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5 Superconductivity I: BCS Theory

5.1 Cooper Problem

A great deal was known about the phenomenology of superconductivity in the 1950's, and it was already suspected that the electron phonon interaction was responsible, but the microscopic form of the wave function was unknown. A clue was provided by Leon Cooper, who showed that the noninteracting Fermi sea is *unstable* towards the addition of a single pair of electrons with attractive interactions. Cooper began by examining the wave function of this pair $\psi(r_1, r_2)$, which can always be written as a sum over plane waves

$$\psi(r_1, r_2) = \sum_{kq} u_k(q) e^{ik\cdot r_1} e^{-i(k+q)\cdot r_2} \zeta \tag{1}$$

where the $u_k(q)$ are expansion coefficients and ζ is the spin part of the wave function, either the singlet $|\uparrow\downarrow - \downarrow\uparrow> /\sqrt{2}$ or one of the triplet, $|\uparrow\uparrow>, |\downarrow\downarrow>, |\uparrow\downarrow + \downarrow\uparrow> /\sqrt{2}$. In fact since we will demand that ψ is the ground state of the two-electron system, we will assume the wave function is realized with zero center of mass momentum of the two electrons, $u_k(q) = u_k \delta_{q,0}$. Then $\psi(r_1, r_2)$ becomes $\Sigma_k u_k e^{ik\cdot(r_1 - r_2)}$. Note that if u_k is *even* in k, the wave function has only terms $\propto \cos k \cdot (r_1 - r_2)$, whereas if it is *odd*, only the $\sin k \cdot (r_1 - r_2)$ will contribute. This is an important distinction, because only in the former case is there an amplitude for the two electrons to live "on top of each other" at the origin. Note further that in order to preserve the proper overall antisymmetry of the wave function, u_k even (odd) in k implies the wave function must be spin singlet (triplet). Let us assume further that there is a general two-body interaction between the two electrons (the rest of the Fermi sea is noninteracting in the model!) $V(r_1, r_2)$, so that the Hamiltonian for the system is

$$H = -\frac{\nabla_1^2}{2m} - \frac{\nabla_2^2}{2m} + V(r_1, r_2). \tag{2}$$

Inserting the assumed form of ψ into the Schrödinger equation $H\psi = E\psi$, and Fourier transforming both sides with respect to the relative coordinate, $r = r_1 - r_2$, we find

$$(E - 2\epsilon_k)u_k = \sum_{k>k_F} V_{kk'}u_{k'}, \tag{3}$$

where $\epsilon_k = k^2/2m$ and the $V_{kk'} = \int d^3r V(r) e^{i(k'-k)\cdot r}$ are the matrix elements of the two-body interaction.

Recall k, k' correspond to energies at the Fermi level ϵ_F in the absence of V. The question was posed by Cooper, is it possible to find an eigenvalue $E < 2\epsilon_F$, i.e. a *bound state* of the two electrons? To simplify the problem, Cooper assumed a model form for $V_{kk'}$ in which $V_{kk'} = -V$ for ξ_k and $\xi_{k'} < \omega_c$, where $\xi_k \equiv \epsilon_k - \epsilon_F$, and $V_{kk'} = 0$ otherwise. The bound state equation becomes

$$u_k = \frac{V \sum'_{k'} u_{k'}}{2\epsilon_k - E}, \tag{4}$$

where the prime on the summation in this context means sum only over k such that $\epsilon_f < \epsilon_k < \epsilon_F + \omega_c$. Now u_k may be eliminated from the equation by summing both sides $\sum_k$, yielding

$$\frac{1}{V} = \sum_k{}' \frac{1}{2\epsilon_k - E} \tag{5}$$

$$\simeq \frac{1}{2} N_0 \int_{\epsilon_F}^{\epsilon_F+\omega_c} d\epsilon \frac{1}{2\epsilon - E} = \frac{1}{2} N_0 \log \frac{2\epsilon_F + 2\omega_c - E}{2\epsilon_F - E}. \tag{6}$$

For a weak interaction $N_0 V \ll 1$, we expect a solution (if at all) just below the Fermi level, so we treat $2\epsilon_F - E$ as a small positive quantity, e.g. negligible compared to $2\omega_c$. We then arrive at the pair binding energy

$$\Delta_{\text{Cooper}} \equiv 2\epsilon_F - E \simeq 2\omega_c e^{-2/N_0 V}. \tag{7}$$

There are several remarks to be made about this result. 1) Note (for your own information–Cooper didn't know this at the time!) that the dependence of the bound state energy on both the interaction V and the cutoff frequency ω_c strongly resembles the famous BCS transition temperature dependence, with ω_c identified as the phonon frequency ω_D, as given in equation (I.1). 2) the dependence on V is that of an essential singularity, i.e. a nonanalytic function of the parameter. Thus we may expect never to arrive at this result at any order in perturbation theory, an unexpected problem which hindered theoretical progress for a long time. 3) The solution found has isotropic or s-symmetry, since it doesn't depend on the $\hat{k}$ on the Fermi surface. [How would an angular dependence arise? Look back over the calculation.] 4) Note the integrand $(2\epsilon_k - E)^{-1} = (2\xi_k + \Delta_{\text{Cooper}})^{-1}$ peaks at the Fermi level with energy spread Δ_{Cooper} of states involved in the pairing. The weak-coupling ($N_0 V \ll 1$) solution therefore provides a bit of *a posteriori* justification for its own existence, since the fact that $\Delta_{Cooper} \ll \omega_c$ implies that the dependence of $V_{kk'}$ on energies out near the cutoff and beyond is in fact not terribly important, so the cutoff procedure used was ok. 5) The spread in momentum is therefore roughly $\Delta_{\text{Cooper}}/v_F$, and the characteristic size of the pair (using Heisenberg's uncertainty relation) about v_F/T_c. This is about 100-1000A in metals, so since there is of order 1 electron/ unit cell in a metal, and if this toy calculation has anything to do with superconductivity, there are certainly many electron pairs overlapping each other in real space in a superconductor.

5.2 Instability of Fermi Sea to Superconductivity

5.2.1 Ferromagnetic Analog.

Obviously one thing is missing from Cooper's picture: if it is energetically favorable for two electrons in the presence of a noninteracting Fermi sea to *pair*, i.e. to form a bound state, why not have the other electrons pair too, and lower the energy of the system still further? This is an *instability* of the normal state, just like magnetism or charge density wave formation, where a ground state of completely different character (and symmetry) than the Fermi liquid is stabilized. The Cooper calculation is a T=0 problem, but we expect that as one lowers the temperature, it will become at some critical temperature T_c energetically favorable for *all* the electrons to pair. Although this picture is appealing, many things about it are unclear: does the pairing of many other electrons alter the attractive interaction which led to the pairing in the first place? Does the bound state energy per pair change? Do all of the electrons in the Fermi sea participate? And most importantly, how does the critical temperature actually depend on the parameters and can we calculate it?

This instability must show up in some quantity we can calculate. Let's use as an example a more familiar system, the ferromagnet. As we saw in the last section, in a ferromagnet the susceptibility diverges at the transition, i.e. the magnetization produced by the application of an infinitesimal external field is suddenly finite.

5.2.2 Pair response function and superconducting T_c.

To investigate the possibility of a superconducting instability of the normal metal, we should do the same thing we did in the case of the itinerant ferromagnet (section 4.6), i.e. consider the appropriate response function, approximated in some simple RPA-type scheme including multiple phonon scattering processes, and look for a divergence. What is the appropriate "susceptibility"? Cooper suggested that the system should have a finite response to the addition of a single zero–momentum pair (infinitesimal perturbation) to the system at or below the transition temperature. So let's add to the electron-phonon Hamiltonian a term which introduces a Cooper pair coupled to a fictitious "external field" h_{pair}:

$$H_{pair} = h_{pair} \sum_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + h.c. \tag{8}$$

The pair, once created, should be allowed to scatter many times before being removed. Once again we will examine the simplest RPA-like approximation to the susceptibility, as illustrated in Fig 2.[1] An arbitrary

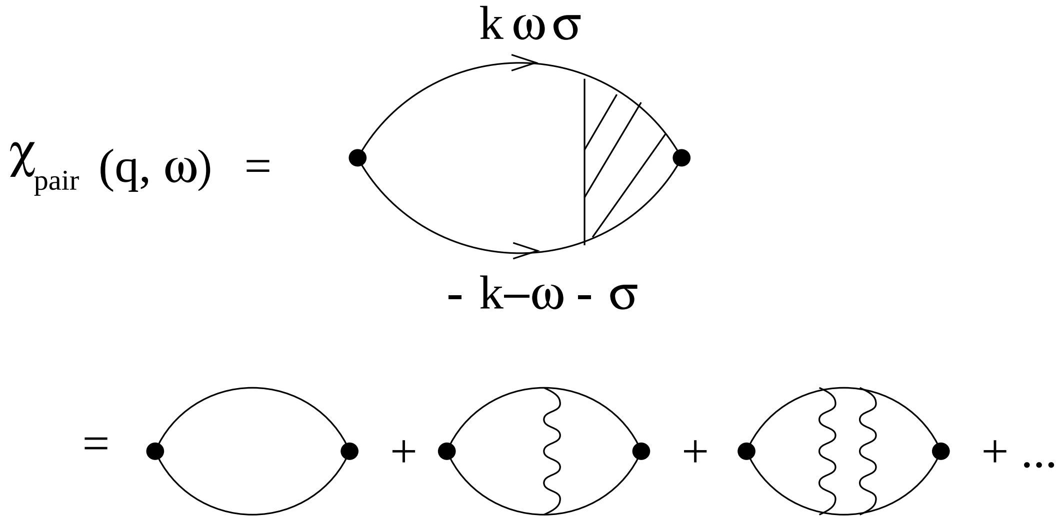


Figure 1: t-matrix (RPA) approximation for pair susceptibility. Note the direction of the arrows!

diagram of nth order contains the element

$$T\sum_{\omega_n'}\sum_{k'}|\bar{g}_{kk'}|^2 D^0(k-k',\omega_n-\omega_n')G^0(k',\omega')G^0(-k',-\omega') \qquad (9)$$

n times, so

$$\begin{aligned}\chi_{\rm pair} &= T\sum_{\omega_n}\sum_{k} G^0(k,\omega)G^0(-k,-\omega)\times \\ &\times\{\frac{1}{1-T\sum_{\omega_n'}\sum_{k'}|g_{kk'}|^2 D^0(k-k',\omega_n-\omega_n')G^0(k',\omega')G^0(-k',-\omega')}\} \qquad (10)\end{aligned}$$

