PHYS 798C Spring 2024 Lecture 12 Summary

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I. PERTURBATIONS TO BCS

We now consider what happens when a superconductor is probed by some means. These probes will be treated as perturbations to the basic pairing Hamiltonian. Our objective is to calculate how the BCS superconductor responds to perturbations. We shall see that this introduces the Case-I and Case-II Coherence Effects, depending on the symmetry of the perturbation, and the response gives rise to clear experimental signatures arising from the quantum mechanical properties of the BCS superconducting state.

A. BCS Density of States

When the energy gap opens up, it pushes states away from the chemical potential, resulting in a singular density of states at the gap edge.

The density of states (DOS) is the rate at which new states are added as the energy increases. For the normal state this is $D_N(\xi) = \frac{dN}{d\xi}$, while for the superconducting state it is $D_S(E) = \frac{dN}{dE_s}$. Taking the ratio yields,

ratio yields, $\frac{D_S(E)}{D_N(E)} = \frac{d\xi}{dE_s}.$ Writing $\xi = \sqrt{E_s^2 - \Delta^2}$ yields, $\frac{D_S(E)}{D_N(E)} = \begin{cases} 0 & E < \Delta \\ \frac{E}{\sqrt{E^2 - \Delta^2}} & E > \Delta \end{cases}$ The singularity at the gap ec

The singularity at the gap edge $E = \Delta$ has important consequences for the physical properties of superconductors, including the 'coherence effects' that we will encounter today.

B. Some Properties of the γ Operators

The γ operators introduced as part of the Bogoliubov-Valatin transformation were written as, $\gamma_{k0}^+ = u_k^* c_{k,\uparrow}^+ - v_k^* c_{-k,\downarrow}$ and, $\gamma_{k1}^+ = u_k^* c_{-k,\downarrow}^+ + v_k^* c_{k,\uparrow}$.

Now look at the effect of γ_{k0} on the BCS ground state. It yields, $\gamma_{k0} |\Psi_{BCS}\rangle = 0$, showing that $|\Psi_{BCS}\rangle$ is the vacuum state for the excitations created by the γ operators.

Acting with $\gamma_{k0}^+ |\Psi_{BCS}\rangle$ creates a quasiparticle with momentum k and spin up with probability 1. It also guarantees that the state -k and spin down is *un-occupied* with probability 1, hence that Cooper pairing state is *excluded* from the wavefunction.

$$\begin{split} \gamma_{k0}^{+} |\Psi_{BCS}\rangle &= \left(u_{k}^{2} + v_{k}^{2}\right)c_{k,\uparrow}^{+} \prod_{l \neq k} \left(u_{l} + v_{l}c_{l,\uparrow}^{+}c_{-l,\downarrow}^{+}\right)|0\rangle \\ &= c_{k,\uparrow}^{+} \prod_{l \neq k} \left(u_{l} + v_{l}c_{l,\uparrow}^{+}c_{-l,\downarrow}^{+}\right)|0\rangle. \end{split}$$

Note that the quasiparticle excitation partly handicaps the BCS wavefunction that describes the remaining superconducting electrons. The γ^+ operators do not conserve particle number. We found that the change in particle number upon acting with γ^+ is $u_k^2 - v_k^2$ which varies from a value of -1 (hole-like) for k-vectors deep inside the Fermi surface to a value of +1 (particle-like) outside the Fermi surface. In general, the excitation created is a coherent superposition of hole and particle.

C. The Perturbing Hamiltonian

We want to now consider how a homogeneous superconductor responds to various kinds of perturbations. This will lead to predictions that test the BCS theory in great detail. The general perturbation will have the form,

 $H_{pert} = \sum_{k\sigma, k'\sigma'} B_{k'\sigma', k\sigma} c^+_{k'\sigma'} c_{k,\sigma}.$

This Hamiltonian scatters an electron from state k, σ to state $k'\sigma'$ with amplitude $B_{k'\sigma',k\sigma}$.

