Physics 505
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Various Topics

12.1 Noninteracting identical fermions - Slater's determinant

Suppose we have a system of n identical particles. Assume that they are not interacting with each other so the Hamiltonian is a sum of n identical single-particle Hamiltonians $\hat{H} = \sum_{i=1}^{n} \hat{H}_i$ where each $\hat{H}_i$ involves only the variables of the i^{th} particle. For bosons, we symmetrize as follows: Let us assume that the eigenfunctions of $\hat{H}_i$ are:

$$\psi_1(x_i), \psi_2(x_i), \ldots$$

Now we can write the wave function of the system of identical particles. Let us assume that we want to have n_1 particles in the 1^{st} state, n_2 particles in the 2^{nd} state, and so on. We have $n_1 + n_2 + \cdots = n$. So we write the wavefunction:

$$\Psi(x_1, x_2, \ldots, x_n) = A\psi_1(x_1)\cdots\psi_1(x_{n_1})\psi_2(x_{n_1+1})\cdots\psi_2(x_{n_1+n_2})\cdots + (\text{all permutations})$$

Here A is a normalization constant. We can write this more formally as:

$$|n_1, n_2, \ldots\rangle \longrightarrow A\sum_{\sigma}\prod_{j}\prod_{l=1}^{n_j}\psi_j(x_{\sigma(l+\sum_{k=1}^{j-1} n_k)}),$$

where A is the normalization factor. For fermions we insert an extra $(-)^{\sigma}$ and use the fact that $n_j = 0, 1$:

$$|n_1, n_2, \ldots\rangle \longrightarrow B\sum_{\sigma}(-)^{\sigma}\prod_{n_j=1}\psi_j(x_{\sigma(1+\sum_{k=1}^{j-1} n_k)}).$$

B is another normalization factor. This can also be written as a (Slater) determinant:

$$\begin{vmatrix} \psi_{j_1}(x_1) & \psi_{j_2}(x_1) & \cdots & \psi_{j_n}(x_1) \\ \psi_{j_1}(x_2) & \psi_{j_2}(x_2) & \cdots & \psi_{j_n}(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ \psi_{j_1}(x_n) & \psi_{j_2}(x_n) & \cdots & \psi_{j_n}(x_n) \end{vmatrix}$$

Here $j_1, \ldots, j_n$ are the subindices, j, for which $n_j = 1$.

Let us calculate the normalization factors. Let us denote:

$$\Psi_\sigma \equiv \prod_j \prod_{l=1}^{n_j} \psi_j(x_{\sigma(l+\sum_{k=1}^{j-1} n_k)}).$$

We have to calculate:

$$\sum_{\sigma,\sigma'} \int \Psi_\sigma^* \Psi_{\sigma'} dx_1 \cdots dx_n.$$

The integral is nonzero only if every x_i appears in the same function ψ_k for both σ and σ'. For a given σ, there are $\prod_k n_k!$ such σ'. So, altogether:

$$A = \frac{1}{\sqrt{n! \prod_k n_k!}}.$$

It is also easy to see that $B = 1/\sqrt{n!}$.

12.2 Exchange interaction

The phenomenon of ferromagnetism and diamagnetism is often explained by an effective interaction between ions with spin. Let us take two ions, one at the origin and one at $\vec{R}$. Let us assume that they are identical fermions with spin-$\frac{1}{2}$. We assume that they are pinned to their places by a strong potential so that $\vec{R}$ does not change. The effective interaction between them is often written as:

$$\hat{V} = -J\vec{S}_1 \cdot \vec{S}_2,$$

where $\vec{S}_1$ and $\vec{S}_2$ are the spin operators of the two ions. Where is this interaction coming from?

