Lecture #5
QM: Basic Postulates

- Topics
  - 6 postulates of QM
  - Examples
- Handouts and Reading assignments
  - van de Ven, Appendix C.
  - Miller, Chapters 2-3 (optional)

First Postulate

At any point in time, t_0, the state of a physical system is defined by a ket $|\psi(t_0)\rangle$ that belongs to the state space F.

- F is a Hilbert Space (linear vector space + metric)
- Superposition holds, $i.e.$ a linear combination of state vectors is also a state vector.

Second Postulate

Every measurable physical quantity $\mathcal{A}$ is described by an operator $\hat{A}$ acting in F. This operator is observable.

Classical mechanics

The state of a system is described by a set of physical parameters (e.g. $\vec{r}, \vec{p}$).

Quantum mechanics

state $\Rightarrow$ ket

physical quantities $\Rightarrow$ operator

What is an <u>observable</u>??

Observables*

- Let $\hat{A}$ be a Hermitian operator with eigenvalues a_n and corresponding normalized eigenkets $|u_n\rangle$ for $n = 1, 2, \ldots N$.
- $\hat{A}$ is an <u>observable</u> if its eigenkets form a basis in state space.
- Things to note:

$$\hat{A} \text{ Hermitian} \quad \Rightarrow \quad a_n \text{ real}$$

$$\langle u_i | u_j \rangle = \delta_{ij}$$

$$\sum_{n=1}^{N} |u_n\rangle\langle u_n| = \hat{E} \quad \text{(closure)}$$

- The set $\{a_n;\ n = 1,2,\ldots N\}$ is called the <u>spectrum</u> of $\hat{A}$.

*discrete, non-degenerate case.

Third Postulate

The only possible result of the measurement of a physical quantity $\mathcal{A}$ is one of the eigenvalues of the corresponding observable $\hat{A}$.

- The measurement of $\mathcal{A}$ always yields a real number.

- If the spectrum of $\hat{A}$ is discrete, the results that can be obtained by measuring $\mathcal{A}$ are quantized.

Fourth Postulate*

When the physical quantity $\mathcal{A}$ is measured the probability $\mathcal{P}(a_n)$ of obtaining eigenvalue a_n of the corresponding observable $\hat{A}$ is:

$$\mathcal{P}(a_n) = \left|\langle u_n|\psi\rangle\right|^2$$

where $|u_n\rangle$ is the eigenket of $\hat{A}$ associated with a_n.

- Consider two kets such that: $|\psi'\rangle = e^{i\theta}|\psi\rangle$.

$$|\psi\rangle:\ \mathcal{P}(a_n) = \left|\langle u_n|\psi\rangle\right|^2 \qquad |\psi'\rangle:\ \mathcal{P}(a_n) = \left|\langle u_n|e^{i\theta}\psi\rangle\right|^2 = \left|\cancelto{1}{e^{i\theta}}\right|^2 \left|\langle u_n|\psi\rangle\right|^2$$

Thus, $|\psi\rangle$ and $|\psi'\rangle$ represent the equivalent states.

* discrete, non-degenerate case. $|u_n\rangle$ and $|\psi\rangle$ normalized.

Phase Factors

- Consider two kets $|\psi\rangle$ and $|\psi'\rangle$ that represent the same state, $i.e.$ $|\psi'\rangle = e^{i\theta}|\psi\rangle$.

- Let $|\psi\rangle = |\psi_1\rangle + |\psi_2\rangle$ and $|\zeta\rangle = e^{i\theta_1}|\psi_1\rangle + e^{i\theta_2}|\psi_2\rangle$.

  Question: does it follow that $|\psi\rangle$ and $|\zeta\rangle$ represent the same state?

  Answer: NO!

$$|\zeta\rangle : \quad \mathcal{P}(a_n) = \left|\langle u_n|\zeta\rangle\right|^2 = \left|e^{i\theta_1}\langle u_n|\psi_1\rangle + e^{i\theta_2}\langle u_n|\psi_2\rangle\right|^2$$

$$= \left|\langle u_n|\psi_1\rangle\right|^2 + \left|\langle u_n|\psi_2\rangle\right|^2 + 2\mathrm{Re}\left\{\underline{e^{i(\theta_1-\theta_2)}}\langle u_n|\psi_1\rangle\langle u_n|\psi_2\rangle^*\right\}$$

In general, interference terms can **not** be ignored.

