37 States of identical particles

Slides: Lecture 37a Multiple particle states

Text reference: Quantum Mechanics for Scientists and Engineers

Section 13.5
States of identical particles

Multiple particle states

Quantum mechanics for scientists and engineers

David Miller
Extension to more than two non-identical particles

If we had \( N \) different (i.e., not identical) particles that were approximately not interacting at least in some region of space and time (e.g., substantially before or after the scattering) then we could construct the state \( |\Psi_{\text{different}}\rangle \) for those by simply multiplying the single-particle states or modes

\[
|\psi_{\text{different}}\rangle = |1,a\rangle|2,b\rangle|3,c\rangle\ldots|N,n\rangle
\]

where the numbers and the letter \( N \) refer to the particles and the small letters refer to the single-particle state the individual particles are in.
More than two bosons

We can write the state as

$$\left| \psi_{\text{identical} \ bosons} \right\rangle \propto \sum_{\hat{P}} \hat{P} \left| 1, a \right\rangle \left| 2, b \right\rangle \left| 3, c \right\rangle \ldots \left| N, n \right\rangle$$

Here $\hat{P}$ is one of the permutation operators.

This is an operator that changes one function in the Hilbert space into another in this case by permuting the particles among the modes.

The meaning of the sum is that it is taken over all of those possible distinct permutation operators.
More than two bosons

The notation here $|\psi_{\text{identical bosons}}\rangle \propto \sum_{\hat{P}} \hat{P}|1, a\rangle|2, b\rangle|3, c\rangle\ldots|N, n\rangle$

is just a mathematical way of saying we are summing over all permutations of the $N$ particles among the chosen set of modes.

Incidentally, for this boson case it is quite allowable for two or more of the modes to be the same mode.

E.g., for mode $b$ to be the same mode as mode $a$ an important and general property of bosons.
More than two bosons

Note that, for any given set of modes $a, b, c, ... n$
with given numbers of these bosons in each mode
there is only one possible such boson state of identical particles

The state $\psi_{\text{identical bosons}} \propto \sum \hat{P} |1, a\rangle |2, b\rangle |3, c\rangle ... |N, n\rangle$

satisfies the symmetry requirement that
swapping any two particles does not change the sign or amplitude of the state

Swapping particles just corresponds to changing the order of the terms, leaving the sum itself unchanged
More than two fermions

We can write the state for \( N \) identical fermions as

\[
\left| \psi_{\text{identical fermions}} \right> = \frac{1}{\sqrt{N!}} \sum_{\hat{P}=1}^{N!} \pm \hat{P} \left| 1, a \right> \left| 2, b \right> \left| 3, c \right> \ldots \left| N, n \right>
\]

where now by \( \pm \hat{P} \) we mean that we use the + sign

when the permutation corresponds to an even number of pair-wise swaps of the individual particles

and the – sign

when the permutation corresponds to an odd number of pair-wise swaps of the individual particles
More than two fermions

Note that for this state

$$|\psi_{\text{identical fermions}}\rangle = \frac{1}{\sqrt{N!}} \sum_{\hat{P}=1}^{N!} \pm \hat{P} |1,a\rangle |2,b\rangle |3,c\rangle \ldots |N,n\rangle$$

if two of the single-particle states are identical
e.g., if $b = a$

then the fermion state is exactly zero because
for each permutation there is an identical one
with opposite sign that exactly cancels it

This is the extension of the Pauli exclusion principle to $N$ particles
Slater determinant

There is a particularly convenient way to write the $N$ particle fermion state which is called the Slater determinant

$$\psi_{\text{identical fermions}} = \frac{1}{\sqrt{N!}} \begin{vmatrix}
1,a & 2,a & \cdots & N,a \\
1,b & 2,b & \cdots & N,b \\
\vdots & \vdots & \ddots & \vdots \\
1,n & 2,n & \cdots & N,n
\end{vmatrix}$$