First there is the magnetic interaction between the two ions. Each ion has a magnetic dipole moment:

$$\vec{M} = g\frac{|e|}{2m_e c}\vec{S},$$

where g is a numerical factor that depends on the ion. Two dipole moments interact and have a potential energy:

$$U = \frac{3(\vec{M}_1 \cdot \vec{R})(\vec{M}_2 \cdot \vec{R}) - (\vec{M}_1 \cdot \vec{M}_2)R^2}{R^5}.$$

This, however, is not the only source! Another source is the exchange interaction. Recall that the wave-function of two spin-$\frac{1}{2}$ particles can be written as $\psi(\vec{r}_1, \vec{r}_2)\chi(s_1, s_2)$ where s_1 and s_2 are the spin variables. If the wave-function of the spin variables,$\chi(s_1, s_2)$, is such that the total spin $\vec{S}_T \equiv \vec{S}_1 + \vec{S}_2$ has value 1 (more precisely $\vec{S}_T^2$ has eigenvalue $\hbar^2 1 \cdot (1+1) = 2\hbar^2$) then $\psi(\vec{r}_1, \vec{r}_2) = -\psi(\vec{r}_2, \vec{r}_1)$. If $\chi(s_1, s_2)$ is such that $\vec{S}_T = 0$ then $\psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2, \vec{r}_1)$.

Now consider the system of the two ions. To a good approximation, the Hamiltonian does not contain the spin variables. We may assume that it is given by:

$$\hat{H} = \frac{\vec{p}_1^2}{2M} + \frac{\vec{p}_1^2}{2M} + V(\vec{r}_1, \vec{r}_2).$$

The eigenstates of the Schrödinger equation associated with this Hamiltonian fall into two types. Those that satisfy $\psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2, \vec{r}_1)$ and those that satisfy $\psi(\vec{r}_1, \vec{r}_2) = -\psi(\vec{r}_2, \vec{r}_1)$. Let us denote the solution with lowest energy and with a wave-function of the first type by ψ_+ and let us denote the solution with lowest energy and wave-function of the second type by ψ_-. Let us denote the corresponding energies by E_+ and E_-. In general, in this case $E_+ < E_-$. The reason is that the ground state energy cannot have any zeroes but all the states of the second type (antisymmetric) have zeroes when $\vec{r}_1 = \vec{r}_2$. So the ground state much be ψ_+.

If the ions are far apart, E_+ and E_- will be close in energy and $\psi_+\chi_0$ and $\psi_-\chi_1$ will be the lowest energy states of the spectrum of the two-ion system. Now, if we the energy scale of a given problem is such that the system is never excited to states beyond the two states $\psi_+\chi_0$ and $\psi_-\chi_1$ we can write the energy of the system in terms of the spin variables as:

$$E = E_+ + (E_- - E_+)\frac{\vec{S}_T^2}{2\hbar^2}.$$

The point is that this expression works for both states. Now we can write:

$$\vec{S}_T^2 \quad = \quad (\vec{S}_1 + \vec{S}_2)^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1 \cdot \vec{S}_2 = \frac{3}{2}\hbar^2 + 2\vec{S}_1 \cdot \vec{S}_2$$

Here we used the fact that for a single spin-$\frac{1}{2}$ particle $\vec{S}^2$ always has the eigenvalue $\frac{1}{2}(\frac{1}{2}+1)\hbar^2 = \frac{3}{4}\hbar^2$. So we can write the energy as:

$$E = E_+ + \frac{3}{4}(E_- - E_+) + \frac{E_- - E_+}{\hbar^2}\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{4}E_+ + \frac{3}{4}E_- + \frac{E_- - E_+}{\hbar^2}\vec{S}_1 \cdot \vec{S}_2.$$

Up to an unimportant constant, this is the exchange interaction.

12.3 Addition of angular momentum

Consider two systems. One with total angular momentum $\hat{L}_1$ with eigenvalue $\hbar^2 l_1(l_1+1)$ and the second with total angular momentum $\hat{L}_2$ and eigenvalue $\hbar^2 l_2(l_2+1)$. The first system has a multiplet of $(2l_1+1)$ states $|m_1\rangle$ with $\hat{L}_{1z}$ eigenvalue $\hbar m_1$ with $m_1 = -l_1, \ldots, l_1$. The second system similarly has $(2l_2+1)$ states. Now let us think about the combined wave-function of teh two-systems together. There are $(2l_1+1)(2l_2+1)$ states that we label as $|m_1 m_2\rangle$. We also have the total angular momentum operator:

$$\vec{L} \equiv \vec{L}_1 + \vec{L}_2.$$

The question is, can we find linear combinations of the $(2l_1+1)(2l_2+1)$ that are eigenstates of $\vec{L}^2$ and $\vec{L}_z$?

