# PHYS 798C Spring 2024
# Lecture 7 Summary

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## I. ELECTRON-PHONON PAIRING MECHANISM, CONCLUDED

### A. Electron-Electron interaction in the Time Domain

Taking the Fourier transform of the $V(q,\omega)$ interaction in to the time domain yields, $V(q,t) \propto \frac{e^2/\epsilon_0}{q^2+k_{TF}^2}\{\delta(t) - \pi\sin(\omega_q t)\}$. This reveals that the two electrons will encounter a strong repulsive interaction if they come to the same location at the same time, but they will enjoy an attractive interaction if one arrives after the other, on the scale of the phonon vibration period. The picture is that the first electron travels through the lattice and leaves behind a time-delayed polarization of the slowly-moving ion lattice. The second electron comes along later, moving in the opposite direction, and enjoys an attractive interaction to the lumbering ion concentration. Note that the time scale for the attractive interaction $V(q,t) < 0$ is up to $\pi/\omega_q \sim 10^{-13}s$. An electron moving at the Fermi velocity will move roughly several hundred nm in this time, which is on the order of the coherence length $\xi_0$. This retarded interaction, mediated by the ion lattice, is the key to avoiding the strong bare electron-electron repulsion.

### B. Consequences of the electron-phonon pairing interaction

Going back to the Cooper pairing calculation, we proposed that the $T_c$ of the superconductor is proportional to the binding energy of the Cooper pair:
$k_B T_c \sim 2\hbar\omega_c e^{-2/D(E_F)V}$.
We now see that Cooper's cutoff energy is in fact the phonon energy $\hbar\omega_q$. The phonon frequency in turn is bounded above by the ion plasma frequency, which scales as $\omega_q \sim \omega_{i,p} \sim \sqrt{1/M}$, where $M$ is the average ion mass. Hence there is an expectation that as the isotope ratio of a superconducting metal changes, one should have $T_c M^\alpha$ =constant, where the simplest expectation is that the "isotope effect exponent" $\alpha = 0.5$. Many experiments have been done to measure the "isotope effect" on $T_c$ in "conventional" elemental superconductors, and they are generally consistent with this dependence. This is considered one piece of "smoking gun evidence" in support of the electron-phonon pairing mechanism (we will see even more compelling evidence later). s-p-bonded metals such as Pb and Hg have $\alpha = 0.5$ to good approximation.

However, 4d and 5d transition metals generally show smaller values of $\alpha$, all the way down to zero. Those metals are thought to have strong Coulomb repulsion, which appears at frequency scales above the phonon frequency. Note that the phonon-mediated interaction $V(q,\omega)$ derived in the last lecture has a positive peak for $\omega > \omega_q$. A model that incorporates this effect successfully predicts a decrease in $\alpha$, as shown on the Supplementary Materials part of the class web site.

Finally, the absence of the superconductivity in Cu, Ag, and Au is presumably due to their small values of electron-phonon coupling. Once again 'good metals make bad superconductors.'

### C. Pairing Interaction in Cuprates

The cuprate pairing interaction is electronic in nature, involving only the electron system. Antiferromagnetic spin fluctuations lead to an entirely repulsive interaction. However when it is Fourier transformed into real space, there are attractive pieces at finite separation of the two electrons, leading to a finite angular momentum "d-wave" ($\ell = 2$ orbital angular momentum of the electrons in the Cooper pair) pairing state.

## II. THE SECOND QUANTIZATION DESCRIPTION

### A. Many Identical Fermion Wavefunctions

Let us suppose that the metal has $N$ electrons and $M >> N$ available single-particle states. Because the electrons in a metal are a gas of many identical Fermions with overlapping wavefunctions, we need to create a wavefunction (WF) for them 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 $QN = (\vec{k}, \sigma)$ which represent the momentum and spin of single-particle solutions to the Schrodinger equation for particles in a box.

The Schrodinger picture makes the mistake of labelling each (identical and indistinguishable) particle in the system $(1, 2, 3, ...i, ...j, ...N)$, and then tries to undo this mistake by creating fully anti-symmetrized wavefunctions using massive Slater determinants. These determinants are a nightmare when $N \sim 10^{23}$. It is best to avoid this approach altogether!

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 labeled by $i$, a list of quantum numbers. The occupation number has values of 0 or 1 for un-occupied and occupied states, respectively.

The wavefunction of a multiparticle system is just the list of occupation numbers of all the states in the system. We use a standard ordering of the states, going from lowest energy to highest energy:

$$|\psi\rangle = |n_1, n_2, n_3, ..., n_i, ...n_M\rangle$$

There are a total of $N$ particles distributed over $M$ states with $M \gg N$. Note that due to the Pauli Exclusion Principle there are only two possible values of the state occupation: $n_i = 0$ (no occupation) or $n_i = 1$ (single occupation). No other values are possible. In our case the states are labeled by $(\vec{k}, \sigma)$, where $\vec{k}$ are the quantized momenta of free electrons in a box, and $\sigma = \uparrow, \downarrow$ are the two spin states of a spin-1/2 particle.

Define operators that create or destroy occupation of specific single-particle states as follows.
$c^+_{\vec{k},\sigma}$ *Creates* an electron in a properly anti-symmetrized state described by the wavenumber $\vec{k}$ and spin $\sigma$, when that state is initially empty. It gives zero when the state is not initially empty.
$c_{\vec{k},\sigma}$ *Destroys* an electron in a properly anti-symmetrized state described by the wavenumber $\vec{k}$ and spin $\sigma$, when that state is initially occupied. It gives zero when the state is initially empty.

Note that these operators not only have the power to create or destroy specific electron occupations, they also have the power to make an entire wavefunction zero!

### B. 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.

### C. 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 the state labeled by $(k, \sigma)$. In other words it's eigenvalue is the occupation of the state $(k, \sigma)$.
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: $[c_{k,\sigma}, c^+_{k,\sigma}]_+ \equiv c_{k,\sigma} c^+_{k,\sigma} + c^+_{k,\sigma} c_{k,\sigma} = 1$.

### D. 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. By the way, you can consider the state $|\Psi\rangle$ as a vector in an $M$-dimensional vector space called "occupation space."

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 $a$, $b$, $c$, ...$N$.
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 (recall that state $i$ appears before state $j$ in the standard order of states). 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 (namely $[c_{k,\sigma}, c^+_{k,\sigma}]_+ = 1$) 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
$[c^+_{k,\sigma}, c^+_{k',\sigma'}]_+ = 0$ for all possible choices of $k$, $k'$, $\sigma$, and $\sigma'$.
These constitute the anti-commutation relations for the Fermionic creation and annihilation operators.

### E. 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 $s$:

$c_s \left|n_1, ...., n_s, ..., n_M\right\rangle = (-1)^{n_1+n_2+...n_{s-1}} \sqrt{n_s} \left|n_1, ...., n_s - 1, ..., n_M\right\rangle$,
and similarly; creating an excitation in state $s$:
$c_s^+ \left|n_1, ...., n_s, ..., n_M\right\rangle = (-1)^{n_1+n_2+...n_{s-1}} \sqrt{1 - n_s} \left|n_1, ...., n_s + 1, ..., n_M\right\rangle$.
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.