This is just another way of writing

$$\psi_{\text{identical fermions}} = \frac{1}{\sqrt{N!}} \sum_{\hat{P}=1}^{N!} \pm \hat{P} |1,a\rangle |2,b\rangle |3,c\rangle \cdots |N,n\rangle$$
37 States of identical particles

Slides: Lecture 37b Multiple particle basis functions

Text reference: Quantum Mechanics for Scientists and Engineers

Section 13.6 up to Eq. 13.50
States of identical particles

Multiple particle basis functions

Quantum mechanics for scientists and engineers

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Multiple particle basis functions

So we can find some complete basis set to represent one of the particles

\[ \psi_i(r_j) \equiv |j,i\rangle \]

and then formally construct a new basis set

\[ \Psi_{ab\ldots n}(r_1, r_2, \ldots, r_N) \equiv |\Psi_{ab\ldots n}\rangle \]

for the \( N \) particle system from products of single particle functions appropriately symmetrized with respect to exchange
Multiple particle basis functions

Depending on the symmetry with respect to exchange there are different forms for this basis function

(i) non-identical particles

$$\psi_{ab...n}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)\cdots\psi_n(\mathbf{r}_N)$$

or equivalently \( |\Psi_{ab...n}\rangle = |1, a\rangle|2, b\rangle\cdots|N, n\rangle \)

where each of the \( \psi_a(\mathbf{r}) \) may be chosen to be any of the single particle basis functions \( \psi_i(\mathbf{r}) \)

(ii) identical bosons

\[ |\Psi_{ab...n}\rangle \propto \sum_{\hat{P}} \hat{P} |1, a\rangle|2, b\rangle\cdots|N, n\rangle \]

(iii) identical fermions

\[ |\Psi_{ab...n}\rangle = \frac{1}{\sqrt{N!}} \sum_{\hat{P}=1}^{N!} \pm \hat{P} |1, a\rangle|2, b\rangle\cdots|N, n\rangle \]
For non-identical particles

there is one basis function for every choice of combination of single particle basis functions

If we imagined there were $M$ possible single particle basis functions

and there are $N$ particles

then there are in general $M^N$ such basis functions for the $N$ particle system
Number of orthogonal states – non-identical particles

So, for $N$ non-identical particles

specifying a state of that $N$ particle system

involves specifying a linear combination

of the $M^N$ different orthogonal $N$-particle basis functions

Because there are only $M^N$ different orthogonal $N$-particle basis functions

there can only be $M^N$ different orthogonal $N$-particle states

even if we now allow them to interact
Number of orthogonal states – non-identical particles

So, for $N$ non-identical particles even allowing them to interact, there are only $M^N$ possible orthogonal $N$-particle states, each of which will be a different combination of the $M^N$ different $N$-particle basis functions.

Number of orthogonal states of $N$ non-identical particles, with $M$ available single-particle states or modes,

$$= M^N$$
Number of distinct basis functions - bosons

In the case of identical bosons

the $N$-particle basis states

corresponding to different permutations

of the same set of choices of basis

modes

are not distinct

and so there are fewer basis

states than for non-identical

particles
Number of distinct basis functions - bosons

For example, we see that in

\[ |\Psi_{ab\ldots n}\rangle \propto \sum_{\hat{P}} \hat{P}|1,a\rangle|2,b\rangle\ldots|N,n\rangle \]

the state \( |\Psi_{ab\ldots n}\rangle \) is not distinct from \( |\Psi_{ba\ldots n}\rangle \)

Since all permutations of the products of basis modes

are already in the sum

these two states are the same sum of products

performed in a different order
Number of distinct basis functions - bosons

The counting of these boson states is complicated, but it corresponds to a standard result in permutations and combinations, which is the problem of counting the number of combinations of \( M \) things here the single particle states or modes taken \( N \) at a time since we always have \( N \) particles with repetitions allowed i.e., we can have more than one particle in a mode with the standard result \((M + N - 1)!/[N!(M - 1)!]\)
Number of distinct basis functions - bosons