Thinking ahead, we will be calculating a transition rate using Fermi's Golden rule as $R \propto | < \sum_{k\sigma,k'\sigma'} B_{k'\sigma',k\sigma} > |^2 D(E_{final})$. In the normal state the wavefunction is incoherent and one can just sum the squares of the *B*'s. In the superconducting state, the wavefunction is a coherent state of Cooper pairs, and one has to add the *B*'s together carefully, before squaring. This leads to what are known as 'coherence effects' in transition and absorption rates.

Example perturbations include **attenuation of longitudinal ultrasound** (ultrasonic attenuation): $H_{pert}^{ua} = \lambda q u_0 e^{i(qx-\omega t)} \sum_{k\sigma,k'\sigma'} c_{k\sigma}^+ c_{k',\sigma'}^+$, where λ is the deformation potential, the longitudinal sound wave is represented by displacement

where λ is the deformation potential, the longitudinal sound wave is represented by displacement $u_0 e^{i(qx-\omega t)}$, and the electron-acoustic wave coupling is proportional to $\nabla u \sim q$. The coupling is provided by electromagnetic fields created by the moving ions, as well as shifted electronic levels created by the deformed ion lattice. Since the electrons are paired by means of phonon 'glue', it is not surprising that perturbations to the lattice vibrations will have a measurable effect on the superconductor.

Nuclear spin relaxation is a contact interaction between the nuclear spins and electron gas, $H_{vert}^{nuc} \sim \vec{I} \cdot \vec{\sigma} \delta(\vec{r} - \vec{r_N})$,

where \vec{I} is the nuclear spin, $\vec{\sigma}$ is the electron spin, and $\vec{r_N}$ is the location of the nucleus. This is very similar to the perturbation giving rise to hyperfine splitting in the Hydrogen atom, which is responsible for the famous 21-cm radiation.

The electromagnetic interaction has a perturbing Hamiltonian of the form,

 $H_{pert}^{em} \sim \frac{e}{2m} \left(\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p} \right),$

where \vec{A} (assumed weak so that we can ignore the $\vec{A} \cdot \vec{A}$ term) is the vector potential of the electromagnetic wave.

D. Time-reversed States

Note that we will eventually evaluate the scattering rate, or absorption rate α , caused by a perturbation. This will involve summing over matrix elements of the form, $\alpha \sim \sum_{k_f,\sigma_f} \sum_{k_i,\sigma_i} \hbar \omega \frac{2\pi}{\hbar} |\langle k_f,\sigma_f| H_{pert} |k_i,\sigma_i \rangle|^2$. The grouping of terms in this sum can be important in the superconducting state. Time-reversed electronic states add coherently in the sums on k and σ in the absorption calculation. (P. W. Anderson showed that pairing of time-reversed states is a more general version of the Cooper pairing that we have considered up to this point. See the paper P. W. Anderson, J. Phys. Chem Solids <u>11</u>, 26 (1959) posted on the class web site)

For example, terms of the form $c_{k',\uparrow}^+ c_{k,\uparrow}$ and $c_{-k,\downarrow}^+ c_{-k',\downarrow}$ connect time-reversed quasiparticle states that are involved in two different Cooper pairs. Note that both terms refer to the same momentum transfer $\Delta k = k' - k$ and same spin change $\Delta \sigma = \sigma' - \sigma$ for the quasiparticles. Note that reversing the direction of time changes k to -k and \uparrow to \downarrow . (Check out the table labeled "Effect of time reversal on some variables of classical physics" at http://en.wikipedia.org/wiki/T-symmetry).

Writing out the products of the coherent pairs of c-operators in terms of the γ operators yields, $c_{k',\uparrow}^+c_{k,\uparrow} = u_{k'}u_k^*\gamma_{k'0}^*\gamma_{k0} - v_{k'}^*v_k\gamma_{k1}^*\gamma_{k'1} + u_{k'}v_k\gamma_{k'0}^*\gamma_{k1}^* + v_{k'}^*u_k^*\gamma_{k'1}\gamma_{k0}$, and $c_{-k,\downarrow}^+c_{-k',\downarrow} = -v_kv_{k'}\gamma_{k'0}^*\gamma_{k0} + u_ku_{k'}^*\gamma_{k1}^*\gamma_{k'1} + u_kv_{k'}\gamma_{k'0}^*\gamma_{k1}^* + v_k^*u_{k'}^*\gamma_{k'1}\gamma_{k0}$. Note that each of the four terms has the same γ operators for both products of c-operators, they differ only in the prefactors. Such terms must be added first before squaring to calculate a transition rate.