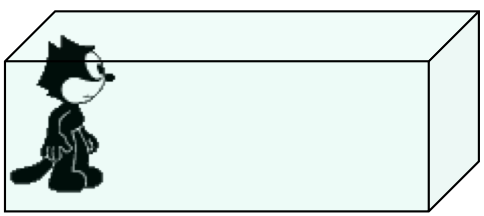
$$|\psi\rangle : \quad \mathcal{P}(a_n) = \left|\langle u_n|\psi_1\rangle\right|^2 + \left|\langle u_n|\psi_2\rangle\right|^2 + 2\mathrm{Re}\left\{\langle u_n|\psi_1\rangle\langle u_n|\psi_2\rangle^*\right\}$$

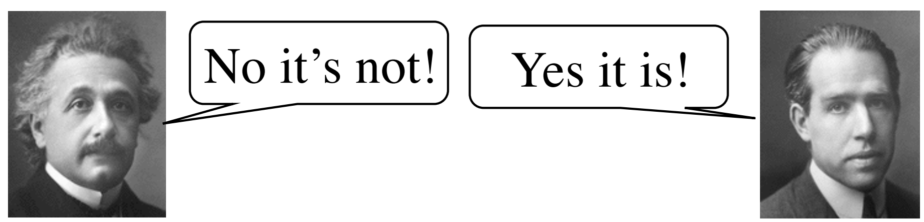
Global phase factors do not affect physical predictions, but the relative phases of the coefficients of an expression are significant.

Fifth Postulate

If the measurement of the physical quantity $\mathcal{A}$ on a system in state $|\psi\rangle$ gives the result a_n, the state of the system immediately after the measurement is $|\psi\rangle = |u_n\rangle$, the eigenket of $\hat{A}$ corresponding to eigenvalue a_n.

- This postulate embodies the non-classical concept of a fundamental interaction between a system and the measurement of that system.
- Hence, probability is *fundamental* to the world in which we live.





Expected Value of an Observable

- Postulates 4 and 5 deal with the measurement process and are expressed in terms of probabilities.

- Most measurements don't involve a single but rather large number of particles (*i.e.* protons, electrons, etc).

- The *expected* (or *mean*) value of an observable $\mathcal{A}$, denoted as $\langle \hat{A} \rangle_{\psi}$ or simply $\langle \hat{A} \rangle$, is defined as the average obtained from a large number of measurements performed on systems all in the same quantum state.

- $\langle \hat{A} \rangle$ generally provides the connection between classical and quantum mechanical physics.

Expected Value of an Observable

Claim: $\left\langle \hat{A} \right\rangle_\psi = \langle \psi | \hat{A} | \psi \rangle$

Proof:

$$\left\langle \hat{A} \right\rangle_\psi = \sum_i a_i \mathcal{P}(a_i) = \sum_i a_i \left| \langle u_i | \psi \rangle \right|^2 \qquad \text{(postulate 4)}$$

$$= \sum_i a_i \langle u_i | \psi \rangle^* \langle u_i | \psi \rangle = \sum_i a_i \langle \psi | u_i \rangle \langle u_i | \psi \rangle$$

$$= \langle \psi | \left[\sum_i a_i | u_i \rangle \langle u_i | \right] | \psi \rangle = \langle \psi | \left[\sum_i \hat{A} | u_i \rangle \langle u_i | \right] | \psi \rangle$$

$$= \langle \psi | \hat{A} \left[\sum_i | u_i \rangle \langle u_i | \right] | \psi \rangle$$