For example think of \( M \) boxes each containing as many blocks as we like of just one color with each box containing a different color of blocks

We are picking \( N \) blocks altogether from these boxes

The number of possible different combinations of blocks we can end up with is

\[
\frac{(M + N - 1)!}{N!(M - 1)!}
\]
Number of distinct basis functions - bosons

For example

the set of combinations of
2 particles among
3 modes, $a$, $b$, and $c$
allowing repetitions is
$ab, ac, bc, aa, bb, cc$
giving six in all

which corresponds to

$\frac{(3+2-1)!}{[2!(3-1)!]} = 6$
Number of orthogonal states - bosons

Just as for the non-identical particle case, this number of basis states is also the number of different orthogonal states we can have for the set of identical boson particles, even if we allow interactions.

Number of orthogonal states of $N$ identical bosons, with $M$ available modes:

$$\frac{(M + N - 1)!}{N!(M - 1)!}$$
Specifically, if there are $M$ choices for the first basis single-particle state $a$ in $\left| \Psi_{ab...n} \right>$

then there are $M - 1$ choices for the second single particle basis state $b$, and so on down to $M - N + 1$ choices for the last single particle basis state $n$

Hence, instead of $M^N$ initial choices, we have only $M (M - 1) \cdots (M - N + 1) = M! / (M - N)!$

Since the order of the choice of states does not matter we divide by the number of different orders, $N!$
Number of orthogonal states - fermions

Hence in the identical fermion case

there are \( M! \left[ (M - N)! N! \right] \) possible basis states

and hence the same number of possible orthogonal states altogether

even if we allow interactions between particles

I.e.,

Number of orthogonal states of \( N \) identical fermions,

with \( M \) available single-particle states

\[
= \frac{M!}{(M - N)! N!}
\]
37 States of identical particles

Slides: Lecture 37c Numbers of states

Text reference: Quantum Mechanics for Scientists and Engineers

Section 13.6 subsection “Example numbers of states”
States of identical particles

Numbers of states

Quantum mechanics for scientists and engineers

David Miller
Example numbers of states

For example, suppose we have two particles

each of which can be in one of two different single-particle states or modes, $a$ and $b$
Example numbers of states

Suppose these particles are in some potential such that there are two single-particle states or modes quite close in energy and all other possible states are sufficiently far away in energy that we can approximately neglect those other states in our counting.
Example numbers of states

We might be considering, for example

two particles in a weakly coupled pair of similar quantum boxes
or a one-dimensional problem such as coupled potential wells
Example numbers of states

Because we know for some other reason that the particles cannot have much energy

for example, the temperature may be low

we presume the particles can only be in one or other of the two lowest coupled single-particle states or modes of these two wells or boxes
Example numbers of states

For each situation we consider

- non-identical particles
- identical bosons, and
- identical fermions

these single-particle states or modes might be different e.g., because of exchange energy but that will not affect our argument here

which is just counting states
Example numbers of states

We can now write out the possible states in each case.

For all of these cases, the number of possible single-particle states or modes of a particle is

\[ M = 2 \]

and the number of particles is

\[ N = 2 \]
Non-identical particles

For non-identical particles such as a proton and a neutron, the possible distinct states of this pair of particles are

\[ |1, a\rangle |2, a\rangle \]
Non-identical particles

For non-identical particles such as a proton and a neutron the possible distinct states of this pair of particles are

$$|1, a\rangle|2, a\rangle \quad |1, b\rangle|2, b\rangle$$
Non-identical particles

For non-identical particles such as a proton and a neutron, the possible distinct states of this pair of particles are:

\[ |1, a\rangle |2, a\rangle \quad |1, b\rangle |2, b\rangle \quad |1, a\rangle |2, b\rangle \]
Non-identical particles

