Lecture 12 Summary

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Finite Temperature BCS

0.1 Meanwhile, Back at the Hamiltonian

Last time, we found that with the substitution of the transformed operators, the model Hamiltonian becomes,
$H_M - \mu N_{op} = \sum_k$ (nice terms involving diagonal operators) + (undesired cross terms)$\left(2\xi_k u_k v_k + \Delta_k^* v_k^2 - \Delta_k u_k^2\right)$.
We can eliminate all of the ugly terms in the transformed Hamiltonian by making a second constraint on the u's and v's, namely to make the bracket term in the model Hamiltonian equal to zero. That leads to a quadratic equation for the quantity $\Delta_k^* v_k/u_k$ whose solution yields $\Delta_k^* v_k/u_k = E_k - \xi_k$, which is real. Here again we have $E_k = \sqrt{\Delta_k^2 + \xi^2}$. If we take the convention that u_k is real (as in the previous calculation), then it must be that v_k and Δ have the same phase. This phase factor is the same for all k and endows the energy gap with the macroscopic quantum phase factor in the superconducting state.
With the two constraints on the u's and v's, we can now solve for them in terms of known quantities, and the result is
$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k - \mu}{\sqrt{\Delta^2 + (\epsilon_k - \mu)^2}}\right]$, and
$u_k^2 = 1 - v_k^2 = \frac{1}{2}\left[1 + \frac{\epsilon_k - \mu}{\sqrt{\Delta^2 + (\epsilon_k - \mu)^2}}\right]$,
exactly as before in the variational calculation!

The resulting diagonalized Hamiltonian is,
$H_M - \mu N_{op} = \sum_k (\xi_k - E_k + \Delta_k b_k^*) + \sum_k E_k \left(\gamma_{k0}^+ \gamma_{k0} + \gamma_{k1}^+ \gamma_{k1}\right)$.
The first sum reproduces the ground state BCS energy. The second sum represents excitations out of the ground state. It counts excitations of energy E_k through the $\gamma^+\gamma$ number operators.
These excitations are gapped by Δ, and as such are very rarely created at low temperatures when $k_B T << \Delta$. Note that there is a gap in the energy spectrum of these excitations, but no gap in the momentum. The excitations are called Bogoliubons or quasi-particles.

0.2 Finite-Temperature Self-Consistent Gap Equation

Now enforce the self-consistency condition on the b_k operators through the energy gap, $\Delta_k \equiv -\sum_l V_{k,l} b_l$ with $b_k = \langle c_{-k,\downarrow} c_{k,\uparrow} \rangle$. Expressing the c-operators in terms of the γ operators eventually yields,
$\Delta_k = -\sum_l V_{k,l} u_l^* v_l \left\langle 1 - \gamma_{l0}^+ \gamma_{l0} - \gamma_{l1}^+ \gamma_{l1} \right\rangle$.
By inspection it seems clear that the $\gamma^+ \gamma$ number operators now serve to decrease the right-hand side of the equation, resulting in a diminished energy gap as more and more excitations are created out of the BCS ground state.

We can set up a finite-temperature version of the self-consistent gap equation as follows. First, propose that the excitations are created at finite temperature by an amount dictated by Fermi-Dirac statistics since we know that the γ operators are Fermionic in nature. Namely the number operator expectation values are replace by the Fermi function for the quasiparticle excitation at energy E_l: $f(E_l) = \frac{1}{e^{\beta E_l}+1}$ with $\beta = 1/k_B T$. This results in a factor of $1 - 2f(E_l) = \tanh(\beta E_l/2)$.
The $u_l^* v_l$ factor can be written as $\frac{\Delta_l}{2E_l}$. The resulting finite-temperature self-consistent gap equation is,
$\Delta_k = -\sum_l V_{k,l} \frac{\Delta_l}{2E_l} \tanh(\beta E_l/2)$.

To proceed, once again put in the Cooper pairing potential as,
$V_{k,l} = \begin{cases} -V & |\xi_k|, |\xi_l| \leqslant \hbar\omega_c \\ 0 & |\xi_k|, |\xi_l| > \hbar\omega_c \end{cases}$
with V a positive number. Again it leads to an isotropic gap, which can be canceled in the numerator, yielding

$1/V = +\frac{1}{2} \sum_l^{Restricted} \frac{\tanh(\beta E_l/2)}{E_l}$

Converting from a sum on l to an integral on energy brings in the density of states $D(E)$ and allows us to write:
$\frac{1}{D(E_F)V} = \int_0^{\hbar\omega_c} \frac{\tanh\left[\frac{\sqrt{\xi^2+\Delta(T)^2}}{2k_B T}\right]}{\sqrt{\xi^2+\Delta(T)^2}} d\xi$

At zero temperature the argument of the tanh is infinity, yielding 1 in the numerator, and the zero-temperature gap result is recovered:
$\Delta(T=0) = \frac{\hbar\omega_c}{\sinh(1/D(E_F)V)}$.

