Contents

5 Superconductivity

5.1 Phenomenology

Superconductivity was discovered in 1911 in the Leiden laboratory of Kamerlingh Onnes when a so-called "blue boy" (local high school student recruited for the tedious job of monitoring experiments) noticed that the resistivity of Hg metal vanished abruptly at about 4K. Although phenomenological models with predictive power were developed in the 30's and 40's, the microscopic mechanism underlying superconductivity was not discovered until 1957 by Bardeen Cooper and Schrieffer. Superconductors have been studied intensively for their fundamental interest and for the promise of technological applications which would be possible if a material which superconducts at room temperature were discovered. Until 1986, critical temperatures (T_c's) at which resistance disappears were always less than about 23K. In 1986, Bednorz and Mueller published a paper, subsequently recognized with the 1987 Nobel prize, for the discovery of a new class of materials which currently include members with T_c's of about 135K.

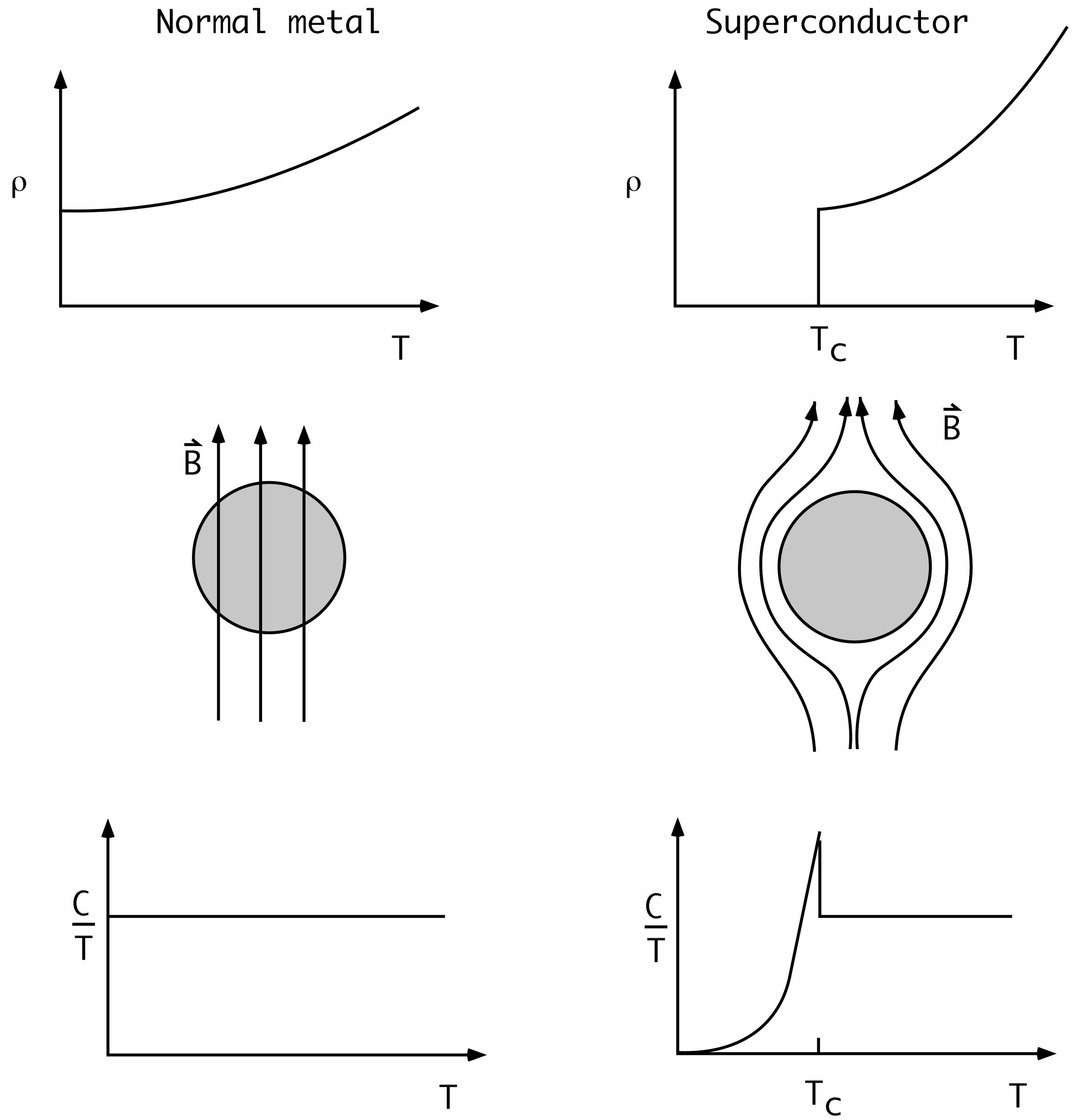

Figure 1: Properties of superconductors.

Superconducting materials exhibit the following unusual behaviors:

1. **Zero resistance**. Below a material's T_c, the DC electrical resistivity ρ is really zero, not just very small. This leads to the possibility of a related effect,

2. **Persistent currents**. If a current is set up in a superconductor with multiply connected topology, e.g. a torus,

it will flow forever without any driving voltage. (In practice experiments have been performed in which persistent currents flow for several years without signs of degrading).

3. **Perfect diamagnetism.** A superconductor expels a weak magnetic field nearly completely from its interior (screening currents flow to compensate the field within a surface layer of a few 100 or 1000 A, and the field at the sample surface drops to zero over this layer).

4. **Energy gap**. Most thermodynamic properties of a superconductor are found to vary as $e^{-\Delta/(k_B T)}$, indicating the existence of a gap, or energy interval with no allowed eigenenergies, in the energy spectrum. Idea: when there is a gap, only an exponentially small number of particles have enough thermal energy to be promoted to the available unoccupied states above the gap. In addition, this gap is visible in electromagnetic absorption: send in a photon at low temperatures (strictly speaking, $T = 0$), and no absorption is possible until the photon energy reaches 2Δ, i.e. until the energy required to break a pair is available.

5.2 Electron-phonon interaction

Superconductivity is due to an effective attraction between conduction electrons. Since two electrons experience a repulsive Coulomb force, there must be an additional attractive force between two electrons when they are placed in a metallic environment. In classic superconductors, this force is known to arise from the interaction with the ionic system. In previous discussion of a normal metal, the ions were replaced by a homogeneous positive background which enforces charge neutrality in the system. In reality, this medium is polarizable– the number of ions per unit volume can fluctuate in time. In particular, if we imagine a snapshot of a single electron entering a region of the metal, it will create a net positive charge density near itself by attracting the oppositely charged ions. Crucial here is that a typical electron close to the Fermi surface moves with velocity $v_F = \hbar k_F/m$ which is much larger than the velocity of the ions, $v_I = V_F m/M$. So by the time ($\tau \sim 2\pi/\omega_D \sim 10^{-13}$ sec) the ions have polarized themselves, 1st electron is long gone (it's moved a distance $v_F\tau \sim 10^8 cm/s \sim 1000\mathring{\text{A}}$, and 2nd electron can happen by to lower its energy with the concentration of positive charge before the ionic fluctuation relaxes away. This gives rise to an effective attraction between the two electrons as shown, which may be large enough to overcome the repulsive Coulomb interaction. Historically, this electron-phonon "pairing" mechanism was suggested by Frölich in 1950, and confirmed by the discovery of the "isotope effect", wherein T_c was found to vary as $M^{-1/2}$ for materials which were identical chemically but which were made with different isotopes.

The simplest model for the total interaction between two electrons in momentum states $\mathbf{k}$ and $\mathbf{k}'$, with $\mathbf{q} \equiv \mathbf{k} - \mathbf{k}'$, interacting both by direct Coulomb and electron-phonon forces, is given by

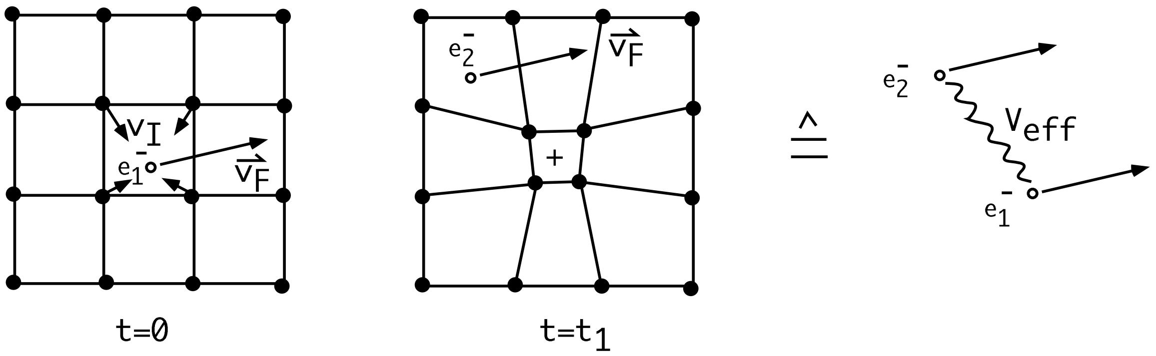

Figure 2: Effective attraction of two electrons due to "phonon exchange"

$$V(\mathbf{q},\omega) = \frac{4\pi e^2}{q^2+k_s^2} + \frac{4\pi e^2}{q^2+k_s^2}\,\frac{\omega_q^2}{\omega^2-\omega_q^2}, \tag{1}$$

in the jellium model. Here first term is Coulomb interaction in the presence of a medium with dielectric constant $\epsilon = 1+k_s^2/q^2$, and ω_q are the phonon frequencies. The screening length k_s^{-1} is $1A$ or so in a good metal. Second term is interaction due to exchange of phonons, i.e. the mechanism pictured in the figure. Note it is frequency-dependent, reflecting the *retarded* nature of interaction (see figure), and in particular that the 2nd term is attractive for $\omega < \omega_q \sim \omega_D$. Something is not quite right here, however; it looks indeed as though the two terms are of the same order as $\omega \to 0$; indeed they cancel each other there, and V is seen to be always repulsive. This indicates that the jellium approximation is too simple. We should probably think about a more careful calculation in a real system as producing two equivalent terms, which vary in approximately the same way with k_{TF} and $\omega_{\mathbf{q}}$, but with prefactors which are arbitrary. In some materials, then, the second term might "win" at low frequencies, depending on details. The BCS interaction is sometimes referred to as a "residual" attractive interaction, i.e. what is left when the long-range Coulomb

5.3 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

$$\psi(r_1, r_2) = \sum_{kq} u_k(q) e^{ik\cdot r_1} e^{-i(k+q)\cdot r_2} \zeta \tag{2}$$