For non-identical particles such as a proton and a neutron, the possible distinct states of this pair of particles are:

\[ |1, a\rangle |2, a\rangle \; |1, b\rangle |2, b\rangle \; |1, a\rangle |2, b\rangle \; |1, b\rangle |2, a\rangle \]

As we expected from the expression \( M^N \), there are \( 2^2 = 4 \) states of the pair of particles.
Bosons

We could consider identical bosons such as two $^4$He (helium-four) atoms (which are bosons) because they are made from 6 particles each with spin $\frac{1}{2}$: two protons, two neutrons and two electrons, which therefore have an integer total spin.

\[ \begin{align*}
  a &= \underline{} \\
  b &= \underline{}
\end{align*} \]
Bosons

The possible distinct states of this pair of identical bosons are

\[ |1,a\rangle|2,a\rangle \]
Bosons

The possible distinct states of this pair of identical bosons are

$$|1,a\rangle|2,a\rangle \quad |1,b\rangle|2,b\rangle$$
Bosons

The possible distinct states of this pair of identical bosons are

\[
|1, a\rangle|2, a\rangle \quad |1, b\rangle|2, b\rangle \quad \frac{1}{\sqrt{2}} \left( |1, a\rangle|2, b\rangle + |2, a\rangle|1, b\rangle \right)
\]

Note there is only one way of having the two identical particles in different states
Bosons

In this list of basis states

$$|1,a\rangle|2,a\rangle, \ |1,b\rangle|2,b\rangle, \ \frac{1}{\sqrt{2}}(|1,a\rangle|2,b\rangle+|2,a\rangle|1,b\rangle)$$

we do not have to write the explicit symmetrized form $$|1,a\rangle|2,a\rangle+|2,a\rangle|1,a\rangle$$

since it is describing the same state as $$|1,a\rangle|2,a\rangle$$

and similarly for the state with both particles in the $b$ mode

(The $1/\sqrt{2}$ normalizes the explicitly symmetric combination state)
Bosons

In this list of basis states

\[ |1, a\rangle|2, a\rangle, |1, b\rangle|2, b\rangle, \frac{1}{\sqrt{2}}(|1, a\rangle|2, b\rangle + |2, a\rangle|1, b\rangle) \]

we therefore have 3 states

which agrees with \((M + N - 1)!/[N!(M - 1)!]\)

i.e., \((2 + 2 - 1)!/2!(2 - 1)! = 3\)

Note that this is not the same as

the case of non-identical particles

where we had 4 states
For identical fermions, there is only one possible state of the pair of particles since the two particles have to be in different single-particle states and here there are only two single-particle states to choose from for each particle.
Fermions

So that one (normalized) state is
\[
\frac{1}{\sqrt{2}} (|1,a\rangle|2,b\rangle - |2,a\rangle|1,b\rangle)
\]
which agrees with the formula

\[
M!/\left[ (M - N)!N! \right]
\]

which gives \(2!/(2!0!) = 1\) state where we remember that \(0! = 1\)
Thermal occupation of states

The differences in the number of available states in the three cases of non-identical particles, identical bosons, and identical fermions leads to very different behavior once we consider the thermal occupation of states.
Thermal occupation of states

For example, if we presume that we are at some relatively high temperature such that the thermal energy, $k_B T$, is much larger than the energy separation of the two single-particle states or modes $a$ and $b$ but still much less than the energy to the next states then the thermal occupation probabilities of all the different allowed combinations of single-particle states or modes will all tend to be similar.
Non-identical particles

For the case of the non-identical particles which behave like classical particles as far as the counting of states is concerned with the 4 states $|1,a\rangle|2,a\rangle |1,b\rangle|2,b\rangle |1,a\rangle|2,b\rangle |1,b\rangle|2,a\rangle$

we therefore expect a probability of $\sim \frac{1}{4}$ of occupation of each of the states.