remember $\hat{A} | u_i \rangle = a_i | u_i \rangle$

$$= \langle \psi | \hat{A} | \psi \rangle$$

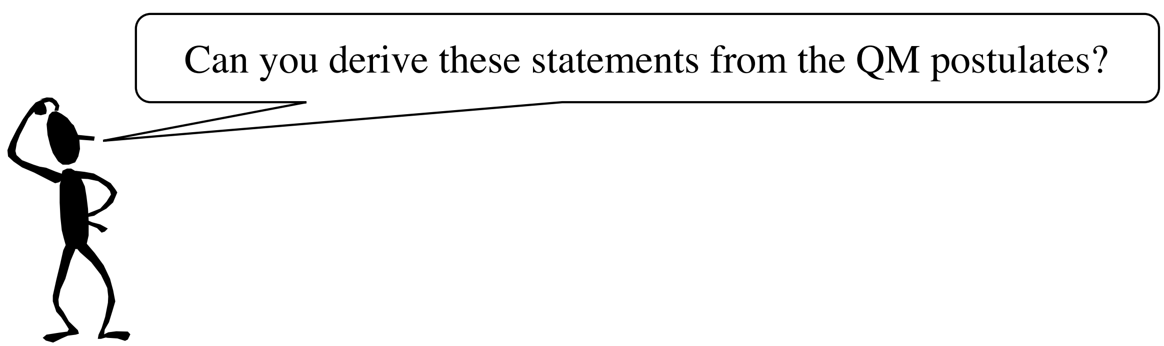
Compatibility of Observables

- Two observables which can be simultaneously determined are called <u>compatible</u>.

- If $\hat{\hat{A}}\hat{B} = 0$, then A and B are compatible.

Remember $\hat{\hat{A}}\hat{B}$ is superoperator notation for the commutator $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

- If $\hat{\hat{A}}\hat{B} \neq 0$, then A and B are incompatible and cannot be measured simultaneously.



Sixth Postulate

The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger equation:

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -i\hat{H}(t)|\psi(t)\rangle$$

where $\hat{H}(t)$ is the operator for the observable $\mathcal{H}$(t) associated with the total energy of the system.

- $\hat{H}(t)$ is called the Hamiltonian operator of the system. As defined above $\hat{H} = \hat{\mathcal{E}}/\hbar$, ($\hbar$ emitted in favor of more compact notation).
- Given an initial state $|\psi(t_0)\rangle$, the state at any subsequent time is determined ($i.e.$ not probabilistic). Probability only enters when a physical quantity is measured, upon which the state vector undergoes an probabilistic change (5th Postulate).

Solving Schrödinger's Equation

$$\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = -i\hat{H}(t)\left|\psi(t)\right\rangle$$

In this class, we'll be interested in addressing three special cases:

- $\hat{H}(t)$ independent of time. Easy to verify solution is:

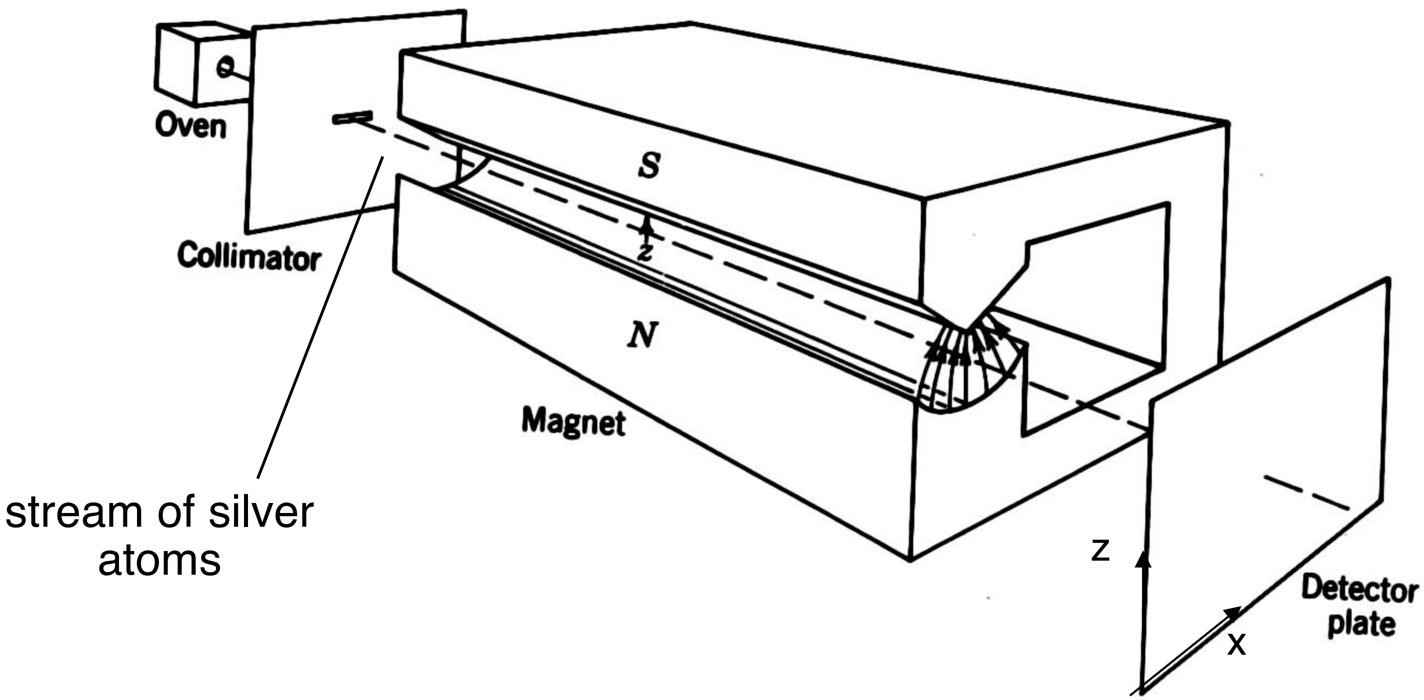
$$\left|\psi(t)\right\rangle = e^{-it\hat{H}}\left|\psi(0)\right\rangle.$$

- $\hat{H}(t)$ is periodic. Solution found by changing to a rotating frame (*i.e.* change of basis) so that Schrödinger's equation becomes time independent. Example: RF excitation.

- $\hat{H}(t)$ random in time. Solution found by considering ensemble of spins. Example: relaxation theory.

Example: Stern-Gerlach Experiment

- In 1922, Stern and Gerlach measured the magnetic dipole moment of silver atoms -- later shown that this moment was due to intrinsic spin (angular momentum) of an unpaired electron.



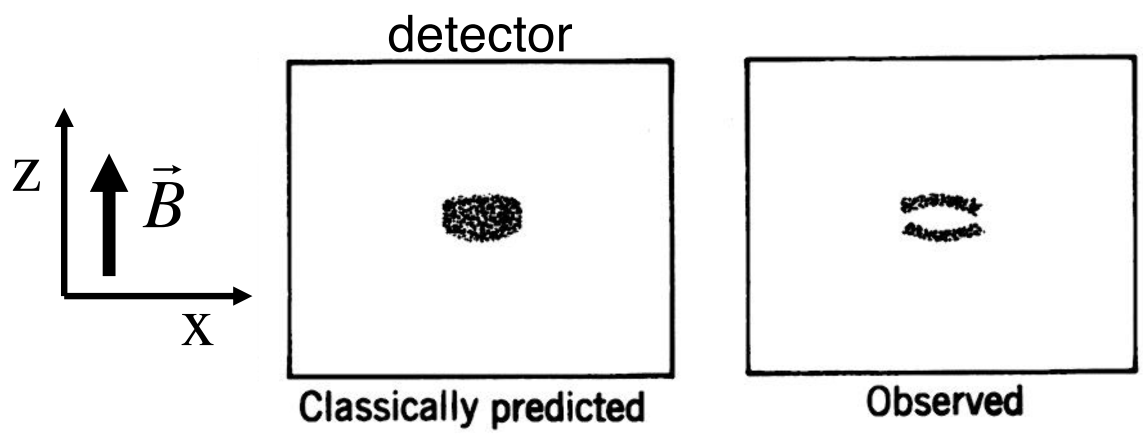
- Magnet designed so that there is a B_z gradient resulting in a z-directed force on the atoms proportional to μ_z, i.e. device measures z component of the angular momentum (see Lecture #2).

