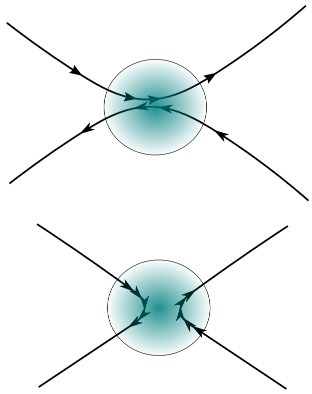
Quantum Mechanics: Identical Particles

Fundamental indistinguishability of particles



Two particles come from opposite directions, scatter off each other, and move away in different directions. We wish to know which particle went which way.

Here we wish to study the quantum mechanical treatment of two or more particles which are identical, e.g., electrons, protons, neutrons etc. One might wonder why a special discussion for identical particles is needed here. Afterall there are identical particles in classical mechanics too, and the same theory works for all the particles. However, consider a scenario depicted in the adjascent figure. Two particles approach each other from opposite directions, scatter off each other, and get deflected in two different directions. Suppose we want to know which particle went which way. Classically it is very easy to infer that, as in the case of billiard balls colliding. Even if the two balls are of the same color and size, one can put a little cross mark on one of the balls, and after the collision, check the balls for the mark to find out which ball went which way. But suppose the same experiment is done with two electrons. They also approach each other from opposite directions, get scattered off because of negative charge on both of them. Electrons being very light, cannot be watched all the time as they interact with each other (the would require repeated collision with photons). An electron has a fixed number of characters, like mass and charge. Unlike a billiard ball one cannot put an additional label on an electron. We also know the electrons are not point particles, but behave like wave-packets, being spread out over a small region in space. Once the wave-packets of the two electrons overlap, it is no longer possible, *even in principle*, to tell which electron went which way. Thus, the indistinguishability of particles in quantum mechanics, is of a fundamental nature, unlike that in classical mechanics.

One may think that the problem described above may be ignored, and we may not wish to know which particle went which way. Howoever, identical particles present difficulty in the formalism of quantum mechanics too. Consider two identical particles which we call particle 1 and particle 2. Suppose particle 1 is in the state $|\psi_a\rangle$ and particle 2 is in the state $|\psi_b\rangle$. In order that the states are distinct, we assume that $|\psi_a\rangle, |\psi_b\rangle$ are orthogonal. We may write the two-particle state as

$$|\psi_a\rangle_1|\psi_b\rangle_2,$$

assuming a convention that the state of particle 1 is written first. But if someone asserts that the state is

$$|\psi_b\rangle_1|\psi_a\rangle_2,$$

meaning particle 1 is in the $|\psi_b\rangle$ and particle 2 is in the state $|\psi_a\rangle$, there is no way we can disprove that assertion. It should be emphasized here that the state $|\psi_a\rangle_1|\psi_b\rangle_2$ and $|\psi_b\rangle_1|\psi_a\rangle_2$ should not be thought of very similar states - in fact they are orthogonal. In fact, our state cannot be distinguished from any state of the form

$$c_1|\psi_a\rangle_1|\psi_b\rangle_2 + c_2|\psi_b\rangle_1|\psi_a\rangle_2.$$

If $|\psi_a\rangle, |\psi_b\rangle$ are eigenstates of an observable, measurement on any of these three states will give identical eigenvalues. So we are faced with a difficulty in our formalism in that there are many different states which give the same eigenvalue - they are all *degenerate*. This degeneracy arises because exchanging particles between two states does not change the eigenvalue. For that reason it is called *exchange degeneracy*. This is the problem of the quantum formalism, not of nature. One may then ask, what actually happens in nature? Are all these degenrate states occur in nature, or is there a restriction? The answer turns out to be very interesting.

Permutation operator

First we will introduce some mathematical tools to analyze the problem of identical particles. We introduce an exange operator with the property

$$\hat{P}_{12}|\psi_a\rangle_1|\psi_b\rangle_2 = |\psi_b\rangle_1|\psi_a\rangle_2.$$