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, $u_k(q) = u_k \delta_{q,0}$. Here is a quick argument related to the electron-phonon origin of the attractive interaction.[1] The electron-phonon interaction is strongest for those electrons with single-particle energies $\xi_{\mathbf{k}}$ within ω_D of the Fermi level. In the scattering process depicted in Fig. 3, momentum is

[1] Thanks to Kevin McCarthy, who forced me to think about this further

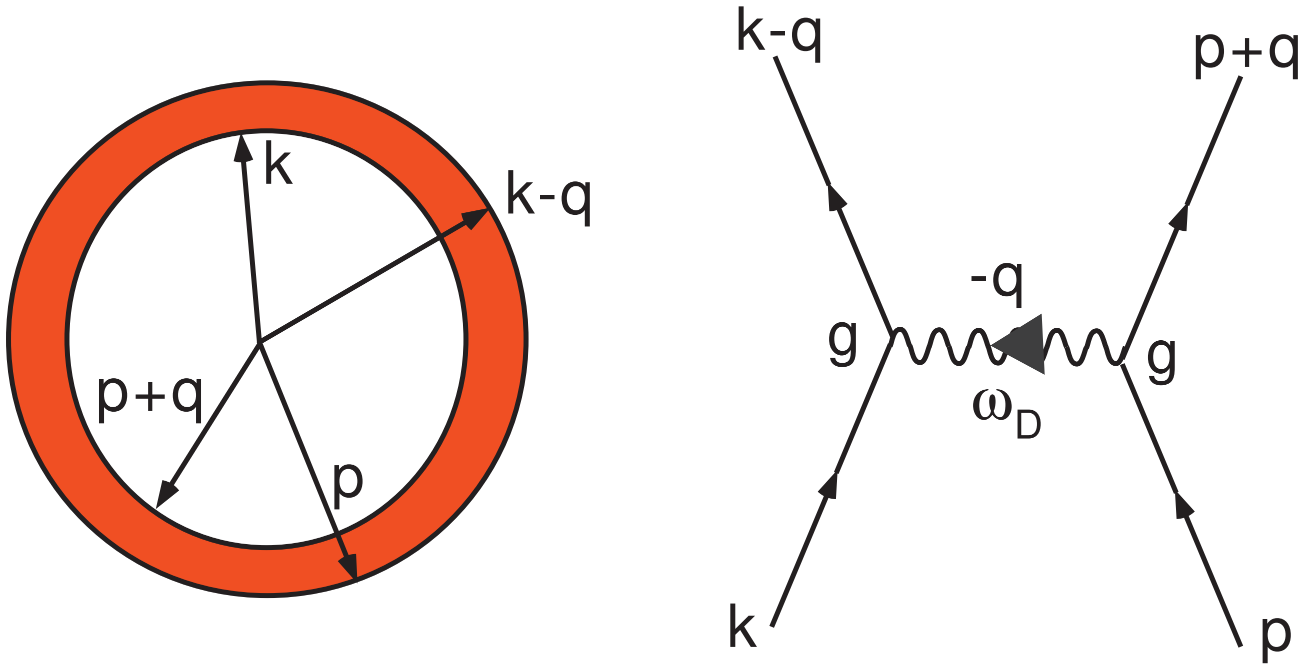

Figure 3: Electrons scattered by phonon exchange are confined to shell of thickness ω_D about Fermi surface.

explicitly conserved, i.e. the total momentum

$$\mathbf{k} + \mathbf{p} = \mathbf{K} \tag{3}$$

is the same in the incoming and outgoing parts of the diagram. Now look at Figure 4, and note that if $\mathbf{K}$ is not ~ 0, the phase space for scattering (attraction) is dramatically reduced. So the system can always lower its energy by creating $\mathbf{K} = 0$ pairs. Henceforth we will make this assumption, as Cooper did.

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

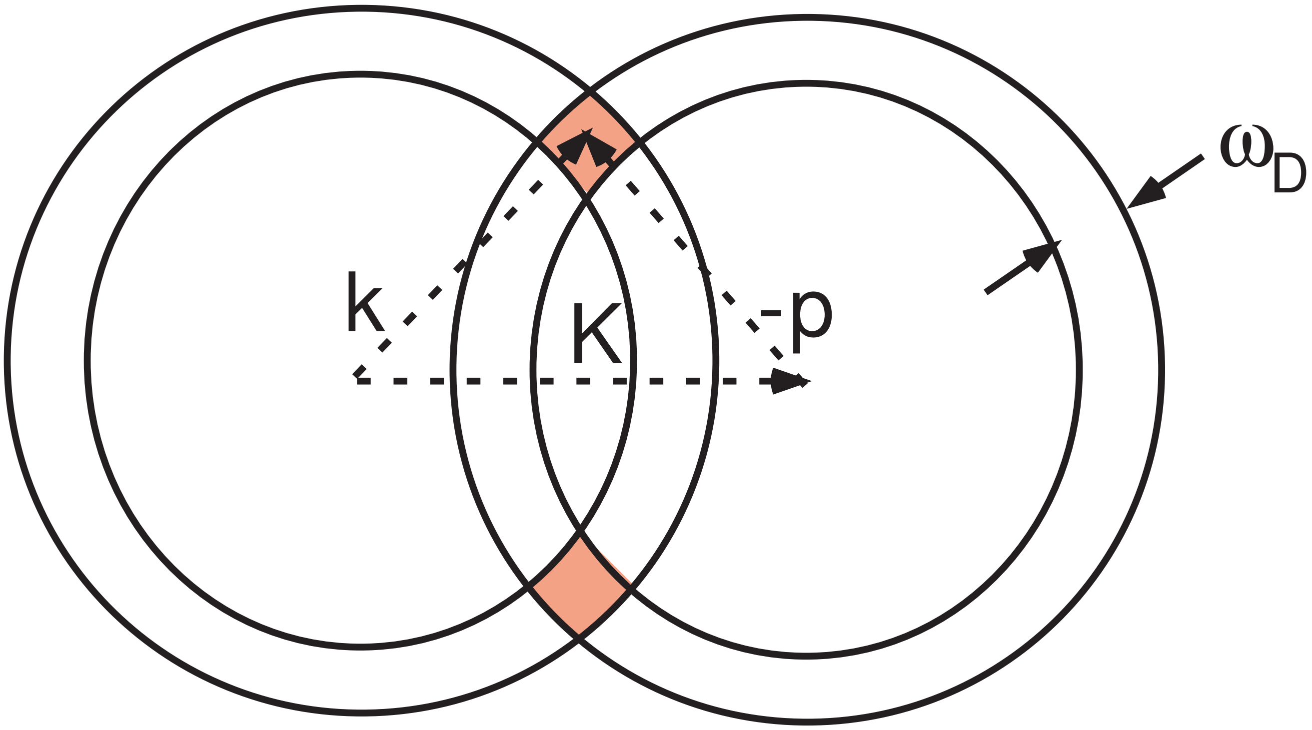

Figure 4: To get (attractive) scattering with finite cm momentum **K**, need both electron energies to be within ω_D of Fermi level– very little phase space.

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

$$H = -\frac{\nabla_1^2}{2m} - \frac{\nabla_2^2}{2m} + V(r_1, r_2). \tag{4}$$

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

$$(E - 2\epsilon_k)u_k = \sum_{k>k_F} V_{kk'}u_{k'}, \tag{5}$$

where $\epsilon_k = k^2/2m$ and the $V_{kk'} = \int d^3rV(r)e^{i(k'-k)\cdot r}$ 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

$$V_{kk'} = \begin{cases} -V & \xi_k, \xi_{k'} < \omega_c \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

where as usual $\xi_k \equiv \epsilon_k - \epsilon_F$. The BCS interaction $V_{kk'}$ is sometimes referred to as a "residual" attractive interaction, i.e. the attractive, short-distance part left when the long-range Coulomb interaction has been subtracted out, as in (1). The bound state equation becomes

$$u_k = \frac{V \sum_{k'}' u_{k'}}{2\epsilon_k - E}, \tag{7}$$

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 Σ_k, yielding

$$\frac{1}{V} = \sum_k' \frac{1}{2\epsilon_k - E} \tag{8}$$

$$\simeq \frac{1}{2} N_0 \int_{\epsilon_F}^{\epsilon_F+\omega_c} d\epsilon \frac{1}{2\epsilon - E} = \frac{1}{2} N_0 \log \frac{2\epsilon_F + 2\omega_c - E}{2\epsilon_F - E}. \tag{9}$$

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

$$\Delta_{\text{Cooper}} \equiv 2\epsilon_F - E \simeq 2\omega_c e^{-2/N_0 V}. \tag{10}$$

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.

5.4 Pair condensate & BCS Wavefctn.

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?

5.5 BCS Model.

A consistent theory of superconductivity may be constructed either using the full "effective interaction" or our approximation $V(\mathbf{q},\omega)$ 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:

$$H = H_0 - V \sum_{\substack{kk'q\\ \sigma\sigma'}}{}' c^\dagger_{k\sigma} c^\dagger_{-k+q\sigma'} c_{-k'+q\sigma'} c_{k'\sigma}, \tag{11}$$

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

[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.

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

$$\begin{aligned} c^\dagger_{k\sigma}c^\dagger_{-k+q\sigma'}c_{-k'+q\sigma'}c_{k'\sigma} &= [\langle c^\dagger_{k\sigma}c^\dagger_{-k+q\sigma'}\rangle + \delta(c^\dagger c^\dagger)] \times \\ &\quad \times[\langle c_{-k'+q\sigma'}c_{k'\sigma}\rangle + \delta(cc)], \quad (12) \end{aligned}$$

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 then becomes (check!)

$$H \simeq H_0 - (\Delta \sum_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow} + h.c.) + \Delta_k \langle c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\rangle^*, \qquad (13)$$

where

$$\Delta = V\sum_k \langle c_{-k\downarrow}c_{k\uparrow}\rangle. \qquad (14)$$

What BCS (actually Bogoliubov, after BCS) did was then to treat the *order parameter* Δ as a (complex) number, and calculate expectation values in the approximate Hamiltonian (13), insisting that Δ be determined self-consistently via Eq. (14) at the same time.

5.5.1 BCS wave function, gauge invariance, and number conservation.

What BCS actually did in their original paper is to treat the Hamiltonian (11) variationally. Their ansatz for the ground state of (11) is a trial state with the pairs $k\uparrow, -k\downarrow$ occupied with amplitude v_k and unoccupied with amplitude u_k, such that $|u_k|^2 + |v_k|^2 = 1$:

$$|\psi>= \Pi_k(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})|0> . \tag{15}$$

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 Hartree-Fock (BCS) Hamiltonian directly, together with the self-consistency equation for the order parameter; the two methods turn out to be equivalent. 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 $c^\dagger_{k\sigma} \rightarrow e^{i\theta}c^\dagger_{k\sigma}$. 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

[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.

simply related by a multiplicative phase factor.[4] Since H is independent of ϕ, however, all 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

$$|\psi(N)>= \int_0^{2\pi} d\phi e^{i\phi N/2}|\psi(\phi)> . \tag{16}$$

[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 calculat-

[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.