Stern-Gerlach Experiment (cont.)

- Potential energy given by: $\mathcal{E} = -\vec{\mu} \cdot \vec{B}$
- Classically, since the atoms can be oriented randomly in space, device should detect continuum of μ_z values.

Force proportional to the gradient of the magnetic field

$$F_z = \mu \frac{\partial B_z}{\partial z}$$



- Forced to conclude that μ_z is not continuous but quantized to two values $\pm\gamma\hbar/2$ (result known as <u>space quantization</u>).

Stern-Gerlach: Theory

QM description of a silver atom (an example of a spin 1/2 particle).

- Associated with the physical quantity $\mathcal{L}_z$ (z-component of angular momentum) is the observable $\hat{L}_z$ with eigenvalues $\pm \hbar/2$.

$$\hat{L}_z|\alpha\rangle = +\frac{\hbar}{2}|\alpha\rangle \text{ and } \hat{L}_z|\beta\rangle = -\frac{\hbar}{2}|\beta\rangle$$

notation for associated eigenkets

$|\alpha\rangle$ "spin up"

$|\beta\rangle$ "spin down"

- State space is 2-D (take as given), hence a general form for $|\psi\rangle$ is:

$$|\psi\rangle = c_\alpha e^{i\theta_\alpha}|\alpha\rangle + c_\beta e^{i\theta_\beta}|\beta\rangle \text{ with } |c_\alpha|^2 + |c_\beta|^2 = 1$$

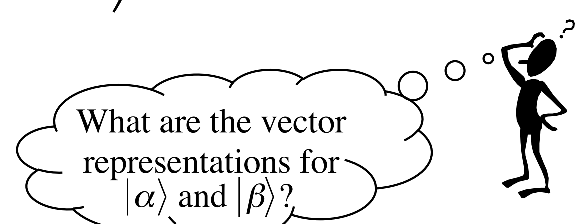
(For now, let's ignore θ_α and θ_β)

- We'll be dealing with spin operators ($\hat{I}_{x,y,z} = \hat{L}_{x,y,z}/\hbar$) and the corresponding matrix representations in the $\{|\alpha\rangle, |\beta\rangle\}$ basis are:

$$\underline{I}_{x,} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \underline{I}_{y,} = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \underline{I}_{z,} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

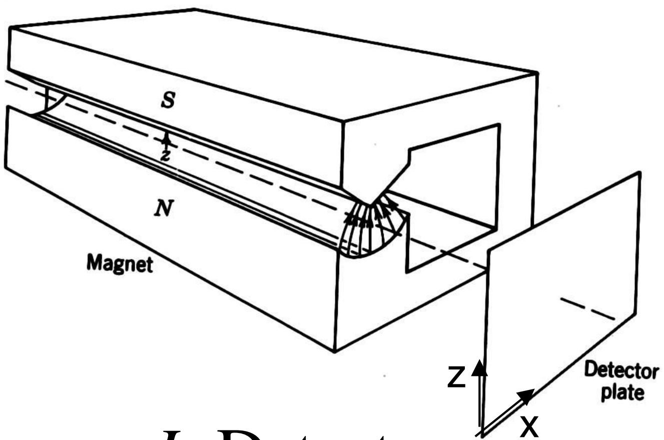
Pauli matrices

Note, $\hat{I}_{x,}$, $\hat{I}_{y,}$, and $\hat{I}_z$ do not commute!

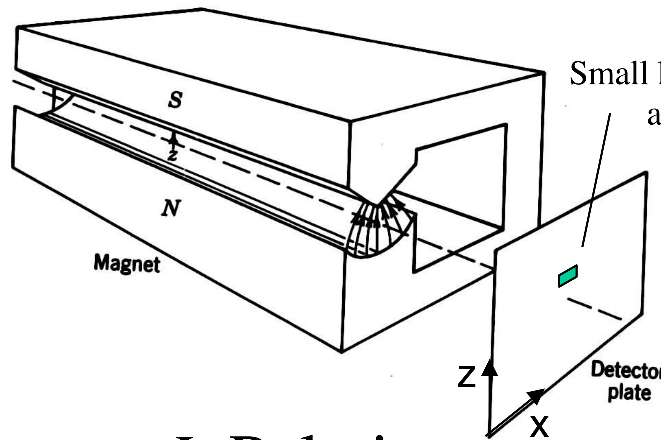


Stern-Gerlach Experiment (cont.)