This is just a mathematical operator, and is not part of any physical process. The effect of the particle is interchanging particles 1 and 2 in their original states. It is obvious then that

$$\hat{P}_{21} = \hat{P}_{12} \quad \text{and} \quad \hat{P}_{12}^2 = \hat{1}$$

Let us assume that $|\psi_a\rangle, |\psi_b\rangle$ are eigenstates of an obeservable $\hat{A}$ for each particle. Obviously, the observables for each particle are different. The state $|\psi_a\rangle_1|\psi_b\rangle_2$ can then be characterized by the eigenvalues of the observables of both the particles

$$\hat{A}_1|\psi_a\rangle_1|\psi_b\rangle_2 = a|\psi_a\rangle_1|\psi_b\rangle_2$$

$$\hat{A}_2|\psi_a\rangle_1|\psi_b\rangle_2 = b|\psi_a\rangle_1|\psi_b\rangle_2.$$

We take the first these two equations and multiply both sides by $\hat{P}_{12}$. We get

$$\hat{P}_{12}\hat{A}_1|\psi_a\rangle_1|\psi_b\rangle_2 = a|\psi_b\rangle_1|\psi_a\rangle_2.$$

Next we insert $\hat{P}_{12}^{-1}\hat{P}_{12}$ between $\hat{A}_1$ and $|\psi_a\rangle_1$, to get

$$\begin{aligned}\hat{P}_{12}\hat{A}_1\hat{P}_{12}^{-1}\hat{P}_{12}|\psi_a\rangle_1|\psi_b\rangle_2 &= a|\psi_b\rangle_1|\psi_a\rangle_2 \\ \hat{P}_{12}\hat{A}_1\hat{P}_{12}^{-1}|\psi_b\rangle_1|\psi_a\rangle_2 &= a|\psi_b\rangle_1|\psi_a\rangle_2. \qquad (1)\end{aligned}$$

But we already know that $\hat{A}_2|\psi_b\rangle_1|\psi_a\rangle_2 = a|\psi_b\rangle_1|\psi_a\rangle_2$. The above equation can be consistent with this only if

$$\hat{P}_{12}\hat{A}_1\hat{P}_{12}^{-1} = \hat{A}_2.$$

So the effect of applying $\hat{P}_{12}$ on the left and $\hat{P}_{12}^{-1}$ on the right of an observable is that it changes the particle label of the observable.

Symmetric & antisymmetric states

Among the various two-particle states that are possible in exchange degeneracy, let us find out if there are states which are eigenstates of the permutation operator. It turns out that there are two eigenstates possible

$$\begin{aligned}\hat{P}_{12}\tfrac{1}{\sqrt{2}}(|\psi_a\rangle_1|\psi_b\rangle_2 + |\psi_b\rangle_1|\psi_a\rangle_2) &= \tfrac{1}{\sqrt{2}}(|\psi_a\rangle_1|\psi_b\rangle_2 + |\psi_b\rangle_1|\psi_a\rangle_2) \\ \hat{P}_{12}\tfrac{1}{\sqrt{2}}(|\psi_a\rangle_1|\psi_b\rangle_2 - |\psi_b\rangle_1|\psi_a\rangle_2) &= -\tfrac{1}{\sqrt{2}}(|\psi_a\rangle_1|\psi_b\rangle_2 - |\psi_b\rangle_1|\psi_a\rangle_2), \qquad (2)\end{aligned}$$

with the eigenvalues ± 1, respectively. Very interestingly it turns out that these are the only two states that occur in nature. If there are two identical particles, their quantum states can only be either symmetric or anti-symmetric under particle permution or particle exchange. Not only that, this property also depends on the *spin* of the particles. Particles having an integer spin can only have symmetric states, and such particles are called *bosons*. Particles having half-integer spins (e.g. electrons, protons, neutrons) can only have antisymmetric states, and are called *fermions*. Within standard quantum mechanics there is no deeper explanation for this surprising connection between the spin and the symmetry of the quantum state. To understand it, one has to go to quantum field theory and look at the *spin-statistics theorem*.

A two-particle state may then be written as

$$|\Phi\rangle = |\psi_a, \psi_b\rangle = \frac{1}{\sqrt{2}}(|\psi_a\rangle_1|\psi_b\rangle_2 \pm |\psi_b\rangle_1|\psi_a\rangle_2), \tag{3}$$

where the states $|\psi_a\rangle, |\psi_b\rangle$ are called *single-particle states*.

