Lecture 8 Summary

PHYS798S Spring 2016

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Second Quantization Description

0.1 Many Identical Fermion Wavefunctions

Let us suppose that the metal has N electrons and $M >> N$ available single-particle states. Because the electrons are many identical Fermions with overlapping wavefunctions, we need to create a wavefunction (WF) that obeys the Pauli exclusion principle and allows at most only single occupation of any microscopic state labeled by a list of quantum numbers QN. Up to now, this list has been $QN = (\overrightarrow{k}, \sigma)$ which represent the momentum and spin of single-particle solutions to the Schrodinger equation for particles in a box.
The easiest way to keep track of things is to use the Wigner-Jordan (second quantization) notation that keeps track of the occupation number n_i of each microscopic state i. The occupation number has values of 0 or 1 for un-occupied and occupied states, respectively.
Define operators that create or destroy occupation of specific single-particle states as follows.
$c^{+}_{\overrightarrow{k},\sigma}$ Creates an electron in a properly anti-symmetrized state described by the wavenumber $\overrightarrow{k}$ and spin σ, when that state is initially empty. It gives zero when the state is not initially empty.
$c_{\overrightarrow{k},\sigma}$ Destroys an electron in a properly anti-symmetrized state described by the wavenumber $\overrightarrow{k}$ and spin σ, when that state is initially occupied. It gives zero when the state is initially empty.

0.2 The Cooper Pair WF in Second Quantized Notation

The Cooper pair WF can be written as
$\Psi(1,2) = \sum_{k>k_F} g_k c^{+}_{k,\uparrow} c^{+}_{-k,\downarrow} |F\rangle$, where $|F\rangle$ represents the filled Fermi sea at $T = 0$. How is the "properly anti-symmetrized" state achieved? The answer is the Slater Determinant. This way of writing the many-electron WF builds in the anti-symmetry constraint, but at the price of other complications. For the Cooper pair wavefunction we can think of the first term in the sum as

$$g_{\vec{k}} c^{+}_{\vec{k},\uparrow} c^{+}_{-\vec{k},\downarrow} |F\rangle = g_{\vec{k}} \begin{vmatrix} e^{i\vec{k}\cdot\vec{r}_a} \begin{pmatrix}1\\0\end{pmatrix}_a & e^{i\vec{k}\cdot\vec{r}_b} \begin{pmatrix}1\\0\end{pmatrix}_b \\ e^{-i\vec{k}\cdot\vec{r}_a} \begin{pmatrix}0\\1\end{pmatrix}_a & e^{-i\vec{k}\cdot\vec{r}_b} \begin{pmatrix}0\\1\end{pmatrix}_b \end{vmatrix} |F\rangle$$

Note that the columns label particles while the rows label states. You will complete this calculation for homework and show that it reduces to the spin-singlet WF that we used in the Cooper pairing calculation.

0.3 Properties of the Creation and Annihilation Operators

The number operator is defined as $n_{k,\sigma} = c^{+}_{k,\sigma} c_{k,\sigma}$. It counts how many excitations exist in state labeled by (k,σ). In other words it's eigenvalue is the occupation of the state (k,σ)

The un-number operator is defined as $c_{k,\sigma} c^{+}_{k,\sigma}$

The anti-commutator of operators $c_{k,\sigma}$ and $c^{+}_{k,\sigma}$ can be found by adding the above two operators: $[c_{k,\sigma}, c^{+}_{k,\sigma}]_{+} \equiv c_{k,\sigma} c^{+}_{k,\sigma} + c^{+}_{k,\sigma} c_{k,\sigma} = 1$.

0.4 Many-Electron WFs

The WF of all the electrons in the metal can now be represented as:
$|\Psi\rangle = |n_{k_1,\sigma_1}, n_{k_2,\sigma_2}, ..., n_{k_M,\sigma_M}\rangle$, where $M >> N$ is the total number of available states for the N particles. An example state is
$|\Psi\rangle = |1,0,0,1,1,0,0,1,0,...,0,0,1,0,0\rangle$.
Note that we have to label each state uniquely and list them in a standard list format whenever the WF is written down or manipulated. Underlying each WF is a massive Slater determinant, as we shall see below.
More generally we can consider this WF, focusing on three states called i, j and k:
$|\Psi\rangle = |...,0(i),...1(j),....,1(k),...\rangle$. In other words, state i is initially un-occupied, while states j, k are initially occupied. The corresponding Slater determinant looks like this:

$$\begin{vmatrix} \vdots & \vdots & \vdots & \vdots & \vdots \\ \psi_j(a) & \psi_j(b) & \psi_j(c) & \cdots & \psi_j(N) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \psi_k(a) & \psi_k(b) & \psi_k(c) & \cdots & \psi_k(N) \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix}$$

, where the particles are labeled a, b, ...N.
Note that the row where state i will appear is somewhere above the row for state j in this standard list format. Also note that switching columns in this determinant is equivalent to switching all of the quantum numbers of two particles, and leads to an overall minus sign in the WF, as expected.
The Slater determinant has N columns for the N particles, and N rows for the $N << M$ uniquely occupied states, out of a possible number M.

Consider the operation of operators c_j and c_i^+ on this WF in opposite orders. The standard procedure to destroy occupation of a state is to move the corresponding row to the bottom of the determinant and then delete it. In doing so one makes many row-by row interchanges, adding many factors of (-1). Adding an excitation in a new state involves introducing a new row at the bottom and permutting it up into it's standard location in the list of states. This also involves permutations of the rows of the determinant, leading to more factors of (-1). Upon keeping careful track of how many factors arise, one finds that $[c_j, c_i^+]_+ = 0$ when $j \neq i$.
This can be combined with the above result to yield the general anti-commutator:
$[c_{k,\sigma}, c^+_{k',\sigma'}]_+ = \delta_{k,k'}\delta_{\sigma,\sigma'}$, in terms of the Kronecker deltas.
Similarly, one can show
$[c_{k,\sigma}, c_{k',\sigma'}]_+ = 0$, and
$[c^+_{k,\sigma}, c^+_{k',\sigma'}]_+ = 0$.

0.5 Construction of a specific state

Consider a specific state of the metal given by a list of M integers:
$|n_1, n_2, n_3, ..., n_s, ..., n_M\rangle = (c_1^+)^{n_1}(c_2^+)^{n_2}...(c_s^+)^{n_s}...(c_M^+)^{n_M}\,|0\rangle$, where $|0\rangle$ is the vacuum state - i.e. empty k-space.
By using the anti-commutator relations, one can show that:
Destroying an excitation in state s:
$c_s\,|n_1, ..., n_s, ..., n_M\rangle = (-1)^{n_1+n_2+...n_{s-1}}\sqrt{n_s}\,|n_1, ..., n_s - 1, ..., n_M\rangle$, and similarly; creating an excitation in state s:
$c_s^+\,|n_1, ..., n_s, ..., n_M\rangle = (-1)^{n_1+n_2+...n_{s-1}}\sqrt{1-n_s}\,|n_1, ..., n_s + 1, ..., n_M\rangle$.
These operations are similar to the lowering and raising operators for (Bosonic) excitations of harmonic oscillators except for the pre-factors of (-1) and the sign in the second radical.