- Consider the following two devices:



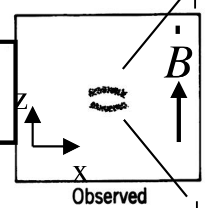
I_z Detector



Small hole that allows +1/2 atoms to pass through.

I_z Polarizer

$|\psi\rangle = c_\alpha|\alpha\rangle + c_\beta|\beta\rangle \longrightarrow$ I_z Detector

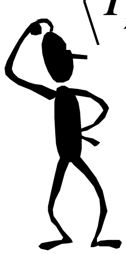


$|\psi\rangle = |\alpha\rangle$

$\vec{B}$

$|\psi\rangle = |\beta\rangle$

$|\psi\rangle = c_\alpha|\alpha\rangle + c_\beta|\beta\rangle \longrightarrow$ I_z Polarizer $\longrightarrow |\psi\rangle = |\alpha\rangle$



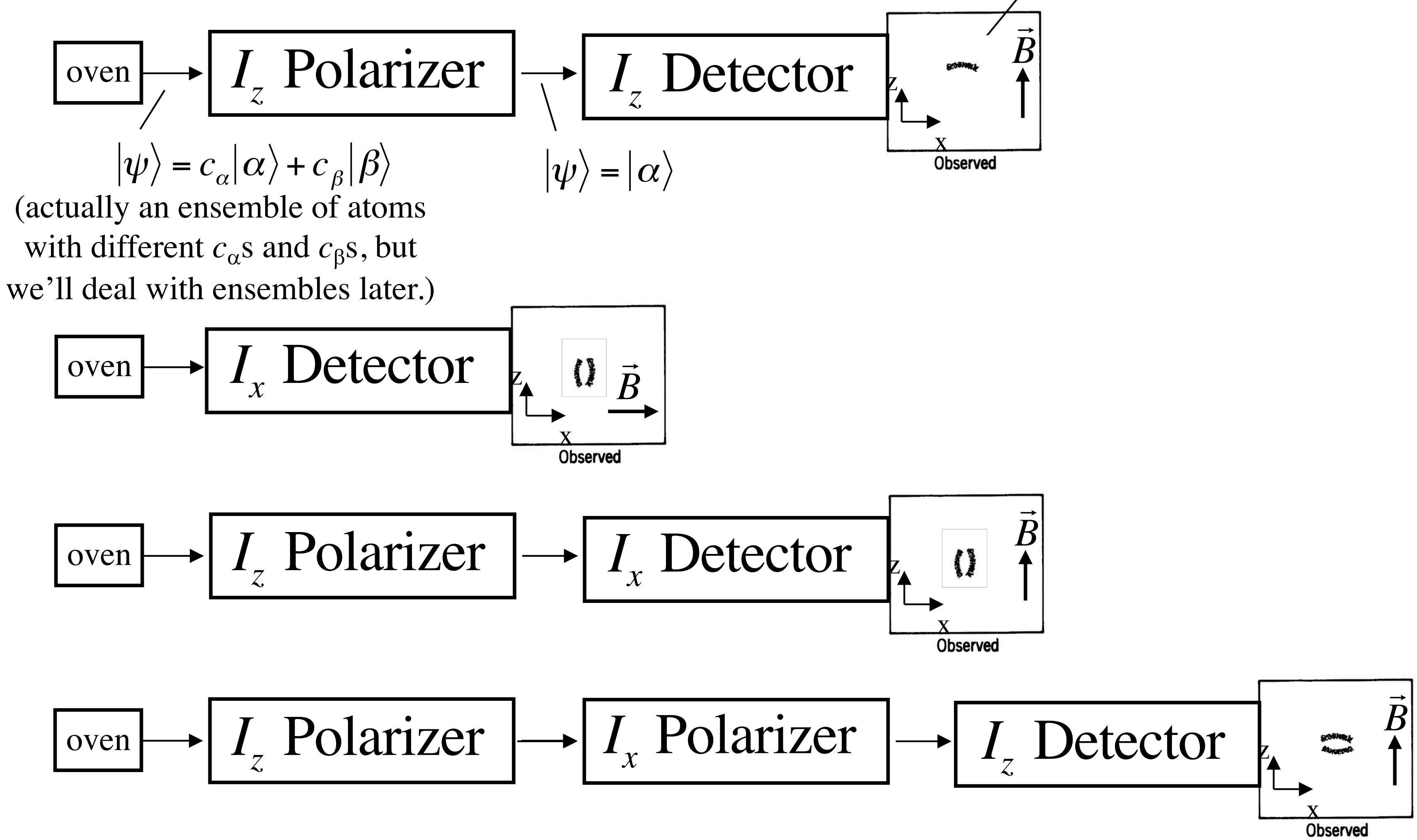
$\left\langle \hat{I}_z \right\rangle = ?$