We many now search for an instability by asking whether the denominator may vanish. Let's first simplify the problem by examining the "effective interaction"

$$V(\omega_n,\omega_n')\equiv|\bar{g}_{kk'}|^2 D^0(k-k',\omega_n-\omega_n'). \qquad (11)$$

Although $V(\omega_n,\omega_n')$ as defined is clearly also a function of momentum, this dependence can be neglected. The idea is that the new renormalized coupling constant $|\bar{g}(q)|^2\sim q$ for small q, so the important contributions

[1]Note instead of the "ring"-type diagrams of Fig. 1b), this sum consists of "ladder"-type diagrams with vertical "rungs". This might suggest a fundamental difference between the two types of series, but note a similar "ladder" series is generated in the ferromagnetic case if we calculate the *transverse* susceptibility $\langle[S_+,S_-]\rangle$, which manifests the same instability. In fact $\chi_{zz}=\chi_{+-}$ in a spin-rotationally invariant system.

to the k' sum in Eq. (10) are at large q (short wavelengths), where the dispersion relation flattens. We may thus replace the phonon frequencies by a characteristic zone boundary frequency, i.e. ω_D. Note further that the Debye frequency serves as an effective *cutoff* for the integral, since the contribution of D^0 will be negligible if $\omega - \omega' \gg \omega_D$. We therefore make the replacement

$$V(\omega_n, \omega_n') \simeq \begin{cases} V & |\omega_n|, |\omega_n'| < \omega_D \\ & 0 \text{ otherwise} \end{cases}. \tag{12}$$

[Q: why don't large frequencies $|\omega| \simeq |\omega'| \gg \omega_D$ contribute?]. This effective interaction is very much in the spirit of the toy interaction proposed by Cooper, except the cutoff on the electron states is made in *frequency* rather than *momentum* space. The original BCS paper used a cutoff in momentum space, but we shall see that we will obtain identical results in the weak-coupling limit of interest. It turns out that the model we have just adopted is actually more physical than that of BCS, since it reflects the retarded nature of the electron-phonon interaction, and for certain subtle calculations differences do arise.

The instability or *critical temperature* is now determined by requiring the denominator to vanish. Inserting the approximate $V(\omega_n, \omega_n')$, we find

$$\begin{aligned} 1 &= T_c V {\sum_{\omega_n}}' \sum_k G^0(k, \omega_n) G^0(-k, \omega_n) && (13) \\ &= T_c V {\sum_{\omega_n}}' N_0 \int d\xi \frac{1}{\omega_n^2 + \xi^2} && (14) \\ &= \pi N_0 V T_c {\sum_{\omega_n}}' \frac{1}{|\omega_n|} && (15) \\ &= N_0 V \sum_{n=0}^{\omega_D/2\pi T_c} \frac{1}{n + \frac{1}{2}}, && (16) \end{aligned}$$

where the prime on the sum indicates a cutoff at ω_D. At temperatures much less than ω_D, the sum may be approximated by an integral, and one obtains $\sim \log(\omega_D/2\pi T_c)$. The exact value may be looked up; it turns out to be $\gamma + \log(\omega_D/2\pi T_c)$, where $\gamma = 0.577$ is Euler's const. The instability equation then reduces to

$$T_c = 1.13\omega_D e^{-\frac{1}{N_0 V}}. \tag{17}$$

This is the famous BCS result, which looks quite similar to the Cooper bound state energy, in that it also corresponds to an essential singularity in its dependence on the coupling constant, and exhibits a solution for infinitesimal V. The cutoff introduced by Cooper is seen explicitly to correspond to a typical short-wavelength phonon frequency. There are some things which ought to trouble you about this neat package, however. The most obvious is the analogy with ferromagnetism. Ferromagnetism corresponds to a spontaneously broken spin-rotational symmetry of the Hamiltonian, with order parameter $< S_z >$. What is the analogous broken symmetry and order parameter for superconductivity? Applying the response function analogy directly, we would expect that the order parameter is something like $< c_{k\sigma} c_{-k-\sigma} >$, since that is what the pair field couples to. But this makes no sense at first glance: the electron-phonon Hamiltonian conserves number, and the expectation value of the pair operator clearly should vanish in a number-conserving ensemble. This is one of the most subtle questions in superconductivity, and it held up acceptance of the BCS theory for a little while. For what BCS theory does is to ignore this "minor point" and say the right thing to do is to take a restricted expectation value, i.e. trace not over all eigenstates, but only over those with fixed overall macroscopic *phase* ϕ [see below]. The theory can actually be formulated in a number-conserving way [Anderson 1958], but it is much less tractable. It is easier to assume that the BCS theory is correct, and then ask how large the corrections to it are [not very!].

5.3 BCS Model.

A consistent theory of superconductivity may be constructed either using the full "effective interaction" or our approximation $V(\omega, \omega')$ to it. However almost all interesting questions can be answered by the even simpler model used by BCS. The essential point is to have an attractive interaction for electrons in a shell near the Fermi surface; retardation is secondary. Therefore BCS proposed starting from a phenomenological Hamiltonian describing free electrons scattering via an effective instantaneous interaction à la Cooper:

$$H = H_0 - V \sum_{\substack{kk'q \\ \sigma\sigma'}}{}' c^\dagger_{k\sigma} c^\dagger_{-k+q\sigma'} c_{-k'+q\sigma'} c_{k'\sigma}, \tag{18}$$

where the prime on the sum indicates that the energies of the states k and k' must lie in the shell of thickness ω_D. Note the interaction term is just the Fourier transform of a completely *local* 4-Fermi interaction $\psi^\dagger(r)\psi^\dagger(r)\psi(r)\psi(r)$.[2]

Recall that in our discussion of the instability of the normal state, we suggested that an infinitesimal pair field could produce a finite amplitude for pairing. That amplitude was the expectation value $\langle c^\dagger_{k\sigma} c^\dagger_{-k-\sigma}\rangle$. We ignore for the moment the problems with number conservation, and ask if we can simplify the Hamiltonian still further with a mean field approximation, again to be justified *a posteriori*. We proceed along the lines of generalized Hartree-Fock theory, and rewrite the interaction as

$$c^\dagger_{k\sigma} c^\dagger_{-k+q\sigma'} c_{-k'+q\sigma'} c_{k'\sigma} = [\langle c^\dagger_{k\sigma} c^\dagger_{-k+q\sigma'}\rangle + \delta(c^\dagger c^\dagger)][\langle c_{-k'+q\sigma'} c_{k'\sigma}\rangle + \delta(cc)], \tag{19}$$

where, e.g. $\delta(cc) = c_{-k'+q\sigma'} c_{k'\sigma} - \langle c_{-k'+q\sigma'} c_{k'\sigma}\rangle$ is the *fluctuation* of this operator about its expectation value. If a mean field description is to be valid, we should be able to neglect terms quadratic in the fluctuations when we expand Eq (20). If we furthermore make the assumption that pairing will take place in a uniform state (zero pair center of mass momentum), then we put $\langle c_{-k'+q\sigma'} c_{k'\sigma}\rangle = \langle c_{-k'\sigma'} c_{k'\sigma}\rangle \delta_{q,0}$. The effective Hamiltonian

[2]Note this is not the most general form leading to superconductivity. Pairing in higher angular momentum channels requires a *bilocal* model Hamiltonian, as we shall see later.

then becomes

$$H \simeq H_0 - \Delta \sum_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + h.c. + const, \tag{20}$$

where

$$\Delta = V \sum_k \langle c_{-k\downarrow} c_{k\uparrow} \rangle. \tag{21}$$

What BCS did was then to treat the *order parameter* Δ as a (complex) number, and calculate expectation values in the approximate Hamiltonian (21), insisting that Δ be determined self-consistently via Eq. (22) at the same time.

BCS wave function, gauge invariance, and number conservation. The BCS ansatz for the ground state of (21) is a state with the pairs $k\uparrow, -k\downarrow$ occupied with amplitude v_k and unoccupied with amplitude u_k, such that $|u_k|^2 + |v_k|^2 = 1$:

$$|\psi >= \Pi_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)|0> . \tag{22}$$

This is a *variational* wave function, so the energy is to be minimized over the space of u_k, v_k. Alternatively, one can diagonalize the Hamiltonian or Green's function directly. I will follow the latter procedure, but first make a few remarks on the form of the wave function. First, note the explicit violation of particle number conservation: $|\psi>$ is a superposition of states describing 0, 2, 4 , N-particle systems.[3] In general a quantum mechanical system with fixed particle number N (like, e.g. a real superconductor!) manifests a global $U(1)$ gauge symmetry, because H is invariant under $c_{k\sigma}^\dagger \to e^{i\theta} c_{k\sigma}^\dagger$. The state $|\psi>$ is characterized by a set of coefficients $\{u_k, v_k\}$, which becomes $\{u_k, e^{2i\theta} v_k\}$ after the gauge transformation. The two states $|\psi>$ and $\psi(\phi)$, where $\phi = 2\theta$, are inequivalent, mutually orthogonal quantum states, since they are not simply related by a multiplicative phase factor.[4] Since H is independent of ϕ, however, all

[3] What happened to the odd numbers? In mesoscopic superconductors, there are actually differences in the properties of even and odd-number particle systems, but for bulk systems the distinction is irrelevant.

[4] In the normal state, $|\psi>$ and $\psi(\phi)$ differ by a global multiplicative phase $e^{i\theta}$, which has no physical consequences, and the ground state is nondegenerate.

states $|\psi(\phi)>$ are continuously degenerate, i.e. the ground state has a $U(1)$ gauge (phase) symmetry. Any state $|\psi(\phi)>$ is said to be a broken symmetry state, becaue it is not invariant under a $U(1)$ transformation, i.e. the system has "chosen" a particular ϕ out of the degenerate range $0<\phi<2\pi$. Nevertheless the absolute value of the overall phase of the ground state is not an observable, but its variations $\delta\phi(r,t)$ in space and time are. It is the *rigidity* of the phase, i.e. the energy cost of any of these fluctuations, which is responsible for superconductivity.

