Identical particles

In classical physics one can distinguish between identical particles in such a way as to leave the dynamics unaltered. Therefore, the exchange of particles of identical particles leads to different configurations. In quantum mechanics, i.e., in nature at the microscopic levels identical particles are indistinguishable. A proton that arrives from a supernova explosion is the same as the proton in your glass of water.\(^1\)

Messiah and Greenberg\(^2\) state the principle of indistinguishability as “states that differ only by a permutation of identical particles cannot be distinguished by any observation whatsoever.”

If we denote the operator which interchanges particles \(i\) and \(j\) by the permutation operator \(P_{ij}\) we have

\[
\langle \Psi | \hat{O} | \Psi \rangle = \langle \Psi | P_{ij}^\dagger \hat{O} P_{ij} | \psi \rangle
\]

which implies that \(P_{ij}\) commutes with an arbitrary observable \(\hat{O}\). In particular, it commutes with the Hamiltonian. All operators are permutation invariant.

**Law of nature:** The wave function of a collection of identical half-odd-integer spin particles is completely antisymmetric while that of integer spin particles or bosons is completely symmetric\(^3\). Defining the permutation operator\(^4\) by

\[
P_{ij} \Psi(1, 2, \cdots, i, \cdots, j, \cdots N) = \Psi(1, 2, \cdots, j, \cdots, i, \cdots N)
\]

we have

\[
P_{ij} \Psi(1, 2, \cdots, i, \cdots, j, \cdots N) = \pm \Psi(1, 2, \cdots, i, \cdots, j, \cdots N)
\]

where the upper sign refers to bosons and the lower to fermions.

Emphasize that the symmetry requirements only apply to identical particles. For the hydrogen molecule if \(I\) and \(II\) represent the coordinates and spins of the two protons and 1 and 2 of the two electrons we have

\[
\Psi(I, II, 1, 2) = -\Psi(II, I, 1, 2) = -\Psi(I, II, 2, 1) = \Psi(II, I, 2, 1)
\]

\(^1\)On the other hand, the elements on earth came from some star/supernova in the distant past.


\(^3\)Identical half-integral spin particles are described by antisymmetric wave functions or are said to obey Fermi-Dirac statistics while integer spin particles are described by symmetric wave functions or are said to obey Bose-Einstein statistics.

\(^4\)Note that the permutation operator \(P_{ij}\) is both Hermitian and unitary.
but there is no symmetry condition if we exchange $I$ with 1.

We also note that since the Hamiltonian commutes with the permutation operator, the symmetry or antisymmetry of the wave function is preserved under time evolution.

**Rule for composite particles** The general rule for a composite particle is that if it contains an even number of fermions and any number of bosons it behaves as a boson and if it contains an odd number of fermions and any number of bosons it behaves as a fermion. Note that the two cases yield integral and half-integral net spins respectively.

$^4He$ has two protons and two neutrons in the nucleus and two electrons and is a boson. Exhibits bosonic superfluidity

$^3He$ has two protons and one neutron in the nucleus and two electrons and is a fermion.

Why does an integral spin particle display bosonic statistics while half-integer spins obey fermionic statistics? Combination of locality, causality, and relativity leads to this result as Pauli showed.

For a two particle system the wave function is written as $\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2)$. For fermions this must be antisymmetric under the interchange of $\{\vec{r}_1, s_1\}$ and $\{\vec{r}_2, s_2\}$. For two spin-1/2 particles (only) it is convenient to impose antisymmetrization by writing the wave function as a product of a spatial wave function $\psi(\vec{r}_1, \vec{r}_2)$ and a spin wave function $\chi(s_1, s_2)$ and making one of them symmetric and the other antisymmetric so that the product is antisymmetric. This is the key point. Note that this is not the only way but is a useful and convenient way. There are other ways of imposing antisymmetry, for example, Slater determinants that will come later.

**Simple Example**

Consider two non-interacting spin-1/2 particles in one-dimensional harmonic oscillator potential. Denote the eigenfunctions of the oscillator by $\phi_n(x)$ with energy $(n + (1/2))\hbar\omega$. One way to proceed since the Hamiltonian is independent of spin (you can add this complication) is to write the spatial part of the wave function for different energies without worrying about statistics. The three lowest energy states are

\[
\phi_0(x_1) \phi_0(x_2) \quad \text{with} \quad E = \hbar\omega.
\]

\[
\phi_1(x_1) \phi_0(x_2) \quad \text{with} \quad E = 2\hbar\omega.
\]
\( \phi_2(x_1) \phi_0(x_2) \) with \( E = 3\hbar \omega \).

\( \phi_1(x_1) \phi_1(x_2) \) with \( E = 3\hbar \omega \).

Now we construct different total wave function by (i) symmetrizing each of the spatial states above and multiplying by the spin singlet state which is antisymmetric (ii) antisymmetrizing each spatial wave function and multiplying by any one of the three triplet states each of which is symmetric. It is useful to observe that if both particles are in the same spatial state anti-symmetrizing yields zero.