[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.

ing 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

$$\langle N\rangle = \langle\psi|\sum_{k\sigma} n_{k\sigma}|\psi\rangle = 2\sum_k |v_k|^2 \ ; \quad \langle(N-\langle N\rangle)^2\rangle = \sum_k u_k^2 v_k^2. \tag{17}$$

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 $< (N- < N >)^2 >\sim V$. 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.

5.5.2 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, since in this case the pairing interaction is most attractive. 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.

5.6 Thermodynamics

5.6.1 Bogoliubov transformation

We now return to (13) and discuss the solution by canonical transformation given by Bogoliubov. After our drastic approximation, we are left with a quadratic Hamiltonian in the c's, but with $c^\dagger c^\dagger$ and cc terms in addition to $c^\dagger c$'s. We can diagonalize it easily, however, by introducing the *quasiparticle operators* $\gamma_{\mathbf{k}0}$ and $\gamma_{\mathbf{k}1}$ by

$$\begin{aligned} c_{\mathbf{k}\uparrow} &= u_{\mathbf{k}}^* \gamma_{\mathbf{k}0} + v_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger \\ c_{-\mathbf{k}\downarrow}^\dagger &= -v_{\mathbf{k}}^* \gamma_{\mathbf{k}0} + u_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger . \end{aligned} \tag{18}$$

You may check that this transformation is canonical (preserves fermion comm. rels.) if $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$. Substituting into (13) and using the commutation relations we get

$$\begin{aligned} H_{BCS} = & \sum_{\mathbf{k}} \xi_{\mathbf{k}} [(|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2)(\gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} + \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1}) + 2|v_{\mathbf{k}}|^2 \\ & + 2u_{\mathbf{k}}^* v_{\mathbf{k}}^* \gamma_{\mathbf{k}1}\gamma_{\mathbf{k}0} + 2u_{\mathbf{k}} v_{\mathbf{k}} \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}0}^\dagger] \\ & + \sum_{\mathbf{k}} [(\Delta_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}^* + \Delta_{\mathbf{k}}^* u_{\mathbf{k}}^* v_{\mathbf{k}})(\gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} + \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1} - 1) \\ & + (\Delta_{\mathbf{k}} v_{\mathbf{k}}^{*2} - \Delta_{\mathbf{k}}^* u_{\mathbf{k}}^{*2}) \gamma_{\mathbf{k}1}\gamma_{\mathbf{k}0} + (\Delta_{\mathbf{k}}^* v_{\mathbf{k}}^2 - \Delta_{\mathbf{k}} u_{\mathbf{k}}^2) \gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}1}^\dagger \\ & + \Delta_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \rangle^* , \end{aligned} \tag{19}$$

which does not seem to be enormous progress, to say the least. But the game is to eliminate the terms which are not of the form $\gamma^\dagger\gamma$, so to be left with a sum of independent number-type terms whose eigenvalues we can write down. The coefficients of the $\gamma^\dagger\gamma^\dagger$ and $\gamma\gamma$ type terms are seen to vanish if we choose

$$2\xi_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} + \Delta^*_{\mathbf{k}}v^2_{\mathbf{k}} - \Delta_{\mathbf{k}}u^2_{\mathbf{k}} = 0. \tag{20}$$

This condition and the normalization condition $|u_{\mathbf{k}}|^2+|v_{\mathbf{k}}|^2 = 1$ are both satisfied by the solutions

$$\begin{matrix} |u_{\mathbf{k}}|^2 \\ |v_{\mathbf{k}}|^2 \end{matrix} = \frac{1}{2}\left(1 \pm \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \tag{21}$$

where I defined the *Bogolibov quasiparticle energy*

$$E_{\mathbf{k}} = \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}. \tag{22}$$

The BCS Hamiltonian has now been *diagonalized*:

$$H_{BCS} = \sum_{\mathbf{k}} E_{\mathbf{k}}\left(\gamma^\dagger_{\mathbf{k}0}\gamma_{\mathbf{k}0} + \gamma^\dagger_{\mathbf{k}1}\gamma_{\mathbf{k}1}\right) + \sum_{\mathbf{k}}\left(\xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}}\langle c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\rangle^*\right). \tag{23}$$

Note the second term is just a constant, which will be important for calculating the ground state energy accurately. The first term, however, just describes a set of *free fermion* excitations above the ground state, with spectrum $E_{\mathbf{k}}$.

5.6.2 Density of states

The BCS spectrum is easily seen to have a minimum $\Delta_{\mathbf{k}}$ for a given direction $\mathbf{k}$ on the Fermi surface; $\Delta_{\mathbf{k}}$ therefore, in addition to playing the role of *order parameter* for the superconducting transition, is also the *energy gap* in the 1-particle spectrum. To see this explicitly, we can simply do a change of variables in all energy integrals from the normal metal eigenenergies $\xi_{\mathbf{k}}$ to the quasiparticle energies $E_{\mathbf{k}}$:

$$N(E)dE = N_N(\xi)d\xi. \tag{24}$$

If we are interested in the standard case where the gap Δ is much smaller than the energy over which the normal state dos $N_N(\xi)$ varies near the Fermi level, we can make the replacement

$$N_N(\xi) \simeq N_N(0) \equiv N_0, \tag{25}$$

so using the form of $E_{\mathbf{k}}$ from (22) we find

$$\frac{N(E)}{N_0} = \begin{cases} \frac{E}{\sqrt{E^2-\Delta^2}} & E > \Delta \\ 0 & E < \Delta \end{cases}. \tag{26}$$

This function is sketched in Figure 5.

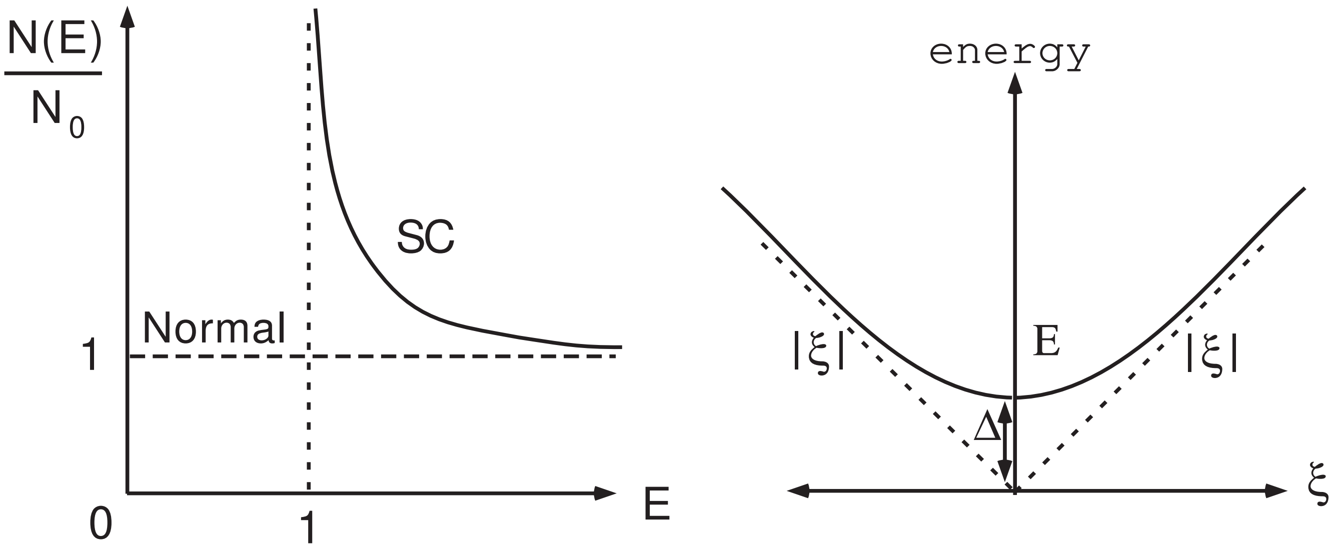

Figure 5: a) Normalized density of states; b) Quasiparticle spectrum.

5.6.3 Critical temperature

The critical temperature is defined as the temperature at which the order parameter $\Delta_{\mathbf{k}}$ vanishes. We can now calculate this with the aid of the diagonalized Hamiltonian. The self-consistency condition is

$$\begin{aligned}
\Delta_{\mathbf{k}}^* &= V \sum_{\mathbf{k}'} \langle c_{\mathbf{k}'\uparrow}^\dagger c_{-\mathbf{k}'\downarrow}^\dagger \rangle^* \\
&= V \sum_{\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}^* \langle 1 - \gamma_{\mathbf{k}0}^\dagger \gamma_{\mathbf{k}0} - \gamma_{\mathbf{k}1}^\dagger \gamma_{\mathbf{k}1} \rangle \\
&= V \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}^*}{2E_{\mathbf{k}}} \left(1 - 2f(E_{\mathbf{k}})\right) . \qquad (27)
\end{aligned}$$

Since $1 - 2f(E) = \tanh[E/(2T)]$, the *BCS gap equation* reads

$$\boxed{\Delta_{\mathbf{k}}^* = V \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}^*}{2E_{\mathbf{k}'}} \tanh \frac{E_{\mathbf{k}'}}{2T}} \qquad (28)$$

This equation may now be solved, first for the critical temperature itself, i.e. 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

$$\frac{1}{N_0 V} = \int_0^{\omega_D} d\xi_k \frac{1}{\xi_k} \tanh \frac{\xi_k}{2T_c}. \tag{29}$$

This integral can be approximated carefully, but it is useful to get a sense of what is going on by doing a crude treatment. Note that since $T_c \ll \omega_D$ generally, most of the integrand weight occurs for $\xi > T$, so we can estimate the tanh factor by 1. The integral is log divergent, which is why the cutoff ω_D is so important. We find

$$\frac{1}{N_0 V_0} = \log \frac{\omega}{T_c} \quad \Rightarrow \quad T_c \simeq \omega_D e^{-1/N_0 V} \tag{30}$$

The more accurate analysis of the integral gives the BCS result

$$\boxed{T_c = 1.14 \omega_D e^{-1/N_0 V}} \tag{31}$$

We can do the same calculation *near* T_c, expanding to leading order in the small quantity $\Delta(T)/T$, to find $\Delta(T)/T_c \simeq 3.06(1 - T/T_c)^{1/2}$. At $T = 0$ we have

$$\frac{1}{N_0 V} = \int_0^{\omega_D} d\xi_k \frac{1}{E_k} = \int_\Delta^{\omega_D} dE N(E)/E \tag{32}$$

$$= \int_\Delta^{\omega_D} dE \frac{1}{\sqrt{E^2 - \Delta^2}} \simeq \ln(2\omega_d/\Delta), \tag{33}$$

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 6). 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.