Earlier I mentioned that it was possible to construct a number conserving theory. It is now instructive to see how: states of definite number are formed [Anderson 1958] by making coherent superpositions of states of definite phase

$$|\psi(N)>=\int_0^{2\pi} d\phi e^{i\phi N/2}|\psi(\phi)>\,. \tag{23}$$

[The integration over ϕ gives zero unless there are in the expansion of the product contained in $|\psi>$ precisely N/2 pair creation terms, each with factor $\exp i\phi$.] Note while this state has maximal uncertainty in the *value* of the phase, the rigidity of the system to phase fluctuations is retained.[5]

It is now straightforward to see why BCS theory works. The BCS wave function $|\psi>$ may be expressed as a sum $|psi>=\Sigma_N\, a_N|\psi(N)>$ [Convince yourself of this by calculating the a_N explicitly!]. IF we can show that the distribution of coefficients a_N is sharply peaked about its mean value $<N>$, then we will get essentially the same answers as working with a state of definite number $N=<N>$. Using the explicit form (23), it is easy to show

$$\langle N\rangle=\langle\psi|\sum_{k\sigma} n_{k\sigma}|\psi\rangle=2\sum_k|v_k|^2\;\;;\quad\langle(N-\langle N\rangle)^2\rangle=\sum_k u_k^2v_k^2. \tag{24}$$

Now the u_k and v_k will typically be numbers of order 1, so since the numbers of allowed k-states appearing in the k sums scale with the volume of the system, we have $<N>\sim V$, and $<(N-<N>)^2>\sim V$.

[5]The phase and number are in fact canonically conjugate variables, $[N/2,\phi]=i$, where $N=2i\partial/\partial\phi$ in the ϕ representation.

Therefore the *width* of the distribution of numbers in the BCS state is $< (N- < N >)^2 >^{1/2} / < N > \sim N^{-1/2}$. As $N \to 10^{23}$ particles, this relative error implied by the number nonconservation in the BCS state becomes negligible.

5.3.1 Is the BCS order parameter general?

Before leaving the subject of the phase in this section, it is worthwhile asking again why we decided to pair states with opposite momenta and spin, $k \uparrow$ and $-k \downarrow$. The BCS argument had to do 1) with minimizing the energy of the entire system by giving the Cooper pairs zero center of mass momentum, and 2) insisting on a spin singlet state because the phonon mechanism leads to electron attraction when the electrons are at the same spatial position (because it is retarded in time!), and a spatially symmetric wavefunction with large amplitude at the origin demands an antisymmetric spin part. Can we relax these assumptions at all? The first requirement seems fairly general, but it should be recalled that one can couple to the pair center of mass with an external magnetic field, so that one will create spatially inhomogeneous (finite-q) states with current flow in the presence of a magnetic field. Even in zero external field, it has been proposed that systems with coexisting antiferromagnetic correlations could have pairing with finite antiferromagnetic nesting vector $\vec{Q}$ [Baltensberger and Strässler 196?]. The requirement for singlet pairing can clearly be relaxed if there is a pairing mechanism which disfavors close approach of the paired particles. This is the case in superfluid ^3He, where the hard core repulsion of two ^3He atoms supresses T_c for s-wave, singlet pairing and enhances T_c for p-wave, triplet pairing where the amplitude for two particles to be together at the origin is always zero.

In general, pairing is possible for some pair mechanism if the single particle energies corresponding to the states $k\sigma$ and $k'\sigma'$ are degenerate. This is necessary because xxx. In the BCS case, a guarantee of this degeneracy for $k\uparrow$ and $-k\downarrow$ in zero field is provided by Kramer's theorem, which says these states must be degenerate because they are connected by *time reversal* symmetry. However, there are other symmetries: in a system with inversion symmetry, *parity* will provide another type of degeneracy, so $k\uparrow$, $k\downarrow$, $-k\uparrow$ and $-k\downarrow$ are all degenerate and may be paired with one another if allowed by the pair interaction.

5.3.2 Green's functions and excitation spectrum of a superconductor.

Let us now calculate the energy spectrum of the superconductor by constructing the Green's function and searching for the poles. Note the equations of motion for the electron operators (using the Heisenberg equation):

$$\begin{aligned}\partial c_{k\sigma}/\partial\tau &= -\xi_k c_{k\sigma} + \sigma\Delta c^\dagger_{-k-\sigma} & (25)\\ \partial c^\dagger_{k\sigma}/\partial\tau &= \xi_k c^\dagger_{k\sigma} - \sigma\Delta^* c_{-k-\sigma}, & (26)\end{aligned}$$

Defining

$$G_\sigma(k,\tau) = -\langle T_\tau c_{k\sigma}(\tau) c^\dagger_{k\sigma}\rangle, \quad (27)$$

as the usual single-particle Green's function and

$$F(k,\tau) = -\langle T_\tau c_{k\uparrow}(\tau) c_{-k\downarrow}\rangle \;\; ; \quad \tilde{F}(k,\tau) = -\langle T_\tau c^\dagger_{-k\downarrow}(\tau) c^\dagger_{k\uparrow}\rangle \quad (28)$$

as "anomalous" Green's functions, which clearly vanish in the normal state, the equations of motion give

$$\begin{aligned}\frac{\partial G(k)}{\partial\tau} &= -\delta(\tau) - \xi_k G(k) + \Delta\tilde{F}(k) & (29)\\ \frac{\partial\tilde{F}(k)}{\partial\tau} &= \xi_k\tilde{F}(k) + \Delta^* G(k). & (30)\end{aligned}$$

A Fourier transform with respect to frequency yields

$$\begin{aligned}i\omega_n G &= -1 - \xi_k G + \Delta\tilde{F} & (31)\\ i\omega_n\tilde{F} &= \xi_k\tilde{F} + \Delta^* G & (32)\end{aligned}$$

which can be solved immediately to yield

$$G(k,\omega_n) = -\frac{i\omega_n+\xi_k}{\omega_n^2+\xi_k^2+|\Delta|^2} \quad (33)$$

$$\tilde{F}(k,\omega_n) = \frac{\Delta^*}{\omega_n^2+\xi_k^2+|\Delta|^2} \quad (34)$$

$$F(k,\omega_n) = \frac{\Delta}{\omega_n^2+\xi_k^2+|\Delta|^2}. \quad (35)$$

As usual, to find the excitation energies of a physical system, we examine the poles of the single-particle Green's function

$$(i\omega_n)^2 = \xi_k^2 + |\Delta_k|^2 \equiv E_k^2 \quad (36)$$

Notice there is a range of disallowed energies E_k between $\pm\Omega_g$, where

$$\Omega_g = \begin{matrix}\min\\ k\end{matrix}\sqrt{\xi_k^2+|\Delta|^2} = \Delta. \quad (37)$$

For this reason the order parameter Δ is frequently referred to as the "gap" or "energy gap", but it is important to remember that these two concepts are in principle distinct. The excitations themselves are called "Bogoliubov quasiparticles", and can be thought of as the final state of two unpaired Landau quasiparticles when a pair is broken by thermal effects or external fields.

It is frequently very useful to be able to draw on one's intuition about perturbation theory in normal metals to calculate various things in the superconducting state. For this reason a *matrix Green's function* was introduced by Nambu, who defined the 2-component fields spanning particle-hole space:

$$\alpha_k = \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow}\end{pmatrix} \quad ; \qquad \alpha_k^\dagger = (c^\dagger_{k\uparrow}\; c_{-k\downarrow}). \quad (38)$$

The Nambu or matrix Green's function is then defined

$$\underline{G}(k,\tau) \equiv -\langle T_\tau \alpha_k(\tau)\alpha_k^\dagger\rangle = \left\{ \begin{matrix} G_\uparrow(k,\tau) & F(k,\tau) \\ \tilde{F}(k,\tau) & G_\downarrow(-k,\tau)\end{matrix} \right\}, \quad (39)$$

The Fourier transformed Nambu Green's function may now be written using the Pauli matrices τ_i spanning the 2×2 particle-hole space:

$$\underline{G}(k, \omega_n) = -\frac{i\omega_n + \xi_k \tau_3 + \Delta \tau_1}{\omega_n^2 + \xi_k^2 + |\Delta|^2}, \tag{40}$$

where I have specialized to the case of real Δ so τ_2 doesn't occur.

The density of single-particle states of a many-body system is related to the imaginary part of the local retarded Green's function : $G^R(r, \omega) = \Sigma_k G^R(k, \omega)$:

$$\begin{aligned}
N(\omega) &= -\frac{1}{\pi} \sum_k \text{Im} G^R(k, \omega) && (41)\\
&= -\frac{1}{\pi} \sum_k \text{Im}[G(k, \omega_n)]_{i\omega_n \to \omega + i0^+} && (42)\\
&= -\frac{1}{\pi} \sum_k \text{Im} \frac{\omega + \xi_k}{(\omega + i0^+)^2 - E_k^2} && (43)\\
&\simeq -\frac{1}{\pi} N_0 \int dE_k \, |\frac{d\xi_k}{dE_k}| \, \omega \, \text{Im}[\frac{1}{\omega + i0 - E_k} - \frac{1}{\omega + i0 + E_k}] \frac{1}{2E_k} && (44)\\
&= N_0 \int dE_k \, |\frac{d\xi_k}{dE_k}| \, \frac{\omega}{2E_k} [\delta(\omega - E_k) - \delta(\omega + E_k)] && (45)\\
&= N_0 \frac{|\omega|}{\sqrt{\omega^2 - \Delta^2}} \theta(\omega^2 - \Delta^2). && (46)
\end{aligned}$$

So the effect of superconductivity on a flat density of states (as per the approximation in step (42)) is to pile up some states just above the "gap edge" at Δ, as shown in Figure 3a.

5.4 Thermodynamics

5.4.1 Specific heat.

The gap in the density of states is reflected in all thermodynamic quantities as an activated behavior $e^{-\Delta/T}$, at low T, due to the exponentially small number of Bogoliubov quasiparticles with thermal energy sufficient to be excited over the gap Δ at low temperatures $T \ll \Delta$. The electronic specific heat is particularly easy to calculate, since the entropy of the BCS

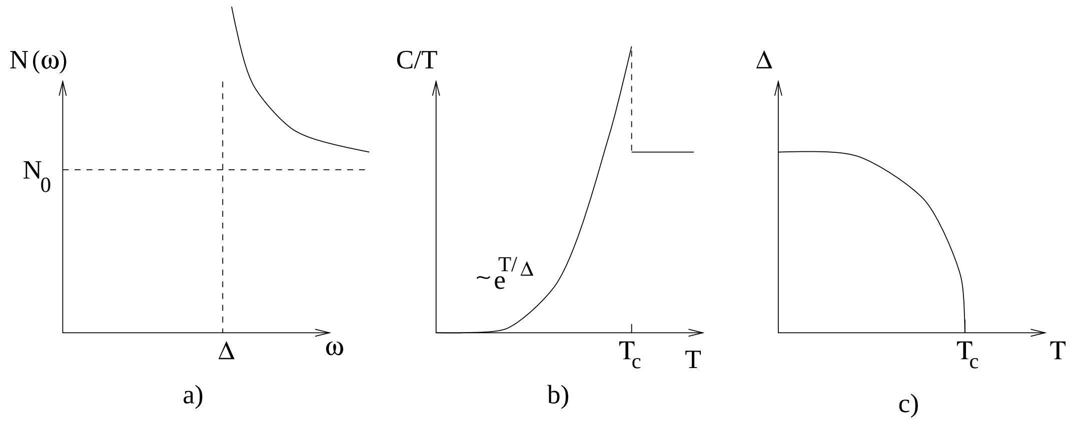


Figure 2: a) BCS density of states $N(\omega)$ vs. ω; b) specific heat vs. T; c) T dependence of order parameter.

superconductor is once again the entropy of a *free* gas of noninteracting quasiparticles, with modified spectrum E_k. The expression (II.6) then gives the entropy directly, and may be rewritten

$$S = -k_B \int_0^\infty d\omega N(\omega)\{f(\omega)\ln f(\omega) + [1 - f(\omega)]\ln[1 - f(\omega)]\}, \quad (47)$$

where $f(\omega)$ is the Fermi function. The constant volume specific heat is just $C_{el,V} = T[dS/dT]_V$, which after a little algebra may be written

$$C_{el,V} = \frac{2}{T}\int d\omega N(\omega)(\frac{-\partial f}{\partial\omega})[\omega^2 - \frac{1}{2}T\frac{d\Delta^2}{dT}]. \quad (48)$$

A sketch of the result of a full numerical evaluation is shown in Figure 3b. Note the discontinuity at T_c and the very rapid falloff at low temperatures.

It is instructive to actually calculate the entropy and specific heat both at low temperatures and near T_c. For $T \ll \Delta$, $f(\omega) \simeq e^{-\omega/T}$ and the density of states factor $N(\omega)$ in the integral cuts off the integration at the lower limit Δ, giving $C \simeq (N_0\Delta^2/T)e^{-\Delta/T}$.

Note the first term in Eq. (47)is continuous through the transition $\Delta \to 0$ (and reduces to the normal state specific heat $(2\pi^2/3)N_0 T$, but the second one gives a discontinuity at T_c. To evaluate this, we need the T dependence of the order parameter.

5.4.2 Gap equation and T_c.

The order parameter in the BCS theory is always determined self-consistently by Eq. (22), and must be temperature dependent since it vanishes at the transition. This dependence may be calculated by expressing the expectation value of the pair operator in terms of the Green's function which we have already calculated,

$$\langle c_{-k\downarrow}c_{k\uparrow}\rangle = F(k,0^-) = T\sum_{\omega_n} e^{-i\omega_n 0^-}F(k,\omega_n) = T\sum_{\omega_n} e^{-i\omega_n 0^-}\frac{\Delta}{\omega_n^2+\xi_k^2+\Delta^2} \quad (49)$$

$$= \oint \frac{dz}{2\pi i} f(z)e^{-z0^-}\frac{\Delta}{z^2-E_k^2} = \Delta\left(\frac{f(E_k)}{2E_k}-\frac{f(-E_k)}{2E_k}\right) \quad (50)$$

$$= \frac{\Delta}{2E_k}\tanh\frac{E_k}{2T} \equiv \Delta\theta_k. \quad (51)$$

Note the importance of the convergence factor $e^{-i\omega_n 0^-}$ in allowing the application of Cauchy's theorem. The gap equation (22) then becomes

$$1 = \sum_{k'} V_{kk'}\theta_{k'} = V{\sum_{k'}}'\frac{1}{2E_{k'}}\tanh\frac{E_{k'}}{2T}. \quad (52)$$

This equation may now be solved, first for the critical temperature itself, being the temperature at which $\Delta \to 0$, and then for the normalized order parameter Δ/T_c for any temperature T. It is the ability to eliminate all normal state parameters from the equation in favor of T_c itself which makes the BCS theory powerful. For in practice the parameters ω_D, N_0, and particularly V are known quite poorly, and the fact that two of them occur in an exponential makes an accurate first principles calculation of T_c nearly impossible. You should always be suspicious of a theory which claims to be able to calculate T_c! On the other hand, T_c is easy to measure, so if it is the only energy scale in the theory, we have a tool with enormous predictive power.

First note that at T_c, the gap equation becomes

$$\frac{1}{N_0 V} = \int_0^{\omega_D} d\xi_k \frac{1}{\xi_k}\tanh\frac{\xi_k}{2T}. \quad (53)$$

Careful evaluation of this integral yields *precisely* the same expression (18) for T_c as we obtained in our instability analysis using the model phonon propagator. We can do the same calculation *near* T_c, expanding to leading order in the small quantity $\Delta(T)/T$, to find $\Delta(T)/T_c \simeq 3.40(1-T/T_c)^{1/2}$. At $T = 0$ we have

$$\frac{1}{N_0 V} = \int_0^{\omega_D} d\xi_k \frac{1}{E_k} = \int_\Delta^{\omega_D} dE N(E)/E \quad (54)$$

$$= \int_\Delta^{\omega_D} dE \frac{1}{\sqrt{E^2 - \Delta^2}} \simeq \ln(2\omega_d/\Delta), \quad (55)$$

so that $\Delta(0) \simeq 2\omega_D \exp -1/N_0 V$, or $\Delta(0)/T_c \simeq 1.76$. The full temperature dependence of $\Delta(T)$ is sketched in Figure 3c). In the halcyon days of superconductivity theory, comparisons with the theory had to be compared with a careful table of Δ/T_c painstakingly calculated and compiled by Mühlschlegl. Nowadays the numerical solution requires a few seconds on a PC. It is frequently even easier to use a phenomenological approximate closed form of the gap, which is correct near $T = 0$ and $= T_c$:

$$\Delta(T) = \delta_{sc} T_c \tanh\{\frac{\pi}{\delta_{sc}} \sqrt{a \frac{\delta C}{C_N} (\frac{T_c}{T} - 1)}\}, \quad (56)$$

where $\delta_{sc} = 1.76$, $a = 2/3$, and $\delta C/C_N = 1.43$ is the normalized specific heat jump. Note to evaluate the last quantity, we need only use the calculated temperature dependence of Δ near T_c, and insert into Eq. (47). This is another of the "universal" ratios which the BCS theory predicted and which helped confirm the theory in classic superconductors.

5.5 Electrodynamics

The existence of an energy gap is not a sufficient condition for superconductivity (actually, it is not even a necessary one!). Insulators, for example, do not possess the *phase rigidity* which leads to perfect conductivity and perfect diamagnetism which are the defining characteristics of superconductivity. We can understand both properties by calculating the current response of the system to an applied magnetic or electric field. The kinetic energy in the presence of an applied vector potential $\mathbf{A}$ is just

$$H_0 = \sum_\sigma \int d^3r \psi^\dagger_\sigma(r)[-i\nabla - (\frac{e}{c})\mathbf{A}]^2 \psi_\sigma(r), \tag{57}$$

and the second quantized current density operator is given by

$$\begin{aligned} \mathbf{j}(r) &= \frac{e}{2m}\{\psi^\dagger(r)(-i\nabla - \frac{e}{c}\mathbf{A})\psi(r) + [(i\nabla - \frac{e}{c}\mathbf{A})\psi^\dagger(r)]\psi(r)\} & (58) \\ &= \mathbf{j}_{para} - \frac{e^2}{mc}\psi^\dagger(r)\psi(r)\mathbf{A}, & (59) \end{aligned}$$

where

$$\mathbf{j}_{para}(r) = \frac{-ie}{2m}\{\psi^\dagger(r)\nabla\psi(r) - (\nabla\psi^\dagger(r))\psi(r)\}, \tag{60}$$

or in Fourier space,

$$\begin{aligned} \mathbf{j}_{para}(q) &= \frac{e}{m}\sum_{k\sigma}(\mathbf{k} + \frac{1}{2}\mathbf{q})c^\dagger_{k\sigma}c_{k+q\sigma} & (61) \\ &= \frac{e}{m}\sum_k(\mathbf{k} + \frac{1}{2}\mathbf{q})\alpha^\dagger_k\alpha_{k+q}, & (62) \end{aligned}$$

where the last step has been to represent the current in terms of Nambu operators. We would like to do a calculation of the linear current response $\mathbf{j}(q,\omega)$ to the application of an external field $\mathbf{A}(q,\omega)$ to the system a long time after the perturbation is turned on. Expanding the Hamiltonian to first order in $\mathbf{A}$ gives the interaction

$$H' = \int d^3r \mathbf{j}_{para} \cdot \mathbf{A}. \tag{63}$$

The expectation value $< \mathbf{j} >$ may now be calculated to linear order via the Kubo formula, yielding

$$\langle \mathbf{j} \rangle(q,\omega) = \underline{K}(q,\omega)\mathbf{A}(q,\omega) \tag{64}$$

with

$$\underline{K}(q,\omega) = -\frac{ne^2}{mc} + \langle[\mathbf{j}_{para}, \mathbf{j}_{para}]\rangle(q,\omega), \tag{65}$$

where the second term is formally the Fourier transform of the *retarded* current-current correlation function.[6] Note the simple product structure of (63) in momentum space implies a *nonlocal* relationship in general between $\mathbf{j}$ and $\mathbf{A}$., i.e. $\mathbf{j}(r)$ depends on the $\mathbf{A}(r')$ at many points r' around r. Note also that the electric field in a gauge where the electrostatic potential is set to zero may be written $\mathbf{E}(q,\omega) = -i\omega\mathbf{A}(q,\omega)$, so that the *complex* conductivity of the system defined by $\mathbf{j} = \underline{\sigma}\mathbf{E}$ may be written

$$\underline{\sigma}(q,\omega) = \frac{i}{\omega}\underline{K}(q,\omega) \tag{66}$$

It remains only to calculate $< [\mathbf{j}_{para}, \mathbf{j}_{para}] >$. Using the definition of the current (60), we see that this may be written as a 4-Fermi expectation value, and is after a little algebra expressible as a retarded 2-particle Green's function as usual in the Kubo approach. We first calculate the Matsubara function, and then analytically continue. In the absence of interactions, the linear response term is just the "bare bubble"

$$\underline{K}_{para}(q,\nu_n) \equiv \langle[\mathbf{j}_{para},\mathbf{j}_{para}]\rangle(q,\nu_n) = \frac{k_F^2 e^2}{m^2 c}\sum_k \hat{k}\hat{k}\; T\sum_{\omega_n}\frac{1}{2}\mathrm{Tr}\underline{G}(k,\omega_n)\underline{G}(k+q,\omega_n+\nu_n), \tag{67}$$

where I've neglected the q-dependence of the vertices and set $k = k_F$ since only electrons at the Fermi surface contribute appreciably.[7]

5.5.1 Meissner Effect.

There is a theorem of classical physics proved by Bohr[8] which states that the ground state of a system of charged particles in an external magnetic field carries zero current. The essential element in the proof of this theorem is the fact that the magnetic forces on the particles are always

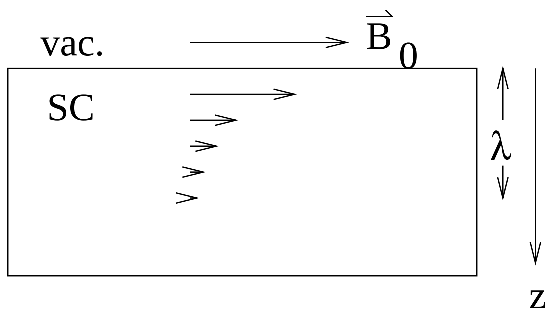
[6] We will see that the first term gives the *diamagnetic* response of the system, and the second the temperature-dependent *paramagnetic* response.

[7] Note the *dyadic product* $\hat{k}\hat{k}$ which makes the right hand side a tensor (the xx component is $\hat{k}_x\hat{k}_x$, etc.).

[8] See "The development of the quantum-mechanical electron theory of metals: 1928-33." L. Hoddeson and G. Baym, Rev. Mod. Phys., 59, 287 (1987).

perpendicular to their velocities. In a quantum mechanical system, the three components of the velocity do not commute in the presence of the field, allowing for a finite current to be created in the ground state. Thus the existence of the Meissner effect in superconductors, wherein magnetic flux is expelled from the interior of a sample below its critical temperature, is a clear proof that superconductivity is a manifestation of quantum mechanics.

The typical theorists' geometry for calculating the penetration of an electromagnetic field into a superconductor is the half-space shown in Figure 4a, and compared to schematics of practical experimental setups involving resonant coils and microwave cavities in Figs. 4b)-c). In the



a) b) c)

Figure 3: 4a) Half-space geometry for penetration depth calculation; 4b) Resonant coil setup; 4c) Microwave cavity

gedanken experiment case, a DC field is applied parallel to the sample surface, and currents and fields are therefore functions only of the coordinate perpendicular to the surface, $\mathbf{A} = \mathbf{A}(z)$, etc. Since we are interested in an external electromagnetic wave of very long wavelength compared to the sample size, and zero frequency, we need the limit $\nu_n = 0, q \to \infty$ of the response. We will assume that in this limit $\underline{K}(0,0) \to$ const, which we will call $-(c/4\pi)\lambda^{-2}$ for reasons which will become clear! Equation (63) then has the form

$$\mathbf{j} = -\frac{c}{4\pi}\lambda^{-2}\mathbf{A}, \tag{68}$$

This is sometimes called London's equation, which must be solved in conjunction with Maxwell's equation

$$\nabla \times \mathbf{B} = -\nabla^2 \mathbf{A} = \frac{4\pi}{c}\mathbf{j} = -\lambda^{-2}\mathbf{A}, \tag{69}$$

which immediately gives $\mathbf{A} \sim e^{-z/\lambda}$, and $\mathbf{B} = \mathbf{B}_0 e^{-z/\lambda}$. The currents evidently screen the fields for distances below the surface greater than about λ. This is precisely the Meissner effect, which therefore follows *only* from our assumption that $K(0,0) =$ const. A BCS calculation will now tell us how the penetration depth depends on temperature. We return to Eq. (66) and put

$$\begin{aligned}\underline{K}(0,0) &= \frac{-ne^2}{mc}\underline{1} + \frac{k_F^2 e^2}{m^2 c}\sum_k \hat{k}\hat{k}\; T\sum_{\omega_n}\frac{1}{2}\mathrm{Tr}\underline{G}(k,\omega_n)\underline{G}(k,\omega_n) &(70)\\ &= \frac{-ne^2}{mc}\{1 + T\sum_{\omega_n}\int d\xi \frac{-\omega_n^2 + E_k^2}{(\omega_n^2+E_k^2)^2}\}\cdot \underline{1}, &(71)\end{aligned}$$

where I've used $N_0 = 3n/\epsilon_F$ (3D), $\Sigma_k \to N_0 \int d\xi \int d\Omega/4\pi$, and $\int (d\Omega/4\pi)\hat{k}\hat{k} = \underline{1}/3$. The frequency sum in (69) may now be evaluated,[9] yielding

$$T\sum_{\omega_n}\frac{-\omega_n^2 + E_k^2}{(\omega_n^2+E_k^2)^2} = \frac{\partial f}{\partial E_k}. \tag{72}$$

The static homogeneous response is therefore

$$\begin{aligned}\underline{K}(0,0) &= \frac{-ne^2}{mc}\{1 - \int d\xi_k (\frac{-\partial f}{\partial E_k})\}\underline{1} &(73)\\ &\equiv \frac{-n_s(T)e^2}{mc}\underline{1} &(74)\end{aligned}$$

where in the last step, I defined the *superfluid density* to be $n_s(T) \equiv n - n_n(T)$, with *normal fluid density* $n_n(T) \equiv n \int d\xi_k \; -\partial f/\partial E_k$. Note at $T = 0$, $\; - \partial f/\partial E_k \to 0$, [Not a delta function, as in the normal state case–do you see why?], while at $T = T_c$ the integral $n_n \to 1$.[10] Correspondingly, the superfluid density as defined varies between n at

[9] Recall the Cauchy rule for the residues of simple poles of degree n, $\oint g(z)/(z-z_0)^n = 2\pi i (d/dz)^{n-1} g(z)|_{z_0}$.

[10] The dimensioness function $n_n(T/T_c)/n$ is sometimes called the Yoshida function, $Y(T)$, and is plotted in Fig. (5).

$T = 0$ and 0 at T_c. This is the BCS microscopic justification for the rather successful phenomenological two-fluid model of superconductivity: the normal fluid consists of the thermally excited Bogoliubov quasiparticle gas, and the superfluid is the condensate of Cooper pairs.[11]

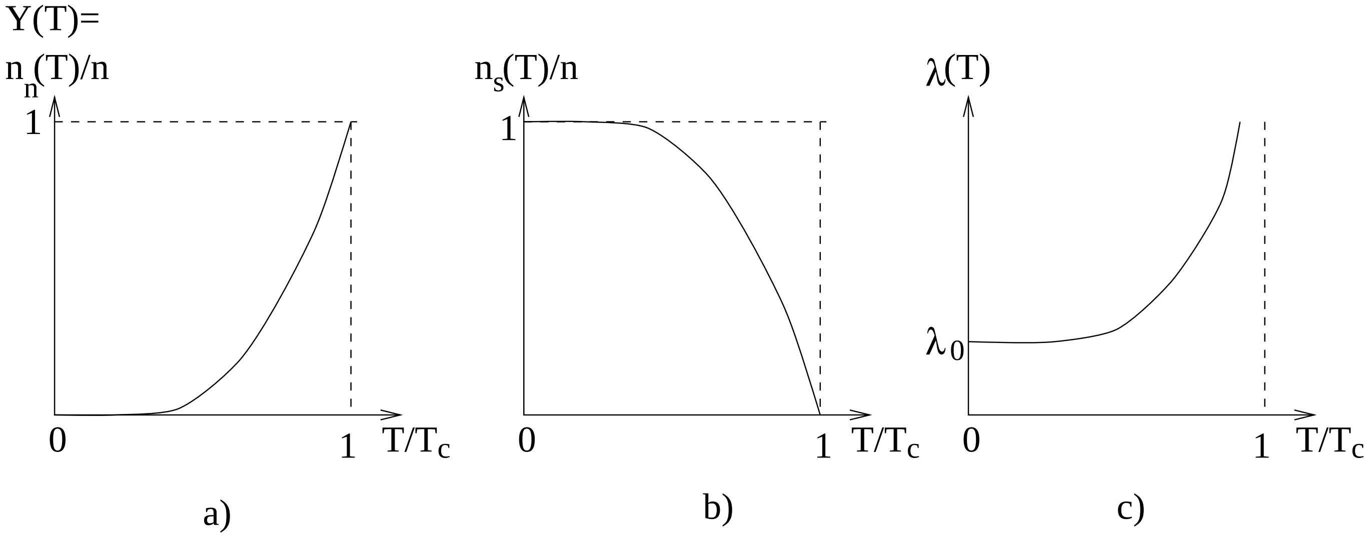


Figure 4: a) Yoshida function; b) superfluid density ; c) penetration depth

Now let's relate the BCS microscopic result for the static homogeneous response to the penetration depth appearing in the macroscopic electrodynamics calculation above. We find immediately

$$\lambda(T) = \Big(\frac{mc^2}{4\pi n_s(T)e^2}\Big)^{1/2}. \qquad (75)$$

At $T = 0$, the supercurrent screening excludes the field from all of the sample except a sheath of thickness $\lambda(0)$. At small but finite temperatures, an exponentially small number of quasiparticles will be excited out of the condensate, depeleting the supercurrent and allowing the field to penetrate further. Both $n_n(T)$ and $\lambda(T) - \lambda(0)$ may therefore be expected to vary as $e^{-\Delta/T}$ for $T \ll T_c$, as may be confirmed by explicit expansion of Eq. (72). [Do it!] Close to T_c, the penetration depth diverges as it must, since in the normal state the field penetrates the sample completely.

[11]The BCS theory and subsequent extensions also allow one to understand the limitations of the two-fluid picture: for example, when one probes the system at sufficiently high frequencies $\omega \sim \Delta$, the normal fluid and superfluid fractions are no longer distinct.

5.5.2 Dynamical conductivity.

This can be a fairly involved subject, but the existence of a 2Δ threshold in the $T = 0$ absorption spectrum of a superconductor is a fundamental property of classic superconductors, and I would like you to see how it comes about. We expect such a result, because at $T = 0$, a photon can only be absorbed by breaking a bound pair of electrons, costing an energy 2Δ, or Δ/particle.

The real part of the conductivity, $\mathrm{Re}\underline{\sigma}(q,\omega)$, given by $-\mathrm{Im}\underline{K}(q,\omega)/\omega$ according to (65), represents the absorption of energy from the electromagnetic wave $\mathbf{E}(q,\omega)$. To show the existence of an absorption threshold, we will do the simplest thing, and calculate the long-wavelength conductivity $\sigma(q = 0,\omega)$.[12] Before we do so, however, let's understand what it takes to get a nonzero absorption. In a normal metal, the photon creates an electron-hole pair which then relax back to the Fermi sea by emission of phonons, collisions with impurities, etc. At $T = 0$ in a superconductor, it clearly requires a photon energy of 2Δ to create a (quasi-) electron-hole pair. Steady-state absorption will only occur, however, if there is a way of relaxing the electronic distribution function back to equilibrium. The $q = 0$ requirement makes phonon emission at energy $\omega = 2\Delta$ impossible in a simple metal; relaxation can therefore only take place via impurities. We will see in the next section that the effect of impurities is to *broaden* the quasiparticle states, giving them an imaginary part $\omega \to \omega + i/2\tau(\omega)$. For now we simply assume a broadening of this type without doing any

[12] Since the electromagnetic wave amplitude decays upon enetering the metal due to the screening currents, in principle all wavelengths contribute to the total power absorption into the material. Solving the electrodynamics problem of an electromagnetic wave normally incident on a specularly reflecting surface yields for the power absorbed at frequency ω

$$P(\omega) \propto \int_0^\infty \mathrm{Im}\frac{K(q,\omega)}{q^2 + (4\pi/c)K(q,\omega)}. \tag{76}$$

At low temperatures, $\mathrm{Re}K \gg \mathrm{Im}K$, so the cutoff in the q integration is set by the size of $(4\pi\mathrm{Re}K/c)^{1/2}$, or λ^{-1}. The only intrinsic length scale over which $\mathrm{Re}K$ can vary in the clean limit of interest is the coherence length $\xi_0 \simeq v_F/\Delta$ (see next chapter). *If* $\xi_0 < \lambda(0)$ ("type II superconductor"), it will be a good approximation to replace $K(q,\omega)$ everywhere by $K(0,\omega)$ [see Fig. 6a]. This situation is called *local electrodynamics* since Fourier transforming Eq. (63) gives approximately $\mathbf{j}(r) \propto \mathbf{A}(\mathbf{r})$. In the local case $\sigma(q = 0,\omega)$ will be a good measure of the absorption. If $\lambda < \xi_0$, however ("type I superconductor"), the full q-dependence of the integrand is required; the q=0 component of σ is not independently useful.

calculations of $1/\tau$, but including the restriction that $1/\tau(\omega) = 0$ for $\omega < \Delta$ since there are no states in the gap to broaden!

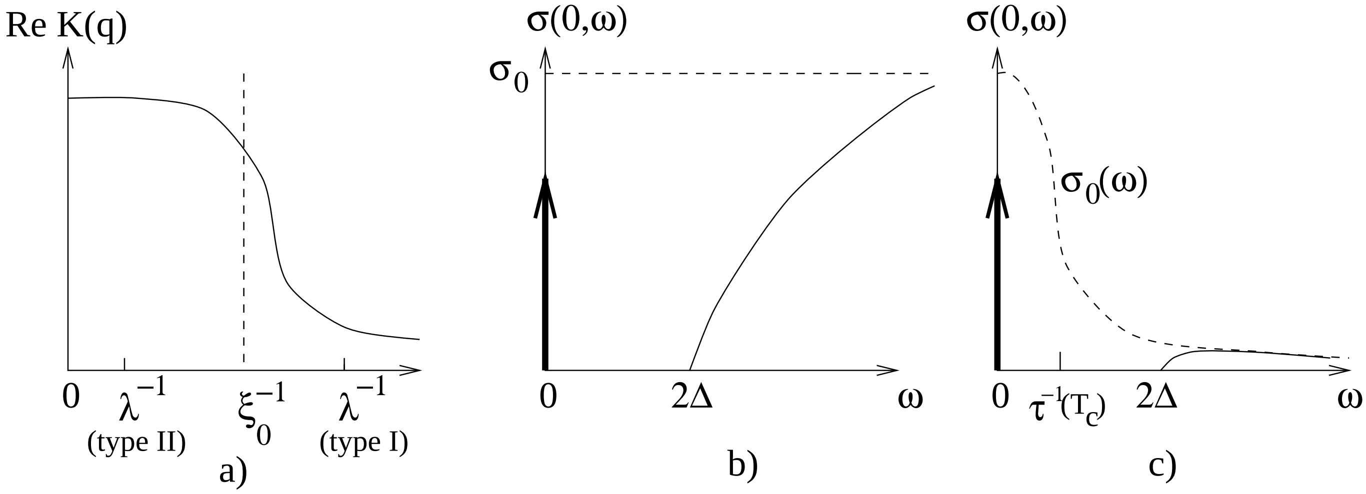


Figure 5: a) q-dependence of response function ; b) conductivity in dirty system; c) conductivity in clean system. Dashed lines are normal state conductivity in both b) and c).

The conductivity is given by

$$\sigma(0,\omega) = -\frac{1}{\omega}\mathrm{Im}\{\frac{k_F^2 e^2}{m^2 c}\sum_k \hat{k}\hat{k}\; T\sum_{\omega_n}\frac{1}{2}\mathrm{Tr}\underline{G}(k,\omega_n)\underline{G}(k,\omega_n+\nu_n)\}_{\nu_n\to\omega+i0^+}. \tag{77}$$

It is now convenient to replace the $\underline{G}$'s by their spectral representations, $\underline{G}(k,\omega_n) = -\int d\epsilon \mathrm{Im}\,\underline{G}^R(k,\epsilon)/(i\omega_n-\epsilon)$, and perform the frequency sum[2]

$$T\sum_{\omega_n}\frac{1}{i\omega_n-\epsilon}\;\frac{1}{i\omega_n+i\nu_n-\epsilon'} = \frac{f(\epsilon)-f(\epsilon')}{\epsilon+i\nu_n-\epsilon'}. \tag{78}$$

We may now perform the analytic continuation, $i\nu_n \to \omega + i0^+$ explicitly, leaving

$$\begin{aligned}\sigma(0,\omega) &= -\frac{1}{\omega}\frac{k_F^2 e^2}{m^2 c}\sum_k \hat{k}\hat{k}\int\frac{d\epsilon d\epsilon'}{\pi^2}\frac{1}{2}\mathrm{Tr}\;\mathrm{Im}\underline{G}^R(k,\epsilon)\mathrm{Im}\underline{G}^R(k,\epsilon')\times \\ &\quad\times\mathrm{Im}\{\frac{f(\epsilon)-f(\epsilon')}{\epsilon+\omega-\epsilon'+i0^+}\} \qquad (79)\\ &= -\frac{1}{\omega}\frac{k_F^2 e^2}{m^2 c}\sum_k \hat{k}\hat{k}\int\frac{d\epsilon}{\pi}\frac{1}{2}\mathrm{Tr}\;\mathrm{Im}\underline{G}^R(k,\epsilon)\mathrm{Im}\underline{G}^R(k,\epsilon+\omega)\times \\ &\quad\times[f(\epsilon)-f(\epsilon+\omega)] \qquad (80)\end{aligned}$$

[2]Remember ν_n is a *boson* frequency, so $f(\epsilon - i\nu_n) = f(\epsilon)$.

$$= -\frac{1}{\omega}\frac{ne^2}{mc}\int d\xi_k \int_{-\omega}^{0} \frac{d\epsilon}{\pi}\frac{1}{2}\mathrm{Tr}\ \mathrm{Im}\underline{G}^R(k,\epsilon)\mathrm{Im}\underline{G}^R(k,\epsilon+\omega) \tag{81}$$

since $[f(\epsilon) - f(\epsilon+\omega)]$ reduces to a window function in ϵ from $-\omega$ to 0 as $T \to 0$. Now note that

$$\mathrm{Im}\ \underline{G}^R(k,\epsilon) = \mathrm{Im}\ \frac{(\omega + i/2\tau)\tau_0 + \xi_k\tau_3 + \Delta\tau_1}{(\omega+i/2\tau)^2 - E_k^2} \propto \frac{1}{\tau(\epsilon)}. \tag{82}$$

So without even performing the integrals, we can already see that

$$\sigma \propto \int_{-\omega}^{0} d\epsilon\ \tau^{-1}(\epsilon)\tau^{-1}(\epsilon+\omega)... \tag{83}$$

Due to the gap Δ in the single-particle spectrum, we must have $|\epsilon| > \Delta$ and $|\epsilon+\omega| > \Delta$ to get a contribution to the integral. But since $-\omega < \epsilon < 0$, we need at least $\omega > 2\Delta$ to satisfy the second condition for positive frequencies ω. So there exists a threshold in the optical absorption spectrum at 2Δ as predicted. Note the *size* of $1/\tau$ does not enter this argument: the optical gap is *not* smeared by disorder if the single-particle threshold remains at Δ (as shown in next section). The full calculation may now be performed for a model of the impurity self-energy such as given in the next section, with the result

$$\frac{\sigma(q=0,\omega)}{\sigma_0} = \frac{1}{\omega}\int_{\Delta}^{\Delta+\omega} d\epsilon[\bar{N}(\epsilon)\bar{N}(\epsilon+\omega) + \bar{D}(\epsilon)\bar{D}(\epsilon+\omega)], \tag{84}$$

where $\sigma_0 = ne^2\tau/m$ is the normal state Drude conductivity, $\bar{N} = N/N_0$ is the normalzed density of states, and $\bar{D}(\epsilon)$ is the normalized *anomalous* density of states, $\bar{D}(\epsilon) = \Delta/\sqrt{\epsilon^2 - \Delta^2}$. This result was first obtained by D. Mattis and J. Bardeen (196..), and looks something like the result sketched in Figure 6b.

The conductivity $\sigma(q=0,\omega)$ may be shown to obey a sum rule such that for any system,

$$\int d\omega\ \sigma(q=0,\omega) = \omega_{pl}^2/xxx \tag{85}$$

We see from Fig. 6b. that at $T = 0$ a good deal of the spectral weight below a frequency of several times Δ has been removed by the onset of superconductivity. Where does the spectral weight go? Our calculation has been complete, except that several steps above did not follow for $\omega = 0$. We therefore suspect, and it may be shown with a bit more care, that the missing spectral weight shows up as a delta-function at the origin whose weight is proportional to the superfluid density $n_s(T)$.

Finally, notice that the schematic in Figure 6b) is unrealistic when compared to the real HTSC materials. The normal state conductivity is shown as a constant on a scale of several Δ, implying $\omega\tau << 1$ over this range. However the actual quasiparticle relaxation $1/\tau$ is much smaller than $\Delta(0)$ at low temperatures in the superconducting state, so the appropriate picture is more like Figure 6c). This is the origin of some of the difficulties optical experiments have had identifying the gap in the superconducting state of the cuprates: most of the spectral weight piles up in the delta function, making the gap hard to see.

5.6 Impurities and Anderson's Theorem.

One of the best ways of learning about the superconducting state is to see what destroys it (and what doesn't). In 1959 P.W. Anderson showed that weak disorder does not affect the thermodynamics of an *isotropic* superconductor. [PW Anderson, J. Phys. Chem. Solids 11, 26 ('59)] "Anderson's theorem" is based on the idea that the most favorable wave function for the ground state of the superconductor consists of pairs containing electrons in time-reversed single-particle eigenstates. That is, momentum $\mathbf{k}$ is no longer a good quantum number of the disordered system. If a Landau quasiparticle description of the normal state is valid, however, there will be analogous single-particle eigenstates with wave functions $\psi_n(r)$ which we index simply by n, with energies ξ_n. The BCS theory may then be reformulated with the new wave functions, and the new energies found to be $E_n = \sqrt{\xi_n^2 + |\Delta|^2}$. It is not hard to see that the reformulated gap equation in the presence of disorder will yield the identical instability temperature

T_c^0, and thermodynamic properties are similarly unaffected.[3]

Experimentally, it is found that the transition temperature of classic superconductors does drop slightly when disorder is added, but then usually levels off until very large levels of disorder are reached, such that the normal state density of states is substantially modified ($1/\tau \sim \epsilon_F$). In the early 60's this behavior was explained by Tsuneto, Markowitz and Kadanoff, and Hohenberg [T. Tsuneto, Prog. Theor. Phys. **28**, 857 (1962); D. Markowitz and L.P. Kadanoff, Phys. Rev. **131**, 563 (1963); P. Hohenberg, Zh. Eksp. Teor. Fiz. **45**, 1208 (1963) (Sov. Phys. JETP **18**, 834 (1964))] as arising from the mixing of the momentum states by the impurity scattering. If the order parameter parameter in the clean system is *anisotropic*, impurity scattering will in general mix regions of large gap and regions of small gap in the gap equation, smearing out the gap anisotropy. The initial drop in T_c takes place while this smearing is occuring, $1/\tau \sim \Delta$, and the levelling out occurs when the gap in the dirty system is approximately isotropic. The sensitivity of highly *anisotropic* superconductors to a small amount of dirt suggested by these early studies was not completely appreciated until people began studying the properties of superconductors with nodes in the presence of dirt [GorkovKalugin,UedaRice]. This will be very relevant to our discussion of HTSC below.

The situation is quite different when the impurity in question is magnetic. The weak scattering case was addressed by Abrikosov and Gor'kov [Sov. Phys JETP 12, 1243 (1961)], who showed that magnetic perturbations break the Cooper pair and lead to T_c supression of the "universal" form shown in Figure 6(b). They also showed that impurities suppress the gap, but that in a narrow range of impurity concentrations just before T_c vanishes, the energy gap would be zero but the order parameter would

[3] Anderson's theorem breaks down, however, if the scattering is magnetic and thus breaks the time reversal symmetry between the two single-particle states (see below), if the scattering is inelastic, if the normal state density of states is strongly modified by disorder if the scattering phase shift is strongly energy dependent, or if the superconducting state is highly anisotropic.

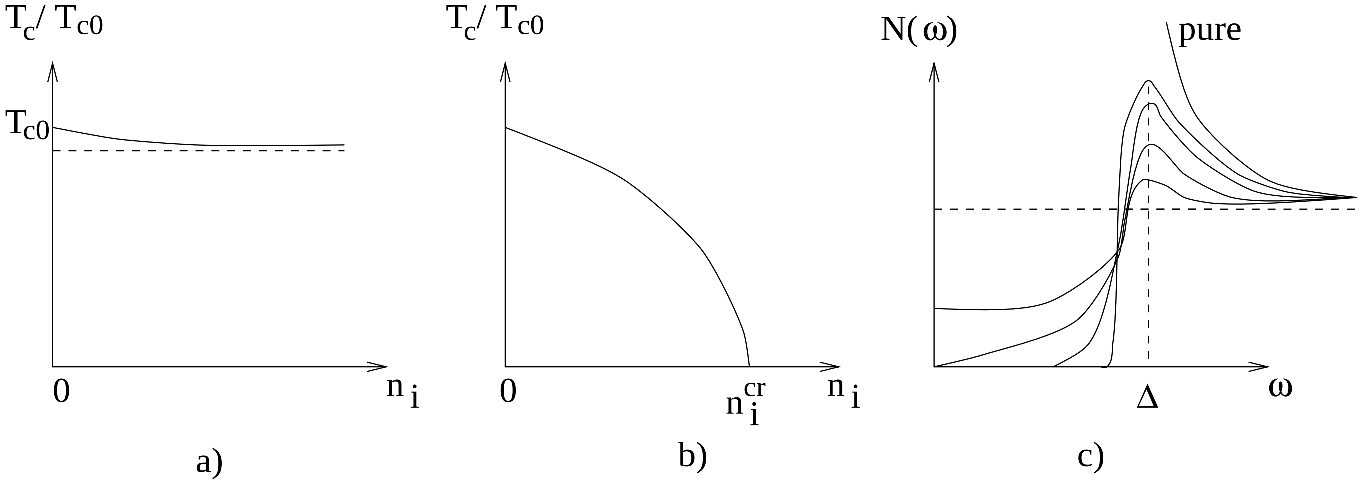


Figure 6: a) Supression of T_c in slightly anisotropic superconductor by potential scatterers; b) Abrikosov-Gor'kov prediction for T_c supression by magnetic impurites; c) schematic density of states for pure classic superconductor and successively more magnetic impurities, showing disappearance of gap.

not, i.e. the system would still exhibit a Meissner effect and perfect conductivity even in the absence of a gap, further evidence that the gap is not the fundamental feature of the superconducting state. This idea is illustrated by plotting the density of states for various impurity concentrations in Figure 6c.

My object in this section is to prove Anderson's theorem using the formalism we have developed. I first need to remind you how one calculates the *disorder-averaged* Green's function. Our use of the Nambu formalism means that you may take what follows as applying to either the normal metal or the superconductor, up to the point where one specifies G^0. First consider the diagrams for the average self-energy in Figure 7a. Each cross represents a scattering from a single impurity, and in Fig. 7a) I have shown that for the case of a single *configuration* of dilute impurities in the sample, the self energy is just the interaction $U(r) = \Sigma_i\, u(r - R_i)$, where R_i are the impurity sites, and $u(r)$ is the single impurity potential measured relative to the impurity position. Note I've assumed the impurities are *nonmagnetic* (U is spin independent) here.

This problem can be solved exactly. However we are really interested in the thermodynamic limit, where many macroscopic blocks of the sample

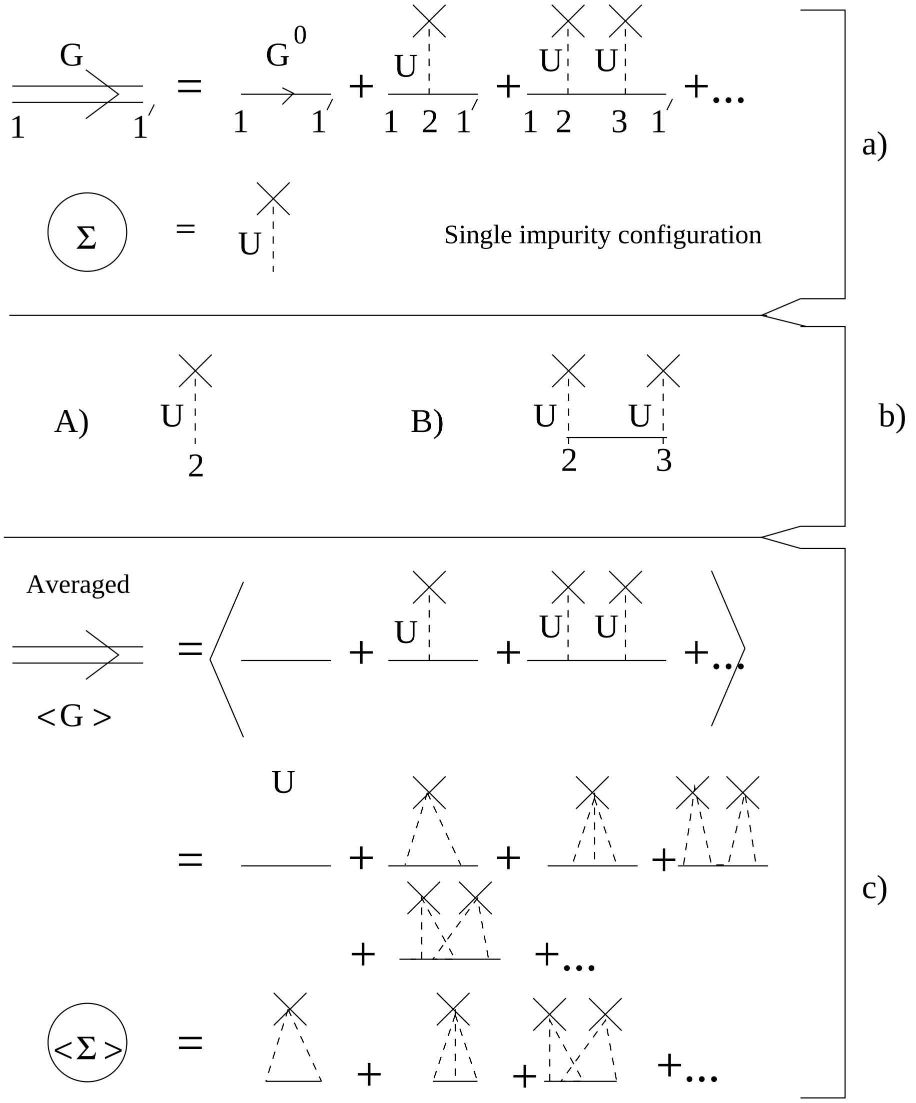


Figure 7: a) Green's function and self-energy for one configuration of impurities; b) leading order diagrams with external legs removed before averaging; c) impurity-averaged quantities.

with different configurations will be averaged over.[4] We therefore perform a disorder average, i.e. average over all possible configurations $\{R_i\}$ with equal weight. The self-energy is now the sum of all diagrams with no external legs irreducible with respect to disorder. Let's calculate the disorder average of the first few diagrams for G with the external legs removed to see which parts we get are irreducible.[5] The disorder average of

[4]How irreversibility and dissipation arise from this averaging is a fascinating and subtle question discussed very nicely by Doniach and Sondheimer [S. Doniach and E. Sondheimer, Green's Functions for Solid State Physicists, Reading, MA: Benjamin, 1974.]

[5]Note the G^0's used in the perturbation theory are independent of disorder, so the average involves only the vertices, represented by crosses.

diagram A) in Figure 7b) is (to simplify notation I've used 2 to represent the coordinate r_2, etc.)

$$\begin{aligned} < U(2) > \delta_{23} &= \sum_i < u(r_2 - R_i) > \delta_{23} & (86) \\ &= \sum_k \sum_i u(k) e^{ik\cdot r} < e^{-ik\cdot R_i} > \delta_{23} & (87) \\ &= n_i u(0) \delta_{23}, & (88) \end{aligned}$$

where the last step follows from the observation that if I average over R_i, the only Fourier component which won't oscillate to zero is the $k = 0$ one, i.e. $< e^{-ik\cdot R_i} >= \delta_{k,0}$. The factor n_i is just the number of impurities. So the average of this diagram represents a constant shift of the chemical potential and may be absorbed in it, which I'll do henceforth.

The second diagram B) is more interesting. Upon averaging we obtain

$$\begin{aligned} < U(2)U(3) > G^0(3-2) &= \sum_{ij} < u(r_2 - R_i) u(r_3 - R_j) > G^0(3-2) & (89) \\ &= \sum_{kk'} \sum_{ij} u(k) u(k') e^{ik\cdot r_2} e^{ik'\cdot r_3} \times \\ & \quad \times < e^{-ik\cdot R_i} e^{-ik'\cdot R_j} > G^0(3-2). & (90) \end{aligned}$$

Now the average of the exponentials has two ways of getting a finite value, one of which where R_i and R_j can be anything, and one in which they are the same, $< e^{-ik\cdot R_i} e^{-ik'\cdot R_j} >= \delta_{k,0}\delta_{k',0} + \delta_{R_i,R_j}\delta_{k,-k'}$. [Make sure you convince yourself of this!] This yields finally

$$n_i^2 u(0)^2 G^0(3-2) + n_i \sum_k |u(k)|^2 G^0(k). \quad (91)$$

Note the first term can't contribute to the irreducible self-energy, since the fact that R_i and R_j aren't "contracted" means I could cut the Green's function line to obtain valid self-energy diagrams. The only remaining term is the second one in Eq. (90), which corresponds, in the diagrammese used for the averaged self-energy, to a picture in which the impurity crosses at R_i and R_j have been identified ("contracted"). Retention of this lowest-order term in the self-energy alone, as depicted in Figure 8a), is called the

Born approximation. Sometimes it is convenient to sum all diagrams of order n_i, as shown in Figure 8b); this is referred to as the t-matrix approximation, and for a normal Fermi system is exact in the dilute limit. (The same is true for a superconductor, but a question has been raised recently about superconductors with order parameter nodes in 2D, see Nersesyan et al., Nucl. Phys. B438, 561 (1995).)

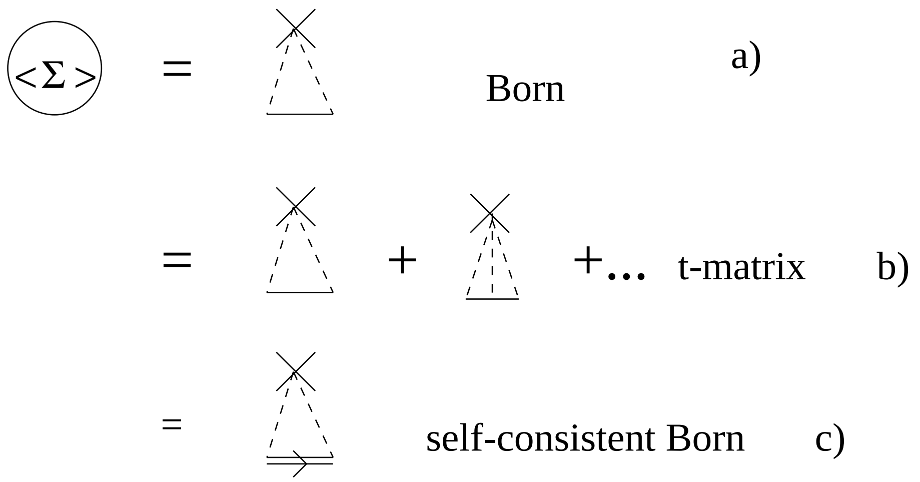


Figure 8: a) Born approx. for self-energy. b) t-matrix approximation; c) self-consistent Born approximation.

To prove Anderson's theorem, it is sufficient to consider the Born approximation of Fig. 8c) in the superconducting state. For simplicity I'll consider δ-function impurities, $u(r) \propto \delta(r)$, such that $u(k) = u = const.$. Note I will use the self-consistent Born approximation 8c) rather than 8a). For my current purposes it won't make a difference: Anderson's theorem will come out in any case. But the effect of replacing the bare G^0 in the intermediate state with the full G in 8c) is to sum all the self-energy processes on the intermediate state line, which will lead to a shift in the pole of the Green's function in the complex plane, and possible new physics.[6] If not, these corrections are of higher order in n_i and may be neglected. One of the additional diagrams included in this way is shown in Figure 9a). Diagrams like crosseddiagb), which are not part of the self-consistent Born although formally of the same order as 9a), represent the interference

[6]These self-consistent corrections are responsible for gapless behavior in the case of the magnetic impurity

of electrons scattering off of two separate impurities, and may (usually) be shown to be of relative order $(k_F\ell)^{-1}$ with respect to 9a), where $\ell = v_F\tau$ is the mean free path.

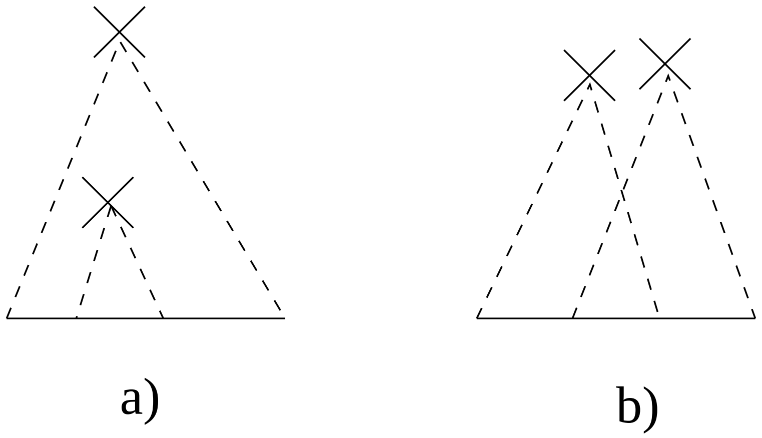


Figure 9: a) Self-energy correction to leading-order Born process; b) Self-energy diagram not included in self-consistent Born or t-matrix approximation.

The approximation we will take for the self-energy in the superconducting state is then

$$\underline{\Sigma} = n_i|u|^2 \sum_k \tau_3 \underline{G}(k,\omega)\tau_3, \tag{92}$$

which, together with the Dyson equation

$$\begin{aligned} \underline{G}^{-1} &= \underline{G}^{0^{-1}} - \underline{\Sigma} && (93) \\ &= (i\omega_n\tau_0 - \xi_k\tau_3 - \Delta\tau_1) - \underline{\Sigma}, && (94) \end{aligned}$$

gives the averaged Green's function, just

$$\underline{G}(k,\omega_n) = -\frac{i\tilde{\omega}_n\tau_0 + \tilde{\xi}_k\tau_3 + \tilde{\Delta}\tau_1}{\tilde{\omega}_n^2 + \tilde{\xi}_k^2 + \tilde{\Delta}^2}, \tag{95}$$

with

$$\begin{aligned} \tilde{\omega}_n &= \omega_n + n_i|u|^2 \sum_{k'} \frac{\omega_n}{\tilde{\omega}_n^2 + \tilde{\xi}_{k'}^2 + \tilde{\Delta}^2} = \omega_n + \Gamma_N \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}^2}} && (96) \\ \tilde{\xi}_k &= \xi_k - n_i|u|^2 \sum_{k'} \frac{\xi_{k'}}{\tilde{\omega}_n^2 + \tilde{\xi}_{k'}^2 + \tilde{\Delta}^2} = \xi_k && (97) \\ \tilde{\Delta} &= \Delta + n_i|u|^2 \sum_{k'} \frac{\Delta}{\tilde{\omega}_n^2 + \tilde{\xi}_{k'}^2 + \tilde{\Delta}^2} = \Delta + \Gamma_N \frac{\tilde{\Delta}}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}^2}}, && (98) \end{aligned}$$

where I've put $\Gamma_N = \pi N_0 |u|^2$. Note also that I assumed as usual a flat density of states in the normal state, and that the self-energy correction to ξ_k vanishes because of the $\xi_{k'}$ integration. The remaining two self-consistency equations, for $\tilde{\omega}_n$ and for $\tilde{\Delta}$, may be combined into a single equation for $\tilde{u} = \tilde{\omega}_n/\tilde{\Delta}$:

$$\tilde{u} = \frac{\omega_n + \frac{\tilde{u}}{\sqrt{\tilde{u}^2+1}}}{\Delta + \frac{1}{\sqrt{\tilde{u}^2+1}}} \tag{99}$$

which may be solved to give $\tilde{u} = \omega_n/\Delta$! This yields the desired result almost immediately, since the gap equation is

$$\begin{aligned} \Delta &= V \sum_k{}' F(k, 0^-) = V \sum_k{}' T \sum_{\omega_n} \frac{1}{2} \mathrm{Tr}[\tau_1 \underline{G}(k, \omega_n)] && (100) \\ &\simeq \pi N_0 V T \sum_{\omega_n}{}' \frac{1}{\sqrt{\tilde{u}^2+1}} = \pi N_0 V T \sum_{\omega_n}{}' \frac{\Delta}{\sqrt{\omega_n^2 + \Delta^2}}, && (101) \end{aligned}$$

where I have used $\tilde{u} = \omega_n/\Delta$ in the last step to show that the gap equation, and hence both $\Delta(T)$ and T_c itself are independent of impurity concentration since Γ_N has dropped out entirely.