Now examine the limit as $T \to T_c$. We expect the gap to decrease continuously to zero, it's value in the normal state. However, a large fraction of the electrons in the metal will be quasi-particles, and their interactions are not included in the Hamiltonian. Nevertheless we proceed. At T_c we expect,
$\frac{1}{D(E_F)V} = \int_0^{\hbar\omega_c} \frac{\tanh\left[\frac{\xi}{2k_B T_c}\right]}{\xi} d\xi$ This integral can be done with some effort and yields an expression for T_c,
$k_B T_c \approx 1.13 \hbar\omega_c e^{-1/D(E_F)V}$, a result similar to that for the zero-temperature

gap. In fact BCS predicts that in the weak coupling limit ($D(E_F)V << 1$) there is a universal result for the "reduced gap",
$\Delta(0)/k_BT_c = 2/1.13 = 1.76$. Data on elemental superconductors show values in this ballpark, or higher.
By the way, the result that $T_c \sim \omega_c$ motivated the study of the "isotope effect" on T_c discussed earlier in the course (i.e. T_cM^α = constant, with $\alpha = 0.5$, where M is the average ionic mass in the metal).

0.3 Temperature Dependent Gap

Numerical solution of the finite-temperature self-consistent gap equation for $\Delta(T)$ is in very good agreement with data obtained by tunneling spectroscopy on weak coupled elemental superconductors, as shown in the Supplementary Material on the class web site.
The gap has two interesting asymptotic temperature dependences:

0.3.1 Low Temperatures

For $T < T_c/3$ one has $\Delta(T) = \Delta(0)\left(1 - e^{-\Delta(0)/k_BT}\right)$. In other words the gap remains very close to it's zero temperature value, dropping only slightly by an activated amount.

0.3.2 Near T_c

For $T \to T_c$ one has $\Delta(T) \approx 1.74\Delta(0)\left(1 - \frac{T}{T_c}\right)^{1/2}$. The superconducting gap goes to zero continuously at T_c, characteristic of a second-order phase transition. This exponent of 1/2 is typical of 'mean field' critical behavior for the order parameter in 3D, and is the same as the mean-field treatment of the ferromagnetic-paramagnetic phase transition. Note that the slope of $\Delta(T)$ is infinite at T_c.

0.4 Thermodynamic Quantities

This simple model Hamiltonian also allows study of the finite-temperature thermodynamic properties of an ideal BCS superconductor. One can calculate the electronic entropy, heat capacity, and free energy vs. temperature. We ignore the lattice contributions.

The BCS ground state is a 'superfluid' in the sense that it cannot carry entropy. The electronic entropy comes from the quasiparticles excited out of the ground state. The electronic entropy for any Fermi gas is given by,
$S_e = -2k_B \sum_k [(1 - f(E_k))\ln(1 - f(E_k)) + f(E_k)\ln(f(E_k))]$.
For a normal metal this becomes,

$S_{en} = \gamma T$, where $\gamma \equiv \frac{2}{3}\pi^2 D(E_F) k_B^2$, and the entropy is just linear in temperature. For a superconductor the situation changes because of the gap in the excitation spectrum, leading to fewer quasiparticle excitations and lower entropy than the normal state at all temperatures below T_c. In fact the electronic entropy is exponentially small for $T < T_c/3$.

The electronic heat capacity is given by $C_e = T\frac{dS_e}{dT}$. Once again this is a linear function of temperature for a normal metal, $C_{en} = \gamma T$. For a superconductor the electronic heat capacity is exponentially small at low temperatures $T < T_c/3$, and enhanced above the normal state value just below T_c. The superconducting electronic specific heat can be written as,
$C_{es} = 2\beta k_B \sum_k -\frac{\partial f(E_k)}{\partial E_k}\left[E_k^2 + \frac{1}{2}\beta\frac{d\Delta^2}{d\beta}\right]$.
The first term in square brackets is common to all Fermi gases. The second term is unique to superconductors and arises from the re-arrangement of states associated with the temperature-dependent gap. At T_c this term gives rise to a discontinuous jump in electronic heat capacity because the singular slope of $\Delta(T)$ there. BCS theory predicts a 'universal specific heat jump' at T_c in the weak-coupling approximation, given by,
$\frac{\Delta C}{C_{en}} = D(E_F)\left(-\frac{d\Delta^2}{dT}\right)/C_{en}$
Using the weak-coupling expression for the gap near T_c, and the universal reduced gap value, one finds,
$\frac{\Delta C}{C_{en}} = 1.43$.
This is found to be in very good agreement with measured results (see the Lecture 1 viewgraphs) on weak-coupled elemental BCS superconductors.

Measurement of the universal specific heat jump is considered a hallmark of "bulk" superconductivity. In higher-T_c superconductors it becomes a challenge to measure $\Delta C/C_{en}$ because of very large lattice contributions (which must be removed to compare to BCS predictions) and the difficulty in determining the normal state electronic heat capacity (because the critical fields are often beyond our ability to generate).

The free energy of the superconductor is lower than that of the normal metal state as shown on the class web site Supplemental Material. This difference in free energy is known as the 'condensation energy.'