The scattering amplitude connecting these time-reversed states will either be even or odd, $B_{k'\sigma',k\sigma} = \pm B_{-k-\sigma,-k'-\sigma'}$

Note that both terms refer to the same momentum transfer $\Delta k = k' - k$ and same spin change $\Delta \sigma = \sigma' - \sigma$ for the quasiparticles. It is simply a question of whether or not the perturbing Hamiltonian is even under time-reversal (+) or odd (-).

 $B_{k'\sigma',k\sigma} \left\{ \left(u_{k'}u_k \mp v_{k'}v_k \right) \left(\gamma_{k'\sigma'}^* \gamma_{k\sigma} \pm \Theta_{\sigma\sigma'} \gamma_{-k-\sigma}^* \gamma_{-k'-\sigma'} \right) + \left(v_k u_{k'} \pm u_k v_{k'} \right) \left(\gamma_{k'\sigma'}^* \gamma_{-k-\sigma}^* \pm \Theta_{\sigma\sigma'} \gamma_{-k'-\sigma'} \gamma_{k\sigma} \right) \right\}$ where the Θ function accounts for spin-flip perturbations, $\left(+1 \quad \sigma = \sigma' \right)$

 $\Theta_{\sigma\sigma'} = \begin{cases} +1 & \sigma = \sigma' \\ -1 & \sigma = -\sigma' \end{cases}, \text{ where the second case is for a spin-flip.}$

Note that the signs \pm and \mp refer to perturbations that are either even (top) or odd (bottom) under time-reversal. Finally note that Tinkham has modified the notation on the γ operators. In this case $\gamma_{k\sigma} = \gamma_{k0}$ for $\sigma = \uparrow$ and $\gamma_{k\sigma} = \gamma_{-k1}$ for $\sigma = \downarrow$. This allows the expression to be written in a way that is 'spin agnostic' and a bit more compact.

The first two products of γ operators correspond to quasiparticle scattering, and the prefactor is called the scattering coherence factor,

 $CF_S = (u_{k'}u_k \mp v_{k'}v_k).$

The second set of γ operators correspond to quasiparticle pair creation and annihilation. These are multiplied by the pair creation coherence factor,

 $CF_{PC} = (v_k u_{k'} \pm u_k v_{k'}).$

Note that the signs flip for quasiparticle scattering vs. quasiparticle creation and annihilation.

E. Absorption Rate

The transition rate associated with the perturbation is given by Fermi's golden rule for Fermionic particles (recall $f(E) = \frac{1}{e^{\beta E} + 1}$, with $\beta = 1/k_B T$):

 $W_{i \to f} = \frac{2\pi}{\hbar} \left| \langle k_f, \sigma_f | H_{pert} | k_i, \sigma_i \rangle \right|^2 \left\{ f(E_i)(1 - f(E_f)) - f(E_f)(1 - f(E_i)) \right\} \delta(E_f - E_i - \hbar \omega).$ Here we are writing $E' = E + \hbar \omega$, and treating the energy change as coming in a unit with energy $\hbar \omega$.

The absorption rate is the sum over all initial and final states of the energy absorbed by the transitions; $\alpha = \frac{1}{(2\pi)^6} \sum_{k_f, \sigma_f} \sum_{k_i, \sigma_i} \hbar \omega W_{i \to f}.$

Converting to an integral on energy brings in the density of states (and it's singularities!),

$$\alpha(\omega) = \int |\langle H_{pert} \rangle|^2 \times \text{Coherence Factors} \times D_s(E) D_s(E + \hbar\omega) \left[f(E) - f(E + \hbar\omega) \right] dE.$$

After some algebra, the coherence factors essentially reduce to Scattering: $(u_{k'}u_k \mp v_{k'}v_k)^2 = \frac{1}{2}\left(1 \mp \frac{\Delta^2}{EE'}\right)$, where $E' = E + \hbar\omega$, and Creation: $(v_k u_{k'} \pm u_k v_{k'})^2 = \frac{1}{2}\left(1 \pm \frac{\Delta^2}{EE'}\right)$. Once again notice the difference in signs.