Since the particles are identical, using the particle labels 1, 2 is unnecessary, and can be completely done away with. One can just represent the two particle state as $|\psi_a, \psi_b\rangle$ which says that one particle is in $|\psi_a\rangle$ and the other in state $|\psi_b\rangle$. The amplitude of these two particles to be found, after a suitable measurement, in the states (say) $|\alpha\rangle$ and $|\beta\rangle$ can be found by using the following simple rule

$$\langle\alpha, \beta|\psi_a, \psi_b\rangle = \langle\alpha|\psi_a\rangle\langle\beta|\psi_b\rangle \pm \langle\alpha|\psi_b\rangle\langle\beta|\psi_a\rangle,$$

where the $+$ and $-$ signs are for the bosonic and fermionic particles, respectively. Replacing the states $|\alpha\rangle$ and $|\beta\rangle$ by two position states $|x_1\rangle$ and $|x_2\rangle$, one gets

$$\begin{aligned}\langle x_1, x_2|\psi_a, \psi_b\rangle &= \langle x_1|\psi_a\rangle\langle x_2|\psi_b\rangle \pm \langle x_1|\psi_b\rangle\langle x_2|\psi_a\rangle \\ \Phi(x_1, x_2) &= \psi_a(x_1)\psi_b(x_2) \pm \psi_b(x_1)\psi_a(x_2),\end{aligned}$$

where $\psi_a(x_1), \psi_b(x_2)$ are the familiar wavefunctions associated with the states $|\psi_a\rangle, \psi_b\rangle$.

The two-particle normalized, symmetric and anti-symmetric, wavefunctions can be written as

$$\Phi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_a(x_1)\psi_b(x_2) \pm \psi_b(x_1)\psi_a(x_2)],$$

the $+, -$ signs corresponding to bosons and fermions, respectively. An interesting thing to notice is that if the two states $|\psi_a\rangle, \psi_b\rangle$ are the same, then the wavefunction $\Phi(x_1, x_2)$ *for fermions* vanishes for all x_1, x_2, which means that the probability of finding two fermions in the same quantum state is zero! This is the familiar *Pauli exclusion principle*. The symmetric and antisymmetric states can be constructed from two single-particle states by using the permutation operator:

$$\begin{aligned}|\Phi_S\rangle &= \frac{1}{\sqrt{2}}(|\psi_a\rangle_1|\psi_b\rangle_2 + \hat{P}_{12}|\psi_b\rangle_1|\psi_a\rangle_2), \\ |\Phi_A\rangle &= \frac{1}{\sqrt{2}}(|\psi_a\rangle_1|\psi_b\rangle_2 - \hat{P}_{12}|\psi_b\rangle_1|\psi_a\rangle_2).\end{aligned} \tag{4}$$

Let us now ask what happens when there are three particles $1,2,3$ and three states, $|\psi_a\rangle, \psi_b\rangle, \psi_c\rangle$. Symmetric and antisymmetric combinations can be formed by applying the permutation operators $\hat{P}_{ij}$ successively:

$$|\Phi_S\rangle=\frac{1}{\sqrt{6}}\Big(|\psi_a\rangle_1|\psi_b\rangle_2|\psi_c\rangle_3 + |\psi_b\rangle_1|\psi_a\rangle_2|\psi_c\rangle_3 + |\psi_b\rangle_1|\psi_c\rangle_2|\psi_a\rangle_3 \\ +|\psi_a\rangle_1|\psi_c\rangle_2|\psi_b\rangle_3 + |\psi_c\rangle_1|\psi_a\rangle_2|\psi_b\rangle_3 + |\psi_c\rangle_1|\psi_b\rangle_2|\psi_a\rangle_3\Big), \tag{5}$$

$$|\Phi_A\rangle=\frac{1}{\sqrt{6}}\Big(|\psi_a\rangle_1|\psi_b\rangle_2|\psi_c\rangle_3 - |\psi_b\rangle_1|\psi_a\rangle_2|\psi_c\rangle_3 + |\psi_b\rangle_1|\psi_c\rangle_2|\psi_a\rangle_3 \\ -|\psi_a\rangle_1|\psi_c\rangle_2|\psi_b\rangle_3 + |\psi_c\rangle_1|\psi_a\rangle_2|\psi_b\rangle_3 - |\psi_c\rangle_1|\psi_b\rangle_2|\psi_a\rangle_3\Big), \tag{6}$$

where $-$ sign comes where there are odd number of permutions involved, and $+$ sign where even number of permutations are involved. One can check that

$$\hat{P}_{ij}|\Phi_S\rangle = |\Phi_S\rangle,$$

$$\hat{P}_{ij}|\Phi_A\rangle = -|\Phi_A\rangle,$$

for all i, j.

