, but we're now reflecting around the $|0\rangle$-axis, so it sends $\boxed{|0\rangle \to |0\rangle}$ and $\boxed{|x\rangle \to -|x\rangle}$ for all $x \neq 0$. (Remember that 0 still represents the n-digit binary integer here, so all $2^n - 1$ other computational basis vectors are flipped – just not $|0\rangle$.) This kind of gate can indeed be implemented using NAND gates, and thus we've indeed managed to construct an R_0 gate.

So thinking geometrically again, we can now return to the state

$$R_0 O_f\,|\psi_0\rangle\,.$$

(Remember that O_f does take in an extra qubit $|q\rangle$ as input, while R_0 does not.) The oracle O_f reflects ψ_0 over the $|\alpha\rangle$-axis, moving us to an angle of $-\theta_0$ in the $|\alpha\rangle\,|\beta\rangle$-plane, and then R_0 reflects the result over the $|\psi_0\rangle$ state. Since the difference in angle is $2\theta_0$, our final result will have an angle of $\theta_1 = 3\theta_0$ in the $|\alpha\rangle\,|\beta\rangle$ plane.

And we can just iterate this again and again: letting $\boxed{G = R_0 O_f}$ be the **Grover operator**, we can just **act with** G **on** $|\psi_0\rangle$ **repeatedly**. If we have some arbitrary state $|\psi\rangle$ at an angle γ from the horizontal $|\alpha\rangle$-axis, then $O_f\,|\psi\rangle$ will be at an angle of $-\gamma$, so applying R_0 (rotating about the $|\psi_0\rangle$ state) to this state will give us $G\,|\psi\rangle$ at an angle of $\boxed{\gamma + 2\theta_0}$, because $O_f\,|\psi\rangle$ is an angle $(\gamma + \theta_0)$ away from $|\psi_0\rangle$.



In summary, $R_0\theta_f$ just **rotates our vector** by an angle $2\theta_0$ in the $|\alpha\rangle\,|\beta\rangle$-plane for **any arbitrary unit vector**, so applying the Grover operator k times to $|\psi_0\rangle$ gives us a vector at an angle of

$$\theta_k = (2k+1)\theta_0 = (2k+1)\sin^{-1}\sqrt{\frac{M}{N}}$$

to the horizontal. And now we know how to carry out our quantum algorithm: if θ_0 is very small, we can apply G

enough times to get $|\psi_k\rangle$ to point **very close** to vertical, meaning that we're in a superposition of mostly states that have $f(x) = 1$. And then measuring along the computational basis states will give us one of the solutions, as desired.

When $M \ll N$, we can approximate the number of steps via

$$\frac{\pi}{2} = \theta_k \approx (2k+1)\sqrt{\frac{M}{N}},$$

and solving for k yields $\boxed{k \approx \frac{\pi}{4}\sqrt{\frac{N}{M}}}$, which is the result that we promised at the beginning! And this quantum algorithm has given us an answer in $O(\sqrt{N})$ queries of the oracle, rather than $O(N)$ as we would have in the classical case.

Fact 353

Suppose that $N = 2^{30} \approx 10^9$ and $M = 1$. Then it takes about 500 million queries with a classical computer to find our solution, while it only takes about 26000 calls with the quantum computer.

But also remember that the quantum algorithm gives us a probability of success very close to 1, but not exactly equal to 1: specifically, the probability of success after we apply the Grover operator k times is

$$\mathbb{P}_k = |\langle\beta|\psi_k\rangle|^2,$$

and this is basically asking us for the squared $|\beta\rangle$-component of $|\psi_k\rangle$, which is $\sin^2(\theta_k)$.

Example 354

Let's examine the probability of success for our quantum algorithm when $N = 2^5 = 32$ and $M = 1$.

Then our starting state has an angle of

$$\theta_0 = \sin^{-1}\sqrt{\frac{M}{N}} = \sin^{-1}\sqrt{\frac{1}{32}} \approx 10.18^\circ,$$

and since $9\theta_0$ is about 90 degrees, we'll want to take $2k+1 = 9 \implies k = 4$, and four calls of the oracle result in

$$\theta_4 = 91.64^\circ \implies |\psi_4\rangle \approx -0.03\,|\alpha\rangle + 0.9996\,|\beta\rangle\,.$$

(Remember that in this case, $|\beta\rangle$ is just a single computational basis state, and $|\alpha\rangle$ is an equal superposition of the other 31 computational basis states.) This yields a probability of

$$\mathbb{P}_4 = \sin^2(91.64^\circ) = 0.9996^2 \approx 0.9991.$$

So more than 99.9 percent of the time, four calls to the oracle will get us the value of x such that $f(x) = 1$: much better than the classical case, where we need sixteen calls on average to get the answer!