Lecture 10 Summary

PHYS798S Spring 2016

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The BCS Variational Calculation

0.1 Expectation values

We first evaluated the expectation value $\langle\Psi_{BCS}|\, H - \mu N_{op}\, |\Psi_{BCS}\rangle$ for the kinetic energy and the potential energy using the properties of the creation and annihilation operators. The result is
$\langle\Psi_{BCS}|\, H - \mu N_{op}\, |\Psi_{BCS}\rangle = 2\sum_k \xi_k \,|v_k|^2 + \sum_{k,l} V_{k,l} u_k v_k^* u_l^* v_l$.
The kinetic energy is the sum over all k-states of the single-particle energies times the probability that the Cooper pair at that momentum state is occupied, times 2 for the two electrons that make up the Cooper pair. The potential energy is constrained by matrix elements. Initially the Cooper pair at $(l, -l)$ must be occupied while that at $(k, -k)$ must be empty. In the final state the pair at $(k, -k)$ must be filled while that at $(l, -l)$ is left empty. This brings in the four factors of u's and v's.

0.2 The variational Calculation

The actual calculation is quite simple and elegant. Assume for now that the u's and v's are real. This is OK because it assumes for the moment that the macroscopic phase of the coherent state Cooper pair WF is fixed at zero. Given the constraint that $|u_k|^2 + |v_k|^2 = 1$, one has just a single parameter, namely the angle θ_k to keep track of, such that $u_k = \sin(\theta_k)$ and $v_k = \cos(\theta_k)$.
The terms in the expectation value can now be written using double angle formulas as $v_k^2 = \cos^2(\theta_k) = \frac{1}{2}(1 + \cos(2\theta_k))$, and $u_k v_k u_l v_l = \frac{1}{2}\sin(2\theta_k)\frac{1}{2}\sin(2\theta_l)$.
The expectation value is now
$\langle\Psi_{BCS}|\, H - \mu N_{op}\, |\Psi_{BCS}\rangle = \sum_k \xi_k(1 + \cos(2\theta_k)) + \frac{1}{4}\sum_{k,l} V_{k,l}\sin(2\theta_k)\sin(2\theta_l)$.
Taking the derivative with respect to $\theta_{k'}$ yields the following result,
$\tan(2\theta_k) = \frac{1}{2\xi_k}\sum_l V_{k,l}\sin(2\theta_l)$.

0.3 Definition of the Energy gap and Quasiparticle Energy

Make the following two definitions:
$\Delta_k \equiv -\sum_l V_{k,l} u_l v_l = -\frac{1}{2}\sum_l V_{k,l}\sin(2\theta_l)$, which defines the "energy gap" of the

superconductor. This will turn out to be the gap in the single-particle excitation spectrum out of the ground state. It can also serve informally as a rough "order parameter" of the superconducting state, although this is not a rigorous definition.
$E_k \equiv \sqrt{\Delta_k^2 + \xi_k^2}$ is the quasiparticle energy.
With these definitions, the variational equation can now be written as,
$\tan(2\theta_k) = -\frac{\Delta_k}{\xi_k}$.

With some further trigonometric gamesmanship, one can write the u's and v's in terms of these newly defined quantities:
$\sin(2\theta_k) = 2u_k v_k = +\frac{\Delta_k}{E_k}$
and, $\cos(2\theta_k) = v_k^2 - u_k^2 = -\frac{\xi_k}{E_k}$

0.4 Self-Consistent Gap Equation

Now use the above expression for the product of $u_k v_k$ back in the definition of the energy gap to obtain the celebrated self-consistent gap equation:
$\Delta_k = -\frac{1}{2}\sum_l \frac{\Delta_l}{\sqrt{\Delta_l^2+\xi_l^2}} V_{k,l}$. In general this can be challenging to solve, but we will consider two simple cases here.

First look at the trivial solution $\Delta_k = 0$ for all k. Going back to the u's and v's, this means that
$\sin(2\theta_k) = 2u_k v_k = 0$ for all k and,
$\cos(2\theta_k) = v_k^2 - u_k^2 = -\frac{\xi_k}{E_k} = \begin{cases} -1 & \xi_k > 0 \\ +1 & \xi_k < 0 \end{cases}$
This is a peculiar situation in which all Cooper states are occupied below $\xi = 0$ and all Cooper pair states are un-occupied above $\xi = 0$. In other words: $u_k = 1$ and $v_k = 0$ for $\xi_k > 0$, and $u_k = 0$ and $v_k = 1$ for $\xi_k < 0$. Roughly speaking this is like the state $|F\rangle$ that we introduced earlier, but it involves all electrons being bound in Cooper pairs with properly anti-symmetrized WFs inside the Fermi sphere, and all states outside un-occupied.
However, consider the potential energy term $\sum_{k,l} V_{k,l} u_k v_k u_l v_l$. This term is identically zero as it has zero contributions from all k because of the result that $2u_k v_k = 0$. Hence this "normal state" does not take advantage of the pairing interaction and is not a superconductor! Next we will find a non-trivial solution to the self-consistent gap equation.