The answer turns out to be that the possible eigenvalues of $\vec{L}^2$ are $\hbar^2 l(l+1)$ where the possible values of l are all the integers that satisfy $|l_1 - l_2| \le l \le l_1 + l_2$, in case $l_1 + l_2$ is an integer. If $l_1 + l_2$ is $\frac{1}{2}$ plus an integer, that l also can takeany value that is an integer plus $\frac{1}{2}$, again in the range $|l_1 - l_2| \le l \le l_1 + l_2$. With $(2l+1)$ states for each l, the total number of states is:

$$\sum_{l=|l_1-l_2|}^{l_1+l_2} (2l+1) = (2l_1+1)(2l_2+1).$$

To find these linear combination, we can write a $(2l_1+1)(2l_2+1) \times (2l_1+1)(2l_2+1)$ matrix corresponding to the operator $\vec{L}^2$ in the basis $|m_1 m_2\rangle$ and diagonalize it. This is, however, very complicated and there is a much simpler way.

Let us consider first the value $l = l_1 + l_2$. Let us also denote the eigenvalue of $\hat{L}_z$ by $\hbar m$. A state $|m_1 m_2\rangle$ is an eigenstate of $\hat{L}_z$ with $m = m_1 + m_2$. Let us look for the state $|l, m\rangle_T$ (we will add a subscript T when we are discussing eigenvalues of the total $\hat{L}$, to avoid confusion with $|m_1 m_2\rangle$) with $m = l = l_1 + l_2$. This is the maximal possible value of m and there is only one such state in the subspace of $(2l_1+1)(2l_2+1)$ states. It is $|l_1 l_2\rangle$. So we conclude that:

$$|l_1+l_2, l_1+l_2\rangle_T = |l_1, l_2\rangle.$$

Now we can apply $\hat{L}_-$ to find:

$$\begin{aligned} |l_1+l_2, l_1+l_2-1\rangle_T &= \frac{\hat{L}_-}{\hbar\sqrt{2(l_1+l_2)}}|l_1+l_2, l_1+l_2\rangle_T = \frac{\hat{L}_{1-}+\hat{L}_{2-}}{\hbar\sqrt{2(l_1+l_2)}}|l_1, l_2\rangle \\ &= \sqrt{\frac{l_1}{l_1+l_2}}|l_1-1, l_2\rangle + \sqrt{\frac{l_2}{l_1+l_2}}|l_1, l_2-1\rangle. \end{aligned}$$

In this way,by repeated application of $\hat{L}_-$, we can find all the states with $l = l_1 + l_2$.

What about the states with $l = l_1 + l_2 - 1$? Let us look for the state with maximal value of $m = l_1 + l_2 - 1$. There are two linearly independent states with this value of m. One is $|l_1 - 1, l_2\rangle$ and the other is $|l_1, l_2 - 1\rangle$. The state that we are looking for, $|l_1+l_2-1, l_1+l_2-1\rangle_T$, is a linear combination of them. But we also know that it is orthogonal to the state

$$|l_1+l_2, l_1+l_2-1\rangle_T = \sqrt{\frac{l_1}{l_1+l_2}}|l_1-1, l_2\rangle + \sqrt{\frac{l_2}{l_1+l_2}}|l_1, l_2-1\rangle,$$

since they have different eigenvalues of the Hermitian operator $\vec{L}_T^2$. So our normalized state is:

$$|l_1+l_2-1, l_1+l_2-1\rangle_T = \sqrt{\frac{l_2}{l_1+l_2}}|l_1-1, l_2\rangle - \sqrt{\frac{l_1}{l_1+l_2}}|l_1, l_2-1\rangle,$$