The coherence factors have the biggest influence when $E \sim E' \sim \Delta$, in which case the factors are either 0 or 1. Also note that the density of states terms in the $\alpha(\omega)$ integral are largest near the gap edge (i.e. the same range of E). Hence the "coherence effects" on absorption rates are quite strong, as we shall see below.

First consider the quasiparticle scattering term. The bare absorption rate has matrix elements that are the same in the normal and superconducting states. Hence it is simpler to compare absorption as a ratio,

$$\frac{\alpha_s}{\alpha_n} = \frac{1}{\hbar\omega} \int_{-\infty}^{+\infty} \frac{\left| E(E+\hbar\omega)\mp\Delta^2 \right| (f(E) - f(E+\hbar\omega))}{\sqrt{E^2 - \Delta^2} \sqrt{(E+\hbar\omega)^2 - \Delta^2}} dE$$

where the single-particle matrix elements cancel out in the ratio. Note that the energy integral excludes the ranges $|E|, |E + \hbar\omega| < \Delta$ where the density of states is zero.

It is pretty clear from the integrand that in the Type-I coherence case (upper sign, perturbation even under time reversal), there is a near-zero when $E \sim \Delta$ in the integral. This coincides with the smallest magnitude of the denominator, significantly reducing the value of the integral. Hence absorption in the type-I case is strongly suppressed in the superconducting state. In the type-II coherence case (lower sign, perturbation odd under time-reversal), the numerator is doubled at the point where the integral picks up it's largest contribution, giving rise to a strong enhancement of the absorption.

F. Ultrasonic Attenuation

The ultrasound waves create a time-reversal invariant (type I) perturbation. The ultrasound waves are in the MHz range, whereas Δ/h is in the THz range. Hence we have $\hbar\omega \ll \Delta$ and the energy factors in the α_s/α_n integral cancel to good approximation, leaving, $\frac{\alpha_s}{\alpha_n} \approx 2f(\Delta) = \frac{2}{1+e^{\Delta(T)/k_BT}}$, a remarkably simple result! Hence the ultrasonic attenuation measures the opening of the superconducting gap at T_c , amplified by being in an exponent.

It turns out that the ultrasonic attenuation becomes a very good way to measure the temperature dependence and anisotropy of the gap!

The ultrasonic attenuation rate $\frac{\alpha_s}{\alpha_n}$ drops dramatically at T_c . (See the data on the class web site.) In fact the rapid drop occurs with nearly infinite slope as the gap opens up. This is a classic example of type-I coherence effects.

The other two perturbations are type-II and involve operators that are odd under time-reversal. They both show a (rather counter-intuitive) strong enhancement of $\frac{\alpha_s}{\alpha_n}$ just below T_c , with exponential suppression at low temperatures.

G. Nuclear Spin Relaxation

The peak in nuclear spin relaxation rate as a function of temperature below T_c was an un-expected prediction of BCS that was confirmed by Hebel and Slichter in Aluminum.

H. Electromagnetic Absorption

Type-II coherence effects cause an increase in electromagnetic absorption (σ_1) below T_c , again an un-expected result. This "coherence peak" in $\sigma_1(T)$ is seen in BCS s-wave superconductors.

The absence of the Hebel-Slichter peak and a "coherence peak" in $\sigma_1(T)$ in the cuprates was an early sign that something different was going on there. In fact, the d-wave gap (with excited states extending all the way down to the Fermi energy), the strongly anisotropic nature of the gap $\Delta_{\vec{k}}$, and the presence of strong spin fluctuations (which serve to de-polarize the nuclear spins and are probably responsible for the pairing interaction between the electrons), alter the coherence factor calculation significantly.

Now consider the pair creation and annihilation coherence factor. Note that the signs flip for cases I and II. Hence type-I pair creation effects are stronger than the type-II kind. In type-II electromagnetic absorption vs. frequency for $\hbar\omega \sim 2\Delta$, the absorption rate simply climbs from zero as the gap edge is exceeded, very different from the coherence peak seen in quasiparticle scattering.