$$\left\langle \hat{I}_z \right\rangle = \langle \psi | \hat{I}_z | \psi \rangle = |c_\alpha|^2 \frac{1}{2} + |c_\beta|^2 \left(-\frac{1}{2}\right)$$

Note: for a given atom we only measure $\pm\frac{1}{2}$.

Stern-Gerlach Experiment (cont.)

- Consider the following cases:



Remember $\left[\hat{I}_x, \hat{I}_z\right] \neq 0.$

Next lecture: NMR in Hilbert Space

Biography: Erwin Schrodinger

(born Aug. 12, 1887, Vienna, Austria—died Jan. 4, 1961, Vienna) Austrian theoretical physicist who contributed to the wave theory of matter and to other fundamentals of quantum mechanics. He shared the 1933 Nobel Prize for Physics with the British physicist Paul Dirac. Schrödinger entered the University of Vienna in 1906 and obtained his doctorate in 1910, upon which he accepted a research post at the university's Second Physics Institute. He saw military service in World War I and then went to the University of Zürich in 1921, where he remained for the next six years. There, in a six-month period in 1926, at the age of 39, a remarkably late age for original work by theoretical physicists, he produced the papers that gave the foundations of quantum wave mechanics. In those papers he described his partial differential equation that is the basic equation of quantum mechanics and bears the same relation to the mechanics of the atom as Newton's equations of motion bear to planetary astronomy. Adopting a proposal made by Louis de Broglie in 1924 that particles of matter have a dual nature and in some situations act like waves, Schrödinger introduced a theory describing the behaviour of such a system by a wave equation that is now known as the Schrödinger equation. The solutions to Schrödinger's equation, unlike the solutions to Newton's equations, are wave functions that can only be related to the probable occurrence of physical events. The definite and readily visualized sequence of events of the planetary orbits of Newton is, in quantum mechanics, replaced by the more abstract notion of probability. (This aspect of the quantum theory made Schrödinger and several other physicists profoundly unhappy, and he devoted much of his later life to formulating philosophical objections to the generally accepted interpretation of the theory that he had done so much to create.)In 1927 Schrödinger accepted an invitation to succeed Max Planck, the inventor of the quantum hypothesis, at the University of Berlin, and he joined an extremely distinguished faculty that included Albert Einstein. He remained at the university until 1933, at which time he reached the decision that he could no longer live in a country in which the persecution of Jews had become a national policy. He then began a seven-year odyssey that took him to Austria, Great Britain, Belgium, the Pontifical Academy of Science in Rome, and—finally in 1940—the Dublin Institute for Advanced Studies, founded under the influence of Premier Eamon de Valera, who had been a mathematician before turning to politics. Schrödinger remained in Ireland for the next 15 years, doing research both in physics and in the philosophy and history of science. During this period he wrote *What Is Life? (1944), an attempt to show how quantum physics can be used to explain the stability of genetic structure. Although much of what Schrödinger had to say in this book has been modified and amplified by later developments in molecular biology, his book remains one of the most useful and profound introductions to the subject. In 1956 Schrödinger retired and returned to Vienna as professor emeritus at the university. Of all of the physicists of his generation, Schrödinger stands out because of his extraordinary intellectual versatility. He was at home in the philosophy and literature of all of the Western languages, and his popular scientific writing in English, which he had learned as a child, is among the best of its kind. His study of ancient Greek science and philosophy, summarized in his Nature and the Greeks (1954), gave him both an admiration for the Greek invention of the scientific view of the world and a skepticism toward the relevance of science as a unique tool with which to unravel the ultimate mysteries of human existence. Schrödinger's own metaphysical outlook, as expressed in his last book, Meine Weltansicht (1961; My View of the World), closely paralleled the mysticism of the Vednta. Because of his exceptional gifts, Schrödinger was able in the course of his life to make significant contributions to nearly all branches of science and philosophy, an almost unique accomplishment at a time when the trend was toward increasing technical specialization in these disciplines.*