We can now find the rest of the states with $l = l_1 + l_2 - 1$ and different m's, by repeated application of $\hat{L}_-$ as before. Next, we look for the state $|l_1+l_2-2, l_1+l_2-2\rangle$. There are three independent states with $m = l_1 + l_2 - 2$. They are:

$$|l_1, l_2-2\rangle,\ |l_1-1, l_2-1\rangle,\ |l_1-2, l_2\rangle.$$

But in the previous steps we have already found two states with total $m = l_1 + l_2 - 2$. They are:

$$|l_1+l_2, l_1+l_2-2\rangle_T,\ |l_1+l_2-1, l_1+l_2-2\rangle_T.$$

The state $|l_1+l_2-2, l_1+l_2-2\rangle_T$ must be the linear combination:

$$A|l_1, l_2-2\rangle + B|l_1-1, l_2-1\rangle + C|l_1-2, l_2\rangle.$$

that is orthogonal to both $|l_1+l_2, l_1+l_2-2\rangle_T$ and $|l_1+l_2-1, l_1+l_2-2\rangle_T$. In this way we proceed until there are no more states to find. This happens when we reach $l = |l_1-l_2|-1$. In this case there all the states with $m = l$ have already been accounted for in previous stages. So there are no more new states.

12.4 A continuum with multi-variables

Recall the Golden Rule for the rate of transitions to the continuum. If the continuum is labeled by a parameter k such that:

$$\langle k'|k\rangle = \delta(k'-k),$$

then:

$$\frac{dP}{dt} = \frac{2\pi}{\hbar}\int |\langle k|\hat{V}|i\rangle|^2 \delta(E_f(k) - E_i - \hbar\omega)dk.$$

It sometimes happens that the continuum is labeled by more than one parameter. For example, a bound state of two particles that is also bound by a potential can dissociate and the final state will be labeled by two particles in the continuum. In this case we can label the continuum by $|k_1, k_2\rangle$. We need to normalize:

$$\langle k_1', k_2'|k_1, k_2\rangle = \delta(k_1'-k_1)\delta(k_2'-k_2),$$

and then:

$$\frac{dP}{dt} = \frac{2\pi}{\hbar}\int |\langle k_1, k_2|\hat{V}|i\rangle|^2 \delta(E_f(k_1, k_2) - E_i - \hbar\omega)dk_1 dk_2.$$

Note that this time there are many different final states, since the equation:

$$E_f(k_1, k_2) - E_i - \hbar\omega = 0,$$

has more than one solution.

12.5 Density of states

There is an alternative way of deriving the normalization of the continuum states in the golden-rule. Let us assume that k is the wave-number of a free particle. For the normalization $\langle k'|k\rangle = \delta(k'-k)$ we took the wave-function

$$\psi_k(x) \equiv \langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}.$$

Let us now pretend that x is restricted to a finite length. We will denote the length by L. We can take the boundary conditions $\psi_k(-\frac{L}{2}) = \psi_k(\frac{L}{2}) = 0$, but it is more convenient to take **periodic** boundary conditions:

$$\psi_k(x) = \psi_k(x+L), \qquad \psi'_k(x) = \psi'_k(x+L).$$

Now k takes on discrete values:

$$k = 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \ldots$$

The wave-functions are now:

$$\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx}.$$

They are normalized such that:

$$\langle k'|k\rangle = \delta_{k'k}.$$

In the limit $L \to \infty$, the number of states between k and $k+dk$, is:

$$\frac{L}{2\pi} dk.$$

In the new normalization: $\langle k|\hat{V}|i\rangle$ is smaller by a factor of $\sqrt{L/2\pi}$. But in this normalization we can write:

$$\frac{dP}{dt} \longrightarrow \sum_k |\langle k|\hat{V}|i\rangle|^2 \delta(E_f(k) - E_i - \hbar\omega) \longrightarrow \int |\langle k|\hat{V}|i\rangle|^2 \delta(E_f(k) - E_i - \hbar\omega) \frac{L}{2\pi} dk$$

and the result is the same. The second arrow is in the limit $L \to \infty$.

In 3D, we can take a finite volume. The normalized wavefunctions are then:

$$\frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

and the number of states in a $\vec{k}$-space volume element $d^3\vec{k}$ is:

$$\frac{V}{(2\pi)^3} d^3\vec{k}.$$

The factor, $V/(2\pi)^3$ is called **the density of states**.