Let us consider the first excited state. Symmetrize it: Write the wave function with all possible permutations of the particle label and add them with the same sign. Works for any number of particles!

\[
\frac{1}{\sqrt{2}} (\phi_1(x_1)\phi_0(x_2) + \phi_1(x_2)\phi_0(x_1))
\]

Clearly, (is it?) this must be accompanied by a spin singlet since it is antisymmetric.

Invent notation. Let \( \alpha \) represents the up state spinor and \( \beta \) the spin down spinor.

\[
\alpha \leftrightarrow \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \quad \beta \leftrightarrow \left( \begin{array}{c} 0 \\ 1 \end{array} \right)
\]

Put a subscript to indicate the particle label. Thus \( \alpha_1 \beta_2 \) represents the first particle with up spin and the second with down spin with respect to the arbitrarily chosen \( z \)-axis.

Thus

\[
\Psi'(x_1, s_1; x_2, s_2) = \frac{1}{\sqrt{2}} (\phi_1(x_1)\phi_0(x_2) + \phi_1(x_2)\phi_0(x_1)) \times \frac{1}{\sqrt{2}} (\alpha_1 \beta_2 - \beta_1 \alpha_2).
\]

One can find other states with the same energy. Antisymmetrize the spatial part of the wave function by writing down all permutations of the particle label with a negative sign for odd number of permutations. We obtain

\[
\frac{1}{\sqrt{2}} (\phi_1(x_1)\phi_0(x_2) - \phi_1(x_2)\phi_0(x_1))
\]

Clearly, (is it?) this must be accompanied by one of the spin triplet states since these are all symmetric. The three states in our newly invented notation are \( \alpha_1 \alpha_2 \), \( (\alpha_1 \beta_2 + \alpha_2 \beta_1)/\sqrt{2} \), and \( \beta_1 \beta_2 \). Thus we have three more state with the same energy that we write down in excruciation detail:

\[
\Psi''(x_1, s_1; x_2, s_2) = \frac{1}{\sqrt{2}} (\phi_1(x_1)\phi_0(x_2) - \phi_1(x_2)\phi_0(x_1)) \times \alpha_1 \alpha_2,.
\]
: The first excited state has a degeneracy of four. Please find the wave functions of next excited state before you come to class.

Given a set of \( n \) orthogonal functions (including spin and space) denoted by \( \{ \phi_{a_j} \} \) the Slater determinant is constructed as the antisymmetrized form of the state \( \phi_{a_1}(1) \cdot \phi_{a_n}(n) \) where 1 denotes \( \vec{r}_1, s_1 \) etc.

\[
\frac{1}{\sqrt{n!}} \left| \begin{array}{cccc}
\phi_{a_1}(\vec{r}_1) & \phi_{a_2}(\vec{r}_1) & \cdots & \phi_{a_n}(\vec{r}_1) \\
\phi_{a_1}(\vec{r}_2) & \phi_{a_2}(\vec{r}_2) & \cdots & \phi_{a_n}(\vec{r}_2) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_{a_1}(\vec{r}_n) & \phi_{a_2}(\vec{r}_n) & \cdots & \phi_{a_n}(\vec{r}_n) \\
\end{array} \right|
\]

The \( n \) orthonormal functions are usually chosen from a complete set of one-particle state. The subscript \( a_j \) denotes a set of four quantum numbers needed to describe a one-particle state in three dimensions such \( \{ n, \ell, m_\ell, m_s \} \) for the hydrogen atom or \( \{ n_x, n_y, n_z, m_s \} \) for a harmonic oscillator wave function. Thus we can have \( \phi_{a_1}(1) = \psi_{2p}(\vec{r}_1) \alpha_1 \) where \( \alpha_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \).

Some simple examples are discussed below:

Consider three electrons with all spins up (chosen for illustrative purposes) in three orthogonal orbitals (spatial wave functions) labeled \( \phi_a, \phi_b, \phi_c \). We will use three-dimensional notation for variety. One can start with the spatial state \( \phi_a(\vec{r}_1)\phi_b(\vec{r}_2)\phi_c(\vec{r}_3) \) and antisymmetrize it or more compactly use Slater determinants.

\[
\frac{1}{\sqrt{3!}} \left| \begin{array}{ccc}
\phi_a(\vec{r}_1) & \phi_b(\vec{r}_1) & \phi_c(\vec{r}_1) \\
\phi_a(\vec{r}_2) & \phi_b(\vec{r}_2) & \phi_c(\vec{r}_2) \\
\phi_a(\vec{r}_3) & \phi_b(\vec{r}_3) & \phi_c(\vec{r}_3) \\
\end{array} \right|
\]