If there are N identical particles, constructing a symmetric state is straightforward, but constructing an antisymmetric state involves some book-keeping with the signs of various terms. A convenient way to write N-particle antisymmetric state is by using a *Slater determinant*:

$$|\Phi_A\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} |\psi_a\rangle_1 & |\psi_b\rangle_1 & |\psi_c\rangle_1 \dots \\ |\psi_a\rangle_2 & |\psi_b\rangle_2 & |\psi_c\rangle_2 \dots \\ |\psi_a\rangle_3 & |\psi_b\rangle_3 & |\psi_c\rangle_3 \dots \\ \vdots & \vdots & \vdots \quad \dots \\ |\psi_a\rangle_N & |\psi_b\rangle_N & |\psi_c\rangle_N \dots \end{vmatrix}.$$

As we will see later, for large number of particles, using *particle number states* or *Fock states* is more convenient. That is a completely different formalism, called *second quantization*.

Second quantization

If we are dealing with a system of many identical particles, it is pointless to ask which particle is in which single-particle state. Even the slater determinant form is not of much use, as the only useful property for the state is $\hat{P}_{ij}|\Phi_S\rangle = |\Phi_S\rangle, \hat{P}_{ij}|\Phi_A\rangle = -|\Phi_A\rangle$. It may be more convenient to ask which single-particle state has how many particles. Clearly, if we are dealing with fermions, any single particle state can be occupied by only one or zero particles, and if we are dealing with bosons, a single-particle state can have any number of particles in it. Let us assume that we have a finite or infinite number of single-particle states:

$$|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, \dots |\psi_i\rangle, \dots,$$

which are the same as the states $|\psi_a\rangle, |\psi_b\rangle, |\psi_c\rangle \dots$ used earlier, but we now use numeric labels intead of alphabetic labels. Let us define a multiparticle *occupation number* state as

$$|n_1, n_2, n_3, \dots, n_i, \dots\rangle,$$

which has a simple meaning: there are n_1 particles in the state $|\psi_1\rangle$, n_2 particles in the state $|\psi_2\rangle$, n_i particles in the state $|\psi_i\rangle$, and so on. If we have don't have any particle, then the state would be

$$|0,0,\ldots,0,\ldots\rangle = |\mathbf{0}\rangle,$$

which we call the *vacuum state*. We have another special state

$$|0,0,\ldots,n_i = 1,\ldots\rangle = |\psi_i\rangle,$$

where there is only one particle, in the single-particle state $|\psi_i\rangle$. So this multiparticle state will just be the same as the single-particle state $|\psi_i\rangle$. Next we introduce the *creation* and *annihilaion* operators such that

$$\begin{aligned} \hat{a}_i^\dagger|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle &\propto |n_1,n_2,n_3,\ldots,n_i+1,\ldots\rangle, \\ \hat{a}_i|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle &\propto |n_1,n_2,n_3,\ldots,n_i-1,\ldots\rangle, \end{aligned} \tag{7}$$

with the priviso $\hat{a}_i|\mathbf{0}\rangle = 0$.

From the above construction it is logical that if $\hat{a}_i^\dagger$ acts on the vacuum state, it should generate the single-particle state $|\psi_i\rangle$

$$\hat{a}_i^\dagger|\mathbf{0}\rangle = |\psi_i\rangle,$$

and the annihilation operator acting on $|\psi_i\rangle$ should lead to the vacuum state: $\hat{a}|\psi_i\rangle = |\mathbf{0}\rangle$. Taking the norm of both sides, we get

$$\langle\mathbf{0}|(\hat{a}_i^\dagger)^\dagger\hat{a}_i^\dagger|\mathbf{0}\rangle = \langle\psi_i|\psi_i\rangle = 1 = \langle\mathbf{0}|(\hat{a}_i^\dagger)^\dagger|\psi_i\rangle.$$

For this to be true, $(\hat{a}_i^\dagger)^\dagger|\psi_i\rangle = |\mathbf{0}\rangle$, which means $(\hat{a}_i^\dagger)^\dagger = \hat{a}$. So the creation and annihilation operators are adjoints of each other. Another logical outcome is

$$\hat{a}_i|\psi_j\rangle = 0 \quad \text{if} \quad i \neq j.$$

By construction, the particle-number states do not tell us if they are for fermions or bosons, or whether they are symmetric or antisymmetric under particle permutation. We assume that the symmetry can be specified by comparing the states where the first particle is put in $|\psi_i\rangle$, and the second particle in $|\psi_j\rangle$, and vice-versa:

$$\hat{a}_i^\dagger\hat{a}_j^\dagger|\mathbf{0}\rangle = \pm\hat{a}_j^\dagger\hat{a}_i^\dagger|\mathbf{0}\rangle.$$

The same logic can be applied to the many-particle states, and not just the vacuum state. The results we get is

$$\hat{a}_i^\dagger\hat{a}_j^\dagger - \hat{a}_j^\dagger\hat{a}_0^\dagger = 0 \quad \text{bosons}$$

$$\hat{a}_i^\dagger\hat{a}_j^\dagger + \hat{a}_j^\dagger\hat{a}_0^\dagger = 0 \quad \text{fermions}$$

Taking the adjoint of the above, we get

$$\begin{aligned} [\hat{a}_i,\hat{a}_j] &= 0 \quad \text{bosons} \\ \{\hat{a}_i,\hat{a}_j\} &= 0 \quad \text{fermions} \end{aligned} \tag{8}$$

where $[,]$ and $\{,\}$ represent the commutator and the anti-commutator, respectively. So one need not bother about the symmetry of the particle number states. It is determined by the commutations rules for the creation-annihilation operators.

Eqn. (7) implies that

$$\begin{aligned} \hat{a}_i^\dagger|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle &= c_+|n_1,n_2,n_3,\ldots,n_i+1,\ldots\rangle, \\ \hat{a}_i|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle &= c_-|n_1,n_2,n_3,\ldots,n_i-1,\ldots\rangle, \end{aligned} \tag{9}$$

where c_+, c_- are the proportionality constants. The above implies that

$$\hat{a}_i^\dagger\hat{a}_i|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle = c_+c_-|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle, \tag{10}$$

meaning, the occupation number states are eigenstates of the operator $\hat{a}_i^\dagger\hat{a}_i$. Using our experience with the harmonic oscillator creation and annihilation operators, we can assume the following commutation relation for bosons, and consequently the anticommutation relation for fermions:

$$\begin{aligned} [\hat{a}_i, \hat{a}_i^\dagger] &= 1 \quad \text{bosons} \\ \{\hat{a}_i, \hat{a}_i^\dagger\} &= 1 \quad \text{fermions.} \end{aligned} \tag{11}$$

Using the above commutation relations it can then be shown that

$$\hat{a}_i^\dagger\hat{a}_i|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle = n_i|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle. \tag{12}$$

This shows that the operator $\hat{a}_i^\dagger\hat{a}_i$ just counts the number of particles in the single-particle state $|\psi_i\rangle$. For fermions n_i can only take values 0 or 1. For bosons, n_i can take positive integer values, starting from 0. The action of the creation, annihilation operators on the number states is given by

$$\begin{aligned} \hat{a}_i^\dagger|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle &= \sqrt{n_i+1}|n_1,n_2,n_3,\ldots,n_i+1,\ldots\rangle, \\ \hat{a}_i|n_1,n_2,n_3,\ldots,n_i,\ldots\rangle &= \sqrt{n_i}|n_1,n_2,n_3,\ldots,n_i-1,\ldots\rangle. \end{aligned} \tag{13}$$

This completes the formulation of second quantization. So to study a quantum mechanical system of many identical particles, one should use the occupation number states. All observables should be defined in terms of the creation, annihilation operators. For example if we have a system of couple Harmonic oscillators, given by the Hamiltonian:

$$\hat{H} = \sum_j \left(\frac{\hat{p}_i^2}{2m} + \tfrac{1}{2}m\omega^2\hat{x}_j^2 + \frac{\gamma}{2}(\hat{x}_j - \hat{x}_{j+1})^2 \right),$$

it can be equivalently represented by the following second-quantized Hamiltonian

$$\hat{H} = \sum_j \hbar\omega(\hat{a}_j^\dagger\hat{a}_j + \tfrac{1}{2}) + \alpha(\hat{a}_j + \hat{a}_j^\dagger - \hat{a}_{j+1} - \hat{a}_{j+1}^\dagger)^2,$$

where α is a constant depending on m, ω, γ. The operators involved here will act on the occupation number states. The single-particle states involved here are the energy eigenstates of a *single* Harmonic oscillator.

The second quantization formalism paves the way for *quantum field theory*.