Therefore, the probability that the two particles are in the same state is $\sim \frac{1}{2}$
Identical bosons

For the case of the identical bosons there are only three possible states so the probability of occupation of any one state is $\sim 1/3$
Identical bosons

Two of the two-particle states have the particles in identical modes $|1, a\rangle |2, a\rangle$, $|1, b\rangle |2, b\rangle$ and only one two-particle state $(1/\sqrt{2})(|1, a\rangle |2, b\rangle + |2, a\rangle |1, b\rangle)$ has the particles in different single particle states.

So the probability of finding the two identical bosons in the same single-particle state (mode) is now $2/3$ larger than the $1/2$ for the non-identical particle case.
Identical fermions

For the case of identical fermions there is only one possible state

\[(\frac{1}{\sqrt{2}})(|1, a\rangle|2, b\rangle - |2, a\rangle|1, b\rangle)\]

which therefore has probability \(~1\)

and it necessarily corresponds to the two particles being in different states

\[b \quad \quad \quad \quad a\]
37 States of identical particles

Slides: Lecture 37d Analogy for counting states

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 13.6 subsection “Bank account analogy for counting states”
States of identical particles

Analogy for counting states

Quantum mechanics for scientists and engineers

David Miller
Bank account analogy

Suppose you have

- an antique jar \((a)\) in the kitchen for your spending money
- and a box \((b)\) under the bed for your savings money

You put your dollar bills

- each labeled with a unique number
- into either the antique jar \((a)\) or the box \((b)\)
Bank account analogy

This is like the quantum mechanical situation of non-identical particles (the dollar bills) and different single-particle states or modes \((a \text{ or } b)\) into which they can be put – the jar or the box.
Bank account analogy

If I have two dollar bills then there are four possible situations i.e., states of the entire system of two dollar bills in the antique jar and/or the box.
Bank account analogy

bill 1 in the box and bill 2 in the box
Bank account analogy

bill 1 in the box and bill 2 in the box

bill 1 in the box and bill 2 in the antique jar
Bank account analogy

bill 1 in the box and bill 2 in the box

bill 1 in the box and bill 2 in the antique jar

bill 1 in the antique jar and bill 2 in the box
Bank account analogy

bill 1 in the box and bill 2 in the box
bill 1 in the box and bill 2 in the antique jar
bill 1 in the antique jar and bill 2 in the box
bill 1 in the antique jar and bill 2 in the antique jar
Bank account analogy

bill 1 in the box and bill 2 in the box
bill 1 in the box and bill 2 in the antique jar
bill 1 in the antique jar and bill 2 in the box
bill 1 in the antique jar and bill 2 in the antique jar

making four states altogether

This reproduces the counting for non-identical particles
Bank account analogy

Consider next that you have two bank accounts
a checking account \((a)\), and a savings account \((b)\)
You may still have the same amount of money
\$2
You may know how much money you have in each account
but the dollars are themselves identical in the accounts
So now there are only three possible states
Two dollars in savings
One dollar in savings and one in checking
Two dollars in checking
Bank account analogy

Note that, in these three possible states

- Two dollars in savings
- One dollar in savings and one in checking
- Two dollars in checking

there are

- 2 states with both dollars in the same account
  - but only one in which they are in different accounts

This bank account argument above gives the counting for boson states
Bank account analogy

Consider now that you have two bank accounts
    a checking account \( (a) \) and a savings account \( (b) \)
but you are living in the Protectorate of Pauliana
    where you may have no more than one dollar in each
    bank account
Then for your two dollars
    there is only one possible state
        one dollar in savings
        one dollar in checking
This gives the counting for fermion states
Counting states with two “bank accounts”

For the case of identical fermions
  there is only one possible state for our two dollars
  with each dollar being in a different bank account

For identical bosons
  there are three possible states for our two dollars
  in two of which both are in the same bank account
  and in one of which they are in different bank accounts

For non-identical (classical) particles
  there are four possible states for our dollar bills
  in two of which both are in the same bank account
  and in two of which they are in different bank accounts