Historical Notes on Spin

Historical Notes on Spin

(from R. Eisberg and R. Resnick, "Quantum Physics", John Wiley & Sons, 1974, pp 300-301)

Credit for the introduction of electron spin is generally given to Goudsmit and Uhlenbreck in 1925 (both were graduate students at the time!). Uhlenbreck described the circumstances as follows:

"Goudsmit and myself hit upon this idea by studying a paper of Pauli, in which the famous exclusion principle (to be treated in Chapter 9) was formulated and in which, for the first time, *four* quantum numbers were ascribed to the electron. This was done rather formally; no concrete picture was connected with it. To us this was a mystery. We were so conversant with the proposition that every quantum number corresponds to a degree of freedom (an independent coordinate), and on the other hand with the idea of a point electron, which obviously had three degrees of freedom only, that we could not place the fourth quantum number. We could understand it only if the electron was assumed to be a small sphere that could rotate . . . .

Somewhat later we found in a paper of Abraham, to which Ehrenfest drew our attention, that for a rotating sphere with surface charge the necessary factor two in the magnetic moment ($g_s = 2$) could be understood classically. This encouraged us, but our enthusiasm was considerably reduced when we saw that the rotational velocity at the surface of the electron had to be many times the velocity of light! I remember that most of these thoughts came to us on an afternoon at the end of September 1925. We were excited, but we had not the slightest intention of publishing anything. It seemed so speculative and bold, that something ought to be wrong with it, especially since Bohr, Heisenberg, and Pauli, our great authorities, had never proposed anything of the kind. But of course we told Ehrenfest. He was impressed at once, mainly, I feel, because of the visual character of our hypothesis, which was very much in his line. He called our attention to several points, e.g., to the fact that in 1921 A. H. Compton already had suggested the idea of a spinning electron as a possible explanation of the natural unit of magnetism, and finally said that it was either highly important or nonsense, and that we should write a short note for *Naturwissenschaften* (a physics research journal) and give it to him. He ended with the words 'and then we will ask Lorentz.' This was done. Lorentz received us with his well known great kindness, and he was very much interested, although, I feel, somewhat skeptical too. He promised to think it over. And in fact, already next week he gave us a manuscript, written in his beautiful handwriting, containing long calculations on the electromagnetic properties of rotating electrons. We could not fully understand it, but it was quite clear that the picture of the rotating electron, if taken seriously, would give rise to serious difficulties. For one thing, the magnetic energy would be so large that by the equivalence of mass and energy the electron would have a larger mass than the proton, or, if one sticks to the known mass, the electron would be bigger than the whole atom! In any case, it seemed to be nonsense. Goudsmit and myself both felt that it might be better for the present not to publish anything; but when we said this to Ehrenfest, he answered: 'I have already sent your letter in long ago; you are both young enough to allow yourselves some foolishness!' " (from *The Conceptual Development of Quantum Mechanics* by Max Jammer, McGraw-Hill, 1966)