Two particle wave functions: Consider

\[
\Psi(\vec{r}_1, s_1; \vec{r}_2, s_2) = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_a(1) & \psi_b(1) \\ \psi_a(2) & \psi_b(2) \end{pmatrix}
\]

with 1 denoting \( \vec{r}_1, s_1 \) etc. We will make different choices for \( \psi_a \) and see what we obtain below.
Assume $\psi_a(1) = \phi_a(\vec{r}_1)\alpha_1$, $\psi_b(1) = \phi_b(\vec{r}_1)\alpha_1$ and you obtain

$$\Psi_{III} = \frac{1}{\sqrt{2}} (\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) - \phi_b(\vec{r}_1)\phi_a(\vec{r}_2)) \alpha_1 \alpha_2.$$  

If we choose $\psi_a(1) = \phi_a(\vec{r}_1)\alpha_1$ and $\psi_b(1) = \phi_b(\vec{r}_1)\beta_1$ etc., we have a

$$\Psi_I = \frac{1}{\sqrt{2}} [\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) \alpha_1 \beta_2 - \phi_a(\vec{r}_2)\phi_b(\vec{r}_1) \beta_1 \alpha_2].$$  

If on the other hand we have $\psi_a(1) = \phi_a(\vec{r}_1)\beta_1$ and $\psi_b(1) = \phi_b(\vec{r}_1)\alpha_1$ etc., we have

$$\Psi_{II} = \frac{1}{\sqrt{2}} [\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) \beta_1 \alpha_2 - \phi_a(\vec{r}_2)\phi_b(\vec{r}_1) \alpha_1 \beta_2].$$  

By adding the two determinants we obtain

$$[\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) - \phi_a(\vec{r}_2)\phi_b(\vec{r}_1)] \times (\alpha_1 \beta_2 + \beta_1 \alpha_2)$$

which is the spin triplet state with $S_z = 0$ and an antisymmetric spatial wave function. Note that this is a sum of two determinants making the naive way preferable.

Check that subtraction yields the $S = 0, S_z = 0$ state.

**An instructive computation illustrating correlations** is given below: Let

$$\Psi_D(x_1, x_2) = \phi_a(x_1)\phi_b(x_2)$$  

$$\Psi_F(x_1, x_2) = \frac{1}{\sqrt{2}} [\phi_a(x_1)\phi_b(x_2) - \phi_a(x_2)\phi_b(x_1)]$$  

$$\Psi_B(x_1, x_2) = \frac{1}{\sqrt{2}} [\phi_a(x_1)\phi_b(x_2) + \phi_a(x_2)\phi_b(x_1)].$$

We wish to evaluate $\langle (x_1 - x_2)^2 \rangle$ for the three wave functions. Defining

$$\langle x^2 \rangle_a = \int dx \phi_a^*(x) x^2 \phi_a(x)$$  

$$\langle x^2 \rangle_b = \int dx \phi_b^*(x) x^2 \phi_b(x)$$  

$$\langle x \rangle_a = \int dx \phi_a^*(x) x \phi_a(x)$$  

$$\langle x \rangle_b = \int dx \phi_b^*(x) x \phi_b(x)$$  

$$\langle x \rangle_{ab} = \int dx \phi_a^*(x) x \phi_b(x)$$  

$$\langle x \rangle_{ba} = \int dx \phi_b^*(x) x \phi_a(x)$$  

$$\langle x \rangle_{aa} = \int dx \phi_a^*(x) x \phi_a(x)$$  

$$\langle x \rangle_{bb} = \int dx \phi_b^*(x) x \phi_b(x)$$  

5
we find by simple expansion

\[ \langle (x_1 - x_2)^2 \rangle_D = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2 \langle x \rangle_a \langle x \rangle_b \] (10)

\[ \langle (x_1 - x_2)^2 \rangle_F = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2 \langle x \rangle_a \langle x \rangle_b + 2 |\langle x \rangle_{ab}|^2 \] (11)

\[ \langle (x_1 - x_2)^2 \rangle_B = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2 \langle x \rangle_a \langle x \rangle_b - 2 |\langle x \rangle_{ab}|^2 \] (12)

Thus one obtains

\[ \langle (x_1 - x_2)^2 \rangle_F = \langle (x_1 - x_2)^2 \rangle_D + 2 |\langle x \rangle_{ab}|^2 \] (13)

\[ \langle (x_1 - x_2)^2 \rangle_B = \langle (x_1 - x_2)^2 \rangle_D - 2 |\langle x \rangle_{ab}|^2 \] (14)

which shows that the root mean squared separation of bosons(fermions) is lesser(greater) than that for distinguishable particles that is very loosely viewed as an effective attractive(repulsive) forces in spite of the fact that the particles are non-interacting. One can do this in three dimensions and for explicit wave functions but is illustrative of the degeneracy pressure that exists for fermions. The Pauli exclusion principle is part of the reason why we do not fall through the floor.