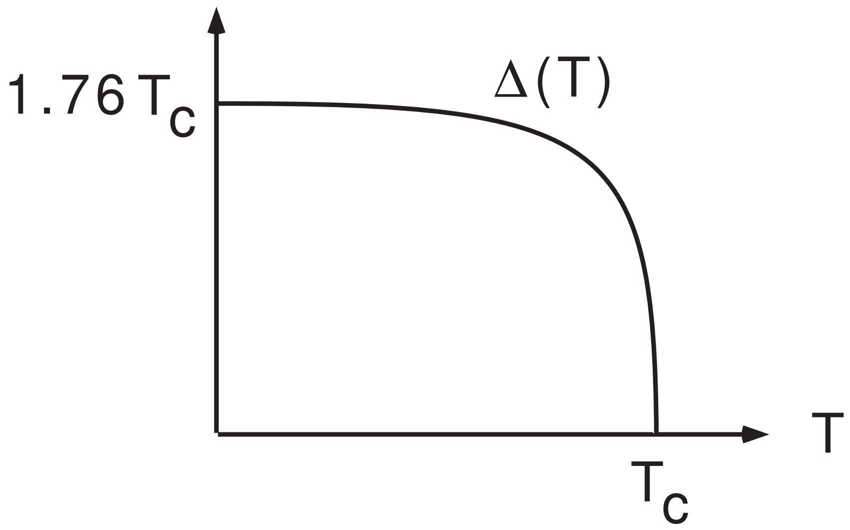

Figure 6: BCS order parameter as fctn. of T.

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 $= T_c$:

$$\Delta(T) = \delta_{sc} T_c \tanh\{\frac{\pi}{\delta_{sc}}\sqrt{a\frac{\delta C}{C_N}(\frac{T_c}{T} - 1)}\}, \tag{34}$$

where $\delta_{sc} = \Delta(0)/T_c = 1.76$, $a = 2/3$, and $\delta C/C_N = 1.43$ is the normalized specific heat jump.[6] This is another of the "universal" ratios which the BCS theory predicted and which helped confirm the theory in classic superconductors.

5.6.4 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 quasi-

[6]Note to evaluate the last quantity, we need only use the calculated temperature dependence of Δ near T_c, and insert into Eq. (47).

particles 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 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

$$S = -k_B \int_0^\infty dE N(E)\{f(E)\ln f(E)+[1-f(E)]\ln[1-f(E)]\}, \tag{35}$$

where $f(E)$ 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

$$C_{el,V} = \frac{2}{T}\int dE N(E)(\frac{-\partial f}{\partial E})[E^2 - \frac{1}{2}T\frac{d\Delta^2}{dT}]. \tag{36}$$

A sketch of the result of a full numerical evaluation is shown in Figure 1. 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 $T \ll \Delta$, $f(E) \simeq e^{-E/T}$ and the density of states factor $N(E)$ in the integral cuts off the integration at the lower limit Δ, giving $C \simeq (N_0\Delta^{5/2}/T^{3/2})e^{-\Delta/T}$.[7]

[7] To obtain this, try the following:

- replace the derivative of Fermi function by exp-E/T
- do integral by parts to remove singularity at Delta
- expand around Delta E = Delta + delta E
- change integration variables from E to delta E

Somebody please check my answer!

Note the first term in Eq. (47)is continuous through the transition $\Delta \to 0$ (and reduces to the normal state specific heat $(2\pi^2/3)N_0T$ above T_c), but the second one gives a discontinuity at T_c of $(C_N - C_S)/C_N = 1.43$, where $C_S = C(T_c^-)$ and $C_N = C(T_c^+)$. To evaluate (36), we need the T dependence of the order parameter from a general solution of (28).

5.7 Electrodynamics

5.7.1 Linear response to vector potential

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

$$H_0 = \frac{1}{2m} \sum_\sigma \int d^3r \psi_\sigma^\dagger(r)[-i\nabla - (\frac{e}{c})\mathbf{A}]^2 \psi_\sigma(r), \qquad (37)$$

and the second quantized current density operator is given by

$$\begin{aligned} \mathbf{j}(r) &= \frac{e}{2m}\{\psi^\dagger(r)(-i\nabla - \frac{e}{c}\mathbf{A})\psi(r) + [(i\nabla - \frac{e}{c}\mathbf{A})\psi^\dagger(r)]\psi(r)\} && (38) \\ &= \mathbf{j}_{para} - \frac{e^2}{mc}\psi^\dagger(r)\psi(r)\mathbf{A}, && (39) \end{aligned}$$

where

$$\mathbf{j}_{para}(r) = \frac{-ie}{2m}\{\psi^\dagger(r)\nabla\psi(r) - (\nabla\psi^\dagger(r))\psi(r)\}, \tag{40}$$

or in Fourier space,

$$\mathbf{j}_{para}(\mathbf{q}) \;=\; \frac{e}{m}\sum_{\mathbf{k}\sigma}\mathbf{k}c^\dagger_{\mathbf{k}-\mathbf{q}\sigma}c_{\mathbf{k}\sigma} \tag{41}$$

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

$$H' = \int d^3r\mathbf{j}_{para}\cdot\mathbf{A} = \frac{e}{mc}\sum_{k\sigma}\mathbf{k}\cdot\mathbf{A}(\mathbf{q})c^\dagger_{\mathbf{k}-\mathbf{q}\sigma}c_{\mathbf{q}\sigma}. \tag{42}$$

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

$$\langle\mathbf{j}\rangle(\mathbf{q},\omega) = \underline{K}(\mathbf{q},\omega)\mathbf{A}(\mathbf{q},\omega) \tag{43}$$

with

$$\underline{K}(\mathbf{q},\omega) = -\frac{ne^2}{mc} + \langle[\mathbf{j}_{para},\mathbf{j}_{para}]\rangle(\mathbf{q},\omega). \tag{44}$$

Note the first term in the current

$$\mathbf{j}_{dia}(\mathbf{q},\omega) \equiv -\frac{ne^2}{mc}\mathbf{A}(\mathbf{q},\omega) \tag{45}$$

is purely *diagmagnetic*, i.e. these currents tend to screen the external field (note sign). The second, *paramagnetic* term is formally the Fourier transform of the current-current correlation function (correlation function used in the sense of our discussion of the Kubo formula).[8] Here are a few remarks on this expression:

- Note the simple product structure of (43) 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.[9]

- Note also that the electric field in a gauge where the electrostatic potential is set to zero may be written $\mathbf{E}(\mathbf{q},\omega) = -i\omega\mathbf{A}(\mathbf{q},\omega)$, so that the *complex* conductivity of the system defined by $\mathbf{j} = \underline{\sigma}\mathbf{E}$ may be written

$$\underline{\sigma}(\mathbf{q},\omega) = \frac{i}{\omega}\underline{K}(\mathbf{q},\omega) \tag{47}$$

- What happens in a normal metal? The paramagnetic second term *cancels* the diamagnetic response at $\omega = 0$, leaving no real part of K (Im part of σ), i.e. the conductivity is purely dissipative and not inductive at $\omega, \mathbf{q} = 0$ in the normal metal.

5.7.2 Meissner Effect.

There is a theorem of classical physics proved by Bohr[10] which states that the ground state of a system of charged particles

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

[9] If we transformed back, we'd get the convolution

$$\mathbf{j}(\mathbf{r}) = \int d^3r' K(\mathbf{r},\mathbf{r}')\mathbf{A}(\mathbf{r}') \tag{46}$$

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

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 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 7, and compared to schematics of practical experimental setups involving resonant coils and microwave cavities in Figs. 7 a)-c). In the *gedanken* experiment

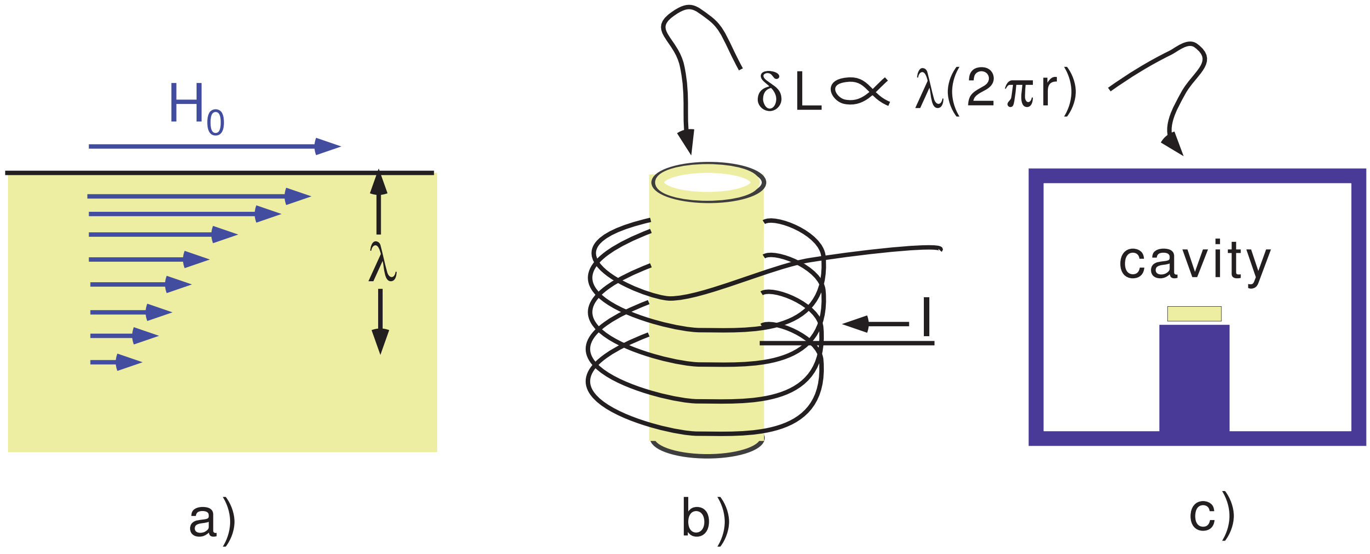

Figure 7: a) Half-space geometry for penetration depth calculation; b) Resonant coil setup; c) Microwave cavity

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 $\omega = 0, q \to \infty$ 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

$$\mathbf{j} = -\frac{c}{4\pi}\lambda^{-2}\mathbf{A}, \tag{48}$$

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

$$\nabla \times \mathbf{B} = -\nabla^2 \mathbf{A} = \frac{4\pi}{c}\mathbf{j} = -\lambda^{-2}\mathbf{A}, \tag{49}$$

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" λ depends on temperature.

Evaluating the expressions in (44) in full generality is tedious and is usually done with standard many-body methods beyond the scope of this course. However for $\mathbf{q} = 0$ the calculation is simple enough to do without resorting to Green's functions. First note that the perturbing Hamiltonian H' may be written in terms of the quasiparticle operators (18) as

$$H' = \tag{50}$$
$$-\frac{e}{mc}\sum_{\mathbf{k}} \mathbf{k}\cdot\mathbf{A}(\mathbf{q})\Big[(u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}} + v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}})(\gamma^\dagger_{\mathbf{k}+\mathbf{q}0}\gamma_{\mathbf{k}0} - \gamma^\dagger_{\mathbf{k}+\mathbf{q}1}\gamma_{\mathbf{k}1})$$
$$+(v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}} - u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}})(\gamma^\dagger_{\mathbf{k}+\mathbf{q}0}\gamma^\dagger_{\mathbf{k}1} - \gamma_{\mathbf{k}+\mathbf{q}1}\gamma_{\mathbf{k}0})\Big]$$

$$\underset{q\to 0}{\rightarrow} \; -\frac{e}{mc}\sum_{\mathbf{k}} \mathbf{k}\cdot\mathbf{A}(0)(\gamma^\dagger_{\mathbf{k}0}\gamma_{\mathbf{k}0} - \gamma^\dagger_{\mathbf{k}1}\gamma_{\mathbf{k}1}) \tag{51}$$

If you compare with the $\mathbf{A} = \mathbf{0}$ Hamiltonian (23), we see that the new excitations of the system are

$$\begin{aligned} E_{\mathbf{k}0} &\rightarrow E_{\mathbf{k}} - \frac{e}{mc}k\cdot\mathbf{A}(0) \\ E_{\mathbf{k}1} &\rightarrow E_{\mathbf{k}} + \frac{e}{mc}k\cdot\mathbf{A}(0) \end{aligned} \tag{52}$$

We may similarly insert the quasiparticle operators (18) into the expression for the expectation value of the paramagnetic current operator(41):

$$\begin{aligned} \langle \mathbf{j}_{para}(\mathbf{q}=0)\rangle &= \frac{e}{m}\sum_{\mathbf{k}}\langle(\gamma^\dagger_{\mathbf{k}0}\gamma_{\mathbf{k}0} - \gamma^\dagger_{\mathbf{k}1}\gamma_{\mathbf{k}1})\rangle \\ &= \frac{e}{m}\sum_{\mathbf{k}}\left(f(E_{\mathbf{k}0}) - f(E_{\mathbf{k}1})\right). \end{aligned} \tag{53}$$

We are interested in the *linear response* $\mathbf{A} \rightarrow 0$, so that when we expand wrt $\mathbf{A}$, the paramagnetic contribution becomes

$$\langle \mathbf{j}_{para}(\mathbf{q}=0)\rangle = \frac{2e^2}{m^2c}\sum_{\mathbf{k}}\left[\mathbf{k}\cdot\mathbf{A}(0)\right]\mathbf{k}\left(-\frac{\partial f}{\partial E_{\mathbf{k}}}\right). \tag{54}$$

Combining now with the definition of the response function K and the diamagnetic current (45), and recalling $\sum_{\mathbf{k}} \rightarrow$

$N_0 \int d\xi_{\mathbf{k}}(d\Omega/4\pi)$, with $N_0 = 3n/(2\epsilon_F)$ and $\int(d\Omega/4\pi)\mathbf{kk} = \underline{1}/3$, we get for the static homogeneous response is therefore

$$\underline{K}(0,0) = \frac{-ne^2}{mc}\{1 - \int d\xi_k(\frac{-\partial f}{\partial E_k})\}\underline{1} \tag{55}$$

$$\equiv \frac{-n_s(T)e^2}{mc}\underline{1} \tag{56}$$

where in the last step, I defined the *superfluid density* to be $n_s(T) \equiv n - n_n(T)$, with *normal fluid density*

$$\boxed{n_n(T) \equiv n \int d\xi_k \ \left(\frac{-\partial f}{\partial E_k}\right)}. \tag{57}$$

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 $n_n \to 1$.[11] Correspondingly, the superfluid density as defined varies between n at $T = 0$ 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.[12]

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

$$\lambda(T) = (\frac{mc^2}{4\pi n_s(T)e^2})^{1/2}. \tag{58}$$

[11] The dimensioness function $n_n(T/T_c)/n$ is sometimes called the Yoshida function, $Y(T)$, and is plotted in Fig.8.

[12] 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.

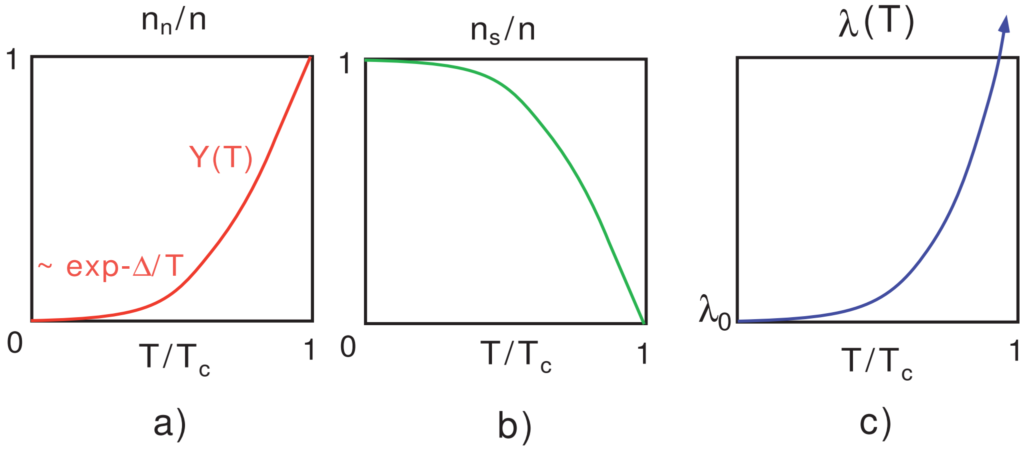

Figure 8: a) Yoshida function; b) superfluid density ; c) penetration depth

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. (57). [See homework.] Close to T_c, the penetration depth diverges as it must, since in the normal state the field penetrates the sample completely.

5.7.3 Dynamical conductivity.

The calculation of the full, frequency dependent conductivity is beyond the scope of this course. If you would like to read an old-fashioned derivation, I refer you to Tinkham's book. The main point to absorb here is that, as in a semiconductor with a gap, at $T = 0$ there is no process by which a photon can be absorbed in a superconductor until its energy exceeds 2Δ, the binding energy of the pair. This "threshold" for optical absorption is one of the most direct measurements of the gaps of the old superconductors.

6 Ginzburg-Landau Theory

6.1 GL Free Energy

While the BCS weak-coupling theory we looked at the last two weeks is very powerful, and provides at least a qualitatively correct description of most aspects of classic superconductors,[13] there is a complementary theory which a) is simpler and more physically transparent, although valid only near the transition; and b) provides exact results under certain circumstances. This is the Ginzburg-Landau theory [V.L. Ginzburg and L.D. Landau, Zh. Eksp. Teor. Fiz. 20, 1064 (1950)], which received remarkably little attention in the west until Gor'kov showed it was derivable from the BCS theory. [L.P. Gor'kov, Zh. Eksp. Teor Fiz. 36, 1918 (1959)]. The theory simply postulated the existence of a macrosopic quantum wave function $\psi(r)$ which was equivalent to an order parameter, and proposed that on symmetry grounds alone, the free energy density of a superconductor should be expressible in terms of an expansion in this quantity:

$$\frac{f_s - f_n}{V} = a|\psi|^2 + b|\psi|^4 + \frac{1}{2m^*}|(\nabla + \frac{ie^*}{c}\vec{A})\psi|^2, \qquad (59)$$

[13] In fact one could make a case that the BCS theory is the most quantitatively accurate theory in all of condensed matter physics

where the subscripts n and s refer to the normal and superconducting states, respectively.

Let's see why GL might have been led to make such a "guess". The superconducting-normal transition was empirically known to be second order in zero field, so it was natural to write down a theory analogous to the Landau theory of a ferromagnet, which is an expansion in powers of the magnetization, **M**. The choice of order parameter for the superconductor corresponding to **M** for the ferromagnet was not obvious, but a complex scalar field ψ was a natural choice because of the analogy with liquid He, where $|\psi|^2$ is known to represent the superfluid density n_s;[14] a quantum mechanical density should be a complex wave function squared. The biggest leap of GL was to specify correctly how electromagnetic fields (which had no analog in superfluid He) would couple to the system. They exploited in this case the similarity of the formalism to ordinary quantum mechanics, and coupled the fields in the usual way to "charges" e^* associated with "particles" of mass m^*. Recall for a real charge in a magnetic field, the kinetic energy is:

$$
\begin{aligned}
< \Psi|\mathcal{H}_{kin}|\Psi > &= -\frac{1}{2m}\int d^3r\Psi^*(\nabla + \frac{ie}{c}\vec{A})^2\Psi && (60)\\
&= \frac{1}{2m}\int d^3r|(\nabla + \frac{ie}{c}\vec{A})\Psi|^2, && (61)
\end{aligned}
$$

after an integration by parts in the second step. GL just replaced e, m with e^*, m^* to obtain the kinetic part of Eq. (59);

[14] ψ in the He case has the microscopic interpretation as the Bose condensate amplitude.

they expected that e^* and m^* were the elementary electron charge and mass, respectively, but did not assume so.

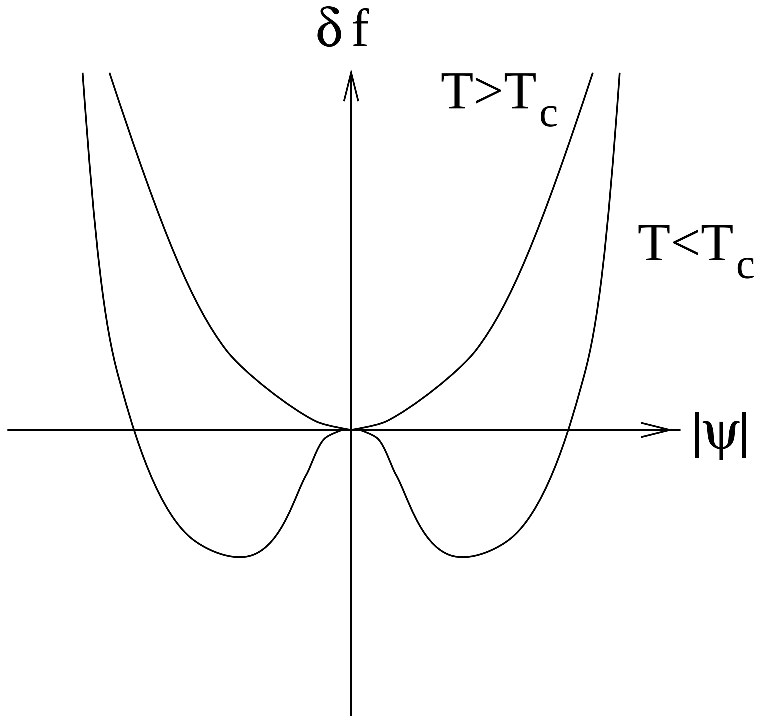

Figure 9: Mexican hat potential for superconductor.

A system described by this free energy will undergo a second-order phase transition in zero field when $a = 0$: clearly when a is positive, the system can minimize δf by having $\psi = 0$ (no superconductivity), whereas if a is negative, δf has a minimum with $\psi \neq 0$. The free energy (59) is a *functional* of the order parameter ψ, meaning the actual value of the order parameter realized in equilibrium satisfies $\delta f/\delta\psi = 0$.[15] Notice f is independent of the phase ϕ of the order parameter, $\psi \equiv |\psi|e^{i\phi}$, and so the ground state for $a < 0$ is equivalent to any state ψ related to it by multiplication by a pure phase. This is the $U(1)$ gauge invariance of which we spoke earlier.

[15]Thus you should not be perturbed by the fact that f apparently depends on ψ even for $a > 0$. The value of f in equilibrium will be $f_n = f[\psi = 0]$.

This symmetry is broken when the system chooses one of the ground states (phases) upon condensation (Fig 1.).

For a uniform system in zero field, the total free energy $F = \int d^3r f$ is minimized when f is, so one find for the order parameter at the minimum,

$$|\psi|_{eq} = [\tfrac{-a}{2b}]^{1/2}, \quad a < 0 \tag{62}$$
$$|\psi|_{eq} = 0, \qquad a > 0. \tag{63}$$

When a changes sign, a minimum with a nonzero value becomes possible. For a second order transition as one lowers the temperature, we assume that a and b are smooth functions of T near T_c. Since we are only interested in the region near T_c, we take only the leading terms in the Taylor series expansions in this region: $a(T,H) = a_0(T - T_c)$ and $b =$ constant. Eqs. (62) and (63) take the form:

$$|\psi(T)|_{eq} = [\tfrac{a_0(T_c-T)}{2b}]^{1/2}, \quad T < T_c \tag{64}$$
$$|\psi(T)|_{eq} = 0, \qquad T > T_c. \tag{65}$$

Substituting back into Eqs.59, we find:

$$f_s(T) - f_n(T) = -\tfrac{a_0^2}{4b}(T_c - T)^2, \quad T < T_c \tag{66}$$
$$f_s(T) - f_n(T) = 0, \qquad T > T_c. \tag{67}$$

The idea now is to calculate various observables, and determine the GL coefficients for a given system. Once they are determined, the theory acquires predictive power due to its extreme simplicity. It should be noted that GL theory is applied to many systems, but it is in classic superconductors that it is most accurate, since the critical region, where deviations from mean field theory are large, is of order 10^{-4} or less. Near the transition it may be taken to be exact for all practical purposes. This is not the case for the HTSC, where the size of the critical region has been claimed to be as much as 10-20K in some samples.

Supercurrents. Let's now focus our attention on the term in the GL free energy which leads to supercurrents, the kinetic energy part:

$$
\begin{aligned}
F_{\rm kin} &= \int d^3r \frac{1}{2m^*}|(\nabla + \frac{ie^*}{c}\vec{A})\psi|^2 & (68)\\
&= \int d^3r \frac{1}{2m^*}[(\nabla|\psi|)^2 + (\nabla\phi - e^*/c\mathbf{A})^2|\psi|^2]. & (69)
\end{aligned}
$$

These expressions deserve several remarks. First, note that the free energy is gauge invariant, if we make the transformation $\vec{A} \rightarrow \vec{A} + \nabla\Lambda$, where Λ is any scalar function of position, while at the same time changing $\psi \rightarrow \psi \exp(-ie^*\Lambda/c)$. Second, note that in the last step above I have split the kinetic part of f into a term dependent on the gradients of the order parameter magnitude $|\psi|$ and on the gradients of the phase ϕ. Let us use a little intuition to guess what these terms mean. The energy of the superconducting state below T_c is lower than that of the normal state by an amount called the *condensation energy.*[16] From Eq. (59) in zero field this is of order $|\psi|^2$ very close to the transition. To make spatial variations of the *magnitude* of ψ must cost a significant fraction of the condensation energy in the region of space in which it

[16]We will see below from the Gorkov derivation of GL from BCS that it is of order $N(0)\Delta^2$.

occurs.[17] On the other hand, the zero-field free energy is actually invariant with respect to changes in ϕ, so fluctuations of ϕ alone actually cost no energy.

With this in mind, let's ask what will happen if we apply a weak magnetic field described by $\mathbf{A}$ to the system. Since it is a small perturbation, we don't expect it to couple to $|\psi|$ but rather to the phase ϕ. The kinetic energy density should then reduce to the second term in Eq. (69), and furthermore we expect that it should reduce to the intuitive two-fluid expression for the kinetic energy due to supercurrents, $\frac{1}{2}mn_sv_s^2$. Recall from the superfluid He analogy, we expect $|\psi|^2 \equiv n_s^*$ to be a kind of density of superconducting electrons, but that we aren't certain of the charge or mass of the "particles". So let's put

$$f_{\text{kin}} \simeq \frac{1}{2m^*}|(\nabla + \frac{ie^*}{c}\vec{A})\psi|^2. = \int d^3r \frac{1}{2m^*}(\nabla\phi - e^*/c\mathbf{A})^2|\psi|^2 \equiv \frac{1}{2}m^*n_s^*v_s^2. \tag{70}$$

Comparing with Eq. (xx), we find that the *superfluid velocity* must be

$$\vec{v_s} = \frac{1}{m^*}(\nabla\phi + \frac{e^*}{c}\vec{A}). \tag{71}$$

Thus the gradient of the phase is related to the superfluid velocity, but the vector potential also appears to keep the entire formalism gauge-invariant.

Meissner effect. The Meissner effect now follows immediately from the two-fluid identifications we have made. The

[17] We can make an analogy with a ferromagnet, where if we have a *domain wall* the magnetization must go to zero at the domain boundary, costing lots of surface energy.

supercurrent density will certainly be just

$$\vec{j}_s = -e^* n_s^* \vec{v}_s = -\frac{e^* n_s^*}{m^*}(\nabla \phi + \frac{e^*}{c}\vec{A}). \tag{72}$$

Taking the curl of this equation, the phase drops out, and we find the magnetic field:

$$\nabla \times \vec{j}_s = -\frac{e^{*2} n_s^*}{m^* c}\vec{B}. \tag{73}$$

Now recall the Maxwell equation

$$\vec{j}_s = \frac{c}{4\pi}\nabla \times \vec{B}, \tag{74}$$

which, when combined with (14), gives

$$\frac{c}{4\pi}\nabla \times \nabla \times \vec{B} = -\frac{c}{4\pi}\nabla^2 \vec{B} = -\frac{e^{*2} n_s}{m^* c}\vec{B}, \tag{75}$$

or

$$\lambda^2 \nabla^2 \vec{B} = \vec{B}, \tag{76}$$

where

$$\lambda = \left(\frac{m^* c^2}{4\pi e^{*2} n_s^*}\right)^{1/2}. \tag{77}$$

Notice now that if we use what we know about Cooper pairs, this expression reduces to the BCS/London penetration depth. We assume e^* is the charge of the pair, namely $e^* = 2e$, and similarly $m^* = 2m$, and $|\psi|^2 = n_s^* = n_s/2$ since n_s^* is the density of pairs.

Flux quantization. If we look at the flux quantization described in Part 1 of these notes, it is clear from our subsequent discussion of the Meissner effect, that the currents which lead to flux quantization will only flow in a small part of the cross section, a layer of thickness λ. This layer encloses the flux passing through the toroid. Draw a contour C in the interior of the toroid, as shown in Figure 10. Then $v_s = 0$ everywhere on C. It follows that

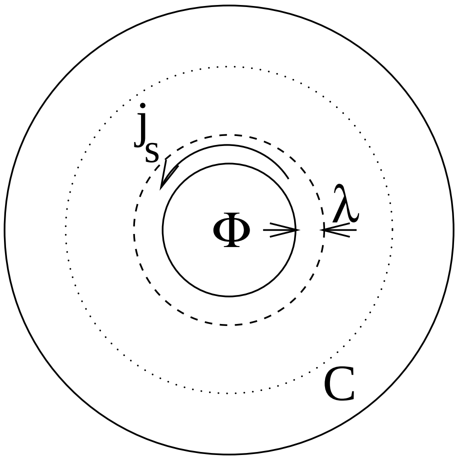

Figure 10: Quantization of flux in a toroid.

$$0 = \oint_C d\vec{\ell} \cdot \vec{v_s} = \frac{1}{m^*} \oint_C d\vec{\ell} \cdot (\nabla\phi + \frac{e^*}{c}\vec{A}). \qquad (78)$$

The last integral may be evaluated using

$$\oint_C d\vec{\ell} \cdot \nabla\phi = 2\pi \times integer, \qquad (79)$$

and

$$\begin{aligned} \frac{e^*}{c} \oint_C d\vec{\ell} \cdot \vec{A} &= \frac{e^*}{c} \int_S d\vec{S} \cdot \nabla \times \vec{A} && (80) \\ &= \frac{e^*}{c} \int_S d\vec{S} \cdot \vec{B} && (81) \\ &= \frac{e^*}{c} \Phi. && (82) \end{aligned}$$

Here S is a surface spanning the hole and Φ the flux through the hole. Combining these results,

$$\Phi = 2\pi \frac{\hbar c}{2e} n = n \frac{hc}{2e} = n\Phi_0, \tag{83}$$

where n is a integer, Φ_0 is the flux quantum, and I've reinserted the correct factor of $\hbar$ in the first step to make the units right. Flux quantization indeed follows from the fact that the current is the result of a phase gradient.[18]

Derivation from Microscopic Theory. One of the reasons the GL theory did not enjoy much success at first was the fact that it is purely phenomenological, in the sense that the parameters a_0, b, m^* are not given within any microscopic framework. The BCS theory is such a framework, and gives values for these coefficients which set the scale for all quantities calculable from the GL free energy. The GL theory is more general, however, since, e.g. for strong coupling superconductors the weak coupling values of the coefficients are simply replaced by different ones of the same order of magnitude, without changing the *form* of the GL free energy. In consequence, the dependence of observables on temperature, field, etc, will obey the same universal forms.

The GL theory was derived from BCS by Gor'kov. The calculation is beyond the scope of this course, but can be found in many texts.

[18]It is important to note, however, that a phase gradient doesn't guarantee that a current is flowing. For example, in the interior of the system depicted in Fig. 2, both $\nabla\phi$ and $\vec{A}$ are nonzero in the most convenient gauge, and cancel each other!

6.2 Type I and Type II superconductivity

Now let's look at the problem of the instability of the normal state to superconductivity in finite magnetic field $\mathbf{H}$. A what magnetic field to we expect superconductivity to be destroyed, for a given $T < T_c$.[19] Well, overall energy is conserved, so the total condensation energy of the system in zero field,$f_s - f_n(T)$ of the system must be equal to the magnetic field energy $\int d^3r H^2/8\pi$ the system *would have* contained at the critical field H_c in the absence of the Meissner effect. For a completely homogeneous system I then have

$$f_s(T) - f_n(T) = -H_c^2/8\pi, \tag{84}$$

and from Eq. (8) this means that, near T_c,

$$H_c = \sqrt{\frac{2\pi a_0^2}{b}}(T_c - T). \tag{85}$$

Whether this *thermodynamic critical field* H_c actually represents the applied field at which flux penetrates the sample depends on geometry. We assumed in the simplified treatment above that the field at the sample surface was the same as the applied field. Clearly for any realistic sample placed in a field, the lines of field will have to follow the contour of the sample if it excludes the field from its interior. This means the value of $\mathbf{H}$ at different points on the surface will be different: the homogeneity assumption we made will not quite hold. If we imagine ramping up the applied field from

[19] Clearly it *will* destroy superconductivity since it breaks the degenerace of between the two componenets of a Cooper pair.

zero, there will inevitably come a point $\mathbf{H}_{appl} = \mathbf{H}_{appl,c}$ where the field at certain points on the sample surface exceeds the critical field, but at other points does not. For applied fields $H_{appl,c} < H_{appl} < H_c$, part of the sample will then be normal, with local field penetration, and other parts will still exclude field and be superconducting. This is the *intermediate state* of a type I superconductor. The structure of this state for a real sample is typically a complicated "striped" pattern of superconducting and normal phases. Even for small fields, edges and corners of samples typically go normal because the field lines bunch up there; these are called "demagnetizing effects", and must be accounted for in a quantitatively accurate measurement of, say, the penetration depth. It is important to note that these patterns are completely geometry dependent, and have no intrinsic length scale associated with them.

In the 50's, there were several materials known, however, in which the flux in sufficiently large fields penetrated the sample in a manner which did *not* appear to be geometry dependent. For example, samples of these so-called "type II" superconductors with nearly zero demagnetizing factors (long thin plates placed parallel to the field) also showed flux penetration in the superconducting state. The type-II materials exhibit a second-order transition at finite field and the flux $\mathbf{B}$ through the sample varies continuously in the superconducting state. Therefore the mixed state must have currents flowing, and yet the Meissner effect is not realized, so that the London equation somehow does not hold.

The answer was provided by Abrikosov in 1957 [A.A.A., Sov. Phys. JETP 5, 1174 (1957).] in a paper which Landau apparently held up for several years because he did not believe it. Let us neglect the effects of geometry again, and go back to our theorist's sample with zero demagnetizing factor. Can we relax any of the assumptions that led to the London equation (72)? Only one is potentially problematic, that $n_s^*(r) = |\psi(r)|^2 =$ constant independent of position. Let's examine–as Abrikosov did–the energy cost of making spatial variations of the order parameter. The free energy in zero field is

$$F = \int d^3r[a|\psi|^2 + \frac{1}{2m^*}|\nabla\psi|^2 + b|\psi|^4], \tag{86}$$

or

$$\frac{1}{-a}F = \int d^3r[-|\psi|^2 + \xi^2|\nabla\psi|^2 + \frac{b}{-a}|\psi|^4], \tag{87}$$

where I've put

$$\xi = [\frac{1}{-2m^*a}]^{1/2} = [\frac{1}{-2m^*a_0(T_c - T)}]^{1/2}. \tag{88}$$

Clearly the length ξ represents some kind of *stiffness* of the quantitiy $|\psi|^2$, the superfluid density. [Check that it does indeed have dimensions of length!] If ξ, the so-called *coherence length*, is small, the energy cost of n_s varying from place to place will be small. If the order parameter is somehow changed from its homogeneous equilibrium value at one point in space by an external force, ξ specifies the length scale over which it "heals". We can then investigate the possibility that, as the kinetic energy of superfluid flow increases with increasing field, if ξ is small enough it might eventually become favorable to "bend" $|\psi|^2$ instead. In typical type I materials, $\xi(T=0)$ is of order several hundreds or even thousands of Angstrom, but in heavy fermion superconductors, for example, coherence lengths are of order 50-100A. The smallest coherence lengths are attained in the HTSC, where ξ_{ab} is of order 12-15A, whereas ξ_c is only 2-3A.

The general problem of minimizing F when ψ depends on position is extremely difficult. However, we are mainly interested in the phase boundary where ψ is small, so life is a bit simpler. Let's recall our quantum mechanics analogy once more so as to write F in the form:

$$F = \int d^3r[a|\psi|^2 + b|\psi|^4] + < \psi|\hat{H}_{kin}|\psi >, \tag{89}$$

where $\hat{H}_{kin}$ is the operator

$$-\frac{1}{2m^*}(\nabla + \frac{ie^*}{c}\vec{A})^2. \tag{90}$$

Now note 1) sufficiently close to the transition, we may always neglect the 4th-order term, which is much smaller; 2) to minimize F, it suffices to minimize $< \hat{H}_{kin} >$, since the $|\psi|^2$ term will simply fix the overall normalization. The variational principle of quantum mechanics states that the minimum value of $< H >$ over all possible ψ is achieved when ψ is the ground state (for a given normalization of ψ). So we need only solve the eigenvalue problem

$$\hat{H}_{kin}\psi_j = E_j\psi_j \tag{91}$$

for the lowest eigenvalue, E_j, and corresponding eigenfunction ψ_j. For the given form of $\hat{H}_{kin}$, this reduces to the classic quantum mechanics problem of a charged particle moving in an applied magnetic field. The applied field H is essentially the same as the microscopic field B since ψ is so small (at the phase boundary only!). I'll remind you of the solution, due to to Landau, in order to fix notation. We choose a convenient gauge,

$$\mathbf{A} = -Hy\hat{x}, \tag{92}$$

in which Eq. 44 becomes

$$\frac{1}{2m^*}[(-i\frac{\partial}{\partial x} + \frac{y}{\ell_M^2})^2 - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}]\psi_j = E_j\psi_j, \tag{93}$$

where $\ell_M = (c/e^*H)^{1/2}$ is the *magnetic length.* Since the coordinates x and z don't appear explicitly, we make the ansatz of a plane wave along those directions:

$$\psi = \eta(y)e^{ik_x x + ik_z z}, \tag{94}$$

yielding

$$\frac{1}{2m^*}[(k_x + \frac{y}{\ell_M^2})^2 - \frac{\partial^2}{\partial y^2} + k_z^2]\eta(y) = E\eta(y). \tag{95}$$

But this you will recognize as just the equation for a one-dimensional harmonic oscillator centered at the point $y = -k_x\ell_M^2$ with an additional additive constant $k_z^2/2m^*$ in the energy. Recall the standard harmonic oscillator equation

$$(-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2)\Psi = E\Psi, \tag{96}$$

with ground state energy

$$E_0 = \frac{\omega_0}{2} = \frac{1}{2}(k/m)^{1/2}, \tag{97}$$

where k is the spring constant, and ground state wavefunction corresponding to the lowest order Hermite polynomial,

$$\Psi_0 \approx \exp[-(mk/4)^{1/2}x^2]. \tag{98}$$

Let's just take over these results, identifying

$$\hat{H}_{kin}\psi_{k_x,k_z} = \frac{e^* H}{2m^* c}\psi_{k_x,k_z}. \tag{99}$$

The ground state eigenfunction may then be chosen as

$$\psi_{k_x,k_z} = \psi_0(\frac{\pi \ell_M^2}{L_y^2})^{-1/4} e^{ik_x x + ik_z z} \exp[-(y + k_x \ell_M^2)^2/2\ell_M^2)], \tag{100}$$

where L_y is the size of the sample in the y direction ($L_x L_y L_z = V = 1$). The wave functions are normalized such that

$$\int d^3r |\psi_{k_x,k_z}|^2 = \psi_0^2 \tag{101}$$

(since I set the volume of the system to 1). The prefactors are chosen such that ψ_0^2 represents the average superfluid denstity. One important aspect of the particle in a field problem seen from the above solution is the large degeneracy of the ground state: the energy is independent of the variable k_x, for example, corresponding to many possible orbit centers.

We have now found the wavefunction which minimizes $< \hat{H}_{kin} >$. Substituting back into (89), we find using (99)

$$F = [a_0(T - T_c) + \frac{e^* H}{2m^* c}] \int d^3r |\psi|^2 + b \int d^3r |\psi|^4. \tag{102}$$

When the coefficient of the quadratic term changes sign, we have a transition. The field at which this occurs is called the *upper critical field* H_{c2},

$$H_{c2}(T) = \frac{2m^* c a_0}{e^*}(T_c - T). \tag{103}$$

What is the criterion which distinguishes type-I and type II materials? Start in the normal state for $T < T_c$ as shown in Figure 3, and reduce the field. Eventually one crosses either H_c or H_{c2} first. Whichever is crossed first determines the nature of the instability in finite field, i.e. whether the sample expels all the field, or allows flux (vortex) penetration (see section C).

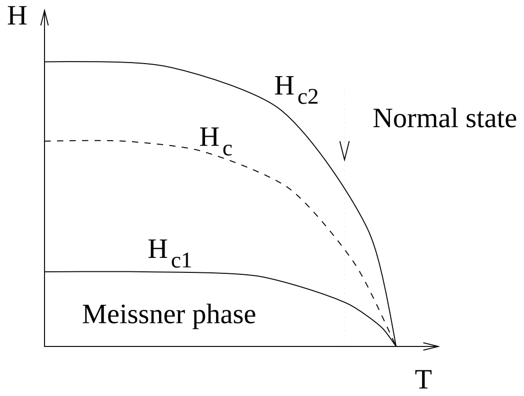

Figure 11: Phase boundaries for classic type II superconductor.

In the figure, I have displayed the situation where H_{c2} is higher, meaning it is encountered first. The criterion for the dividing line between type 1 and type II is simply

$$|\frac{dH_c}{dT}| = |\frac{dH_{c2}}{dT}| \tag{104}$$

or, using the results (38) and (56),

$$\frac{(m^*)^2 c^2 b}{\pi (e^*)^2} = \frac{1}{2}. \tag{105}$$

This criterion is a bit difficult to extract information from in its current form. Let's define the *GL parameter* κ to be the ratio of the two fundamental lengths we have identified so far, the penetration depth and the coherence length:

$$\kappa = \frac{\lambda}{\xi}. \tag{106}$$

Recalling that

$$\lambda^2 = -\frac{m^* c^2}{4\pi e^{*2} n_s^*} = -\frac{m^* c^2 b}{2\pi e^{*2} a} \tag{107}$$

and

$$\xi^2 = -\frac{1}{2m^* a}. \tag{108}$$

The criterion (58) now becomes

$$\kappa^2 = \frac{m^* c^2 b / 2\pi e^{*2} a}{1/2m^* a} = \frac{(m^*)^2 c^2 b}{\pi e^{*2}} = \frac{1}{2}. \tag{109}$$

Therefore a material is type I (II) if κ is less than (greater than) $\frac{1}{\sqrt{2}}$. In type-I superconductors, the coherence length is large compared to the penetration depth, and the system is stiff with respect to changes in the superfluid density. This gives rise to the Meissner effect, where n_s is nearly constant over the screened part of the sample. Type-II systems can't screen out the field close to H_{c2} since their stiffness is too small. The screening is incomplete, and the system must decide what pattern of spatial variation and flux penetration is most favorable from an energetic point of view. The result is the *vortex lattice* first described by Abrikosov.

6.3 Vortex Lattice

I commented above on the huge degeneracy of the wave functions (53). In particular, for fixed $k_z = 0$, there are as many ground states as allowed values of the parameter k_x. At H_{c2} it didn't matter, since we could use the eigenvalue alone to determine the phase boundary. Below H_{c2} the fourth order term becomes important, and the minimization of f is no longer an eigenvalue problem. Let's make the plausible assumption that if some spatially varying order parameter structure is going to form below H_{c2}, it will be periodic with period $2\pi/q$, i.e. the system *selects* some wave vector $\mathbf{q}$ for energetic reasons. The x-dependence of the wave functions

$$\psi_{k_x,k_z=0} = \psi_0(\frac{\pi\ell_M^2}{L_y^2})^{-1/4} e^{ik_x x} \exp[-(y+k_x\ell_M^2)^2/2\ell_M^2)]. \quad (110)$$

is given through plane wave phases, $e^{ik_x x}$. If we choose $k_x = qn_x$, with n_x =integer, all such functions will be invariant under $x \to x + 2\pi/q$. Not all n_x's are allowed, however: the center of the "orbit", $k_x\ell_M^2$ should be inside the sample:

$$-L_y/2 < k_x\ell_M^2 = q\ell_M^2 n_x < L_y/2, \quad (111)$$

Thus n_x is restricted such that

$$-\frac{L_y}{2q\ell^2} = -n_{max}/2 < n_x < n_{max}/2 = \frac{L_y}{2q\ell^2} \tag{112}$$

and the total number of degenerate functions is $L_y/(q\ell_M^2)$.

Clearly we need to build up a periodic spatially varying structure out of wave functions of this type, with "centers" distributed somehow. What is the criterion which determines this structure? All the wave functions (110) minimize $< \hat{H}_{kin} >$, and are normalized to $\int d^3r|\psi|^2 = |\psi_0|^2$. They are all therefore degenerate at the level of the quadratic GL free energy, $F = \int d^3r|\psi|^2 + < \hat{H}_{kin} >$. The fourth order term must stabilize some linear combination of them. We therefore write

$$\psi(r) = \sum_{n_x} C_{n_x}\psi_{n_x}(r), \tag{113}$$

with the normalization $\Sigma_{n_x} |C_{n_x}|^2 = 1$, which enforces $\int d^3r|\psi(r)|^2 = \psi_0^2$. Note this must minimize $< \hat{H}_{kin} >$. Let's therefore choose the C_{n_x} and q to minimize the remaining terms in F, $\int d^3r[a|\psi|^2 + b|\psi|^4]$. Substituting and using the normalization condition and orthogonality of the different ψ_{k_z,k_x}, we find

$$f \;=\; \tilde{a}\psi_0^2 + \tilde{b}\psi_0^4. \tag{114}$$

with

$$\tilde{a}(H,T) \;=\; a_0(T-T_c) + \frac{e^*H}{2m^*c} = \frac{e^*}{2m^*c}(H - H_{c2}(T)), \tag{115}$$

$$\tilde{b}(H) \;=\; sb, \tag{116}$$

and

$$s \;=\; \left(\frac{\pi\ell_M^2}{L_y^2}\right)^{-1} \sum_{n_{x1},n_{x2},n_{x3},n_{x4}}^{n_{max}} C^*_{n_{x1}}C^*_{n_{x2}}C_{n_{x3}}C_{n_{x4}} \tag{117}$$

$$\int dz \ \int dx \ e^{iq(-n_{x1}-n_{x2}+n_{x3}+n_{x4})x} \times \tag{118}$$
$$\int dy \ e^{\{-\frac{1}{2\ell_M^2}[(y+qn_{x1}\ell_M^2)^2+(y+qn_{x2}\ell_M^2)^2+(y+qn_{x3}\ell_M^2)^2+(y+qn_{x4}\ell_M^2)^2]\}} \tag{119}$$

The *form* of $f[\psi_0]$ is now the same as in zero field, so we immediately find that in equilibrium,

$$\psi_0|_{eq} = (\frac{-\tilde{a}}{2\tilde{b}})^{1/2}. \tag{120}$$

and

$$f = \frac{-\tilde{a}^2}{4\tilde{b}}. \tag{121}$$

This expression depends on the variational parameters C_{n_x}, q only through the quantity s appearing in $\tilde{b}$. Thus if we minimize s, we will minimize f (remember $b > 0$, so $f < 0$). The minimization of the complicated expression (xx) with constraint $\Sigma_{n_x} |C_{n_x}|^2 = 1$ is difficult enough that A. Abrikosov made a mistake the first time he did it, and I won't inflict the full solution on you. To get an idea what it might look like, however, let's look at a very symmetric linear combination, one where all the C_{n_x}'s are equal:

$$C_n = n_{max}^{-1/2}. \tag{122}$$

Then

$$\psi(r) \sim \sum_n e^{inqx} \exp[-(y + nq\ell^2)^2/2\ell_M^2], \tag{123}$$

which is periodic in x with period $2\pi/q$,

$$\psi(x + 2\pi/q, y) = \psi(x, y), \tag{124}$$

and periodic in q with period $q\ell_M^2$, up to a phase factor

$$\psi(x, y + q\ell_M^2) = e^{-iqx}\psi(x, y). \tag{125}$$

Note if $q = \sqrt{2\pi}/\ell_M$, $|\psi|^2$ forms a square lattice! The area of a unit cell is $(2\pi/q) \times (q\ell_M^2) = 2\pi\ell_M^2$, and the flux through each one is therefore

$$\Phi_{cell} = 2\pi\ell_M^2 H = 2\pi\frac{c}{e^* H}H = \frac{hc}{2e} = \Phi_0 \qquad (126)$$

where I inserted a factor of $\hbar$ in the last step. We haven't performed the minimization explicitly, but this is a characteristic of the solution, that each cell contains just one flux quantum. The picture is crudely depicted in Fig. 12a). Note by symmetry that the currents must cancel on the boundaries

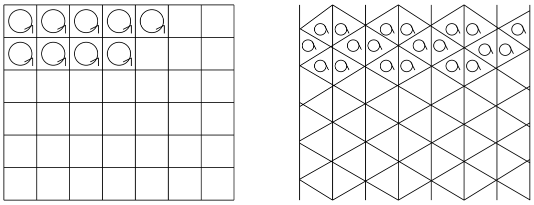

Figure 12: a) Square vortex lattice; b) triangular vortex lattice.

of the cells. Since $\vec{j_s} = -en_s\vec{v_s}$, integrating $\nabla\phi + \frac{2e}{\hbar c}\vec{A} = 0$ around each square must give, as in our previous discussion of flux quantization in a toroid,

$$\Phi_{cell} = n\Phi_0, n = integer. \qquad (127)$$

Somehow the vortex lattice consists of many such rings. The problem with this idea is that the only way $\oint \nabla\phi \cdot d\vec{\ell} = \delta\phi$ around the boundary can be nonzero and the usual argument about single-valuedness of the wave function carried through is if there is a "hole" in the wave function. If there is no hole, or region from which the wave function is excluded, the path can be shrunk to a point, but the value of the integral must remain the same since the integrand is the gradient of a scalar field. This is unphysical because it would imply a finite phase change along an infinitesimal path (and a divergence of the kinetic energy!) The only way out of the paradox is to have the system introduce its own "hole" in itself, i.e. have the amplitude of the order parameter density $|\psi|^2$ go to zero at the center of each cell. Intuitively, the magnetic field will have an accompanying maximum here, since the screening tendency will be minimized. This reduction in order parameter amplitude, magnetic flux bundle, and winding of the phase once by 2π constitute a magnetic "vortex", which I'll discuss in more detail next time.

Assuming $C_n =$ constant, which leads to the square lattice does give a relatively good (small) value for the dimensionless quantity s, which turns out to be 1.18. This was Abrikosov's claim for the absolute minimum of $f[|\psi|^2]$. But his paper contained a (now famous) numerical error, and it turns out that the actual minimum $s = 1.16$ is attained for another set of the C_n's, to wit

$$C_n = n_{max}^{-1/2}, \quad n = even \tag{128}$$

$$C_n = i n_{max}^{-1/2}, \quad n = odd. \tag{129}$$

This turns out to be a *triangular* lattice (Fig. 12b), for which the optimal value of q is found to be

$$q = \frac{3^{1/4}\pi^{1/2}}{\ell}, \tag{130}$$

Again the area of the unit cell is $2\pi\ell^2$, and there is one flux quantum per unit cell.

6.4 Properties of Single Vortex. Lower critical field H_{c1}

Given that the flux per unit cell is quantized, it is very easy to see that the lattice spacing d is actually of order the coherence length near H_{c2}. Using (103) and (88) we have

$$H_{c2} = \frac{c}{e^*}\frac{1}{\xi^2} = \frac{\Phi_0}{2\pi\xi^2}. \tag{131}$$

On the other hand, as H is reduced, d must increase. To see this, note that the area of the triangular lattice unit cell is $A = \sqrt{3}d^2/2$, and that there is one quantum of flux per cell, $A = \Phi_0/H$. Then the lattice constant may be expressed as

$$d = \frac{4\pi}{\sqrt{3}}\xi(\frac{H_{c2}}{H})^{1/2}. \tag{132}$$

Since $\lambda \gg \xi$ is the length scale on which supercurrents and magnetic fields vary, we expect the size of a magnetic vortex to be about λ. This means at H_{c2} vortices are strongly overlapping, but as the field is lowered, the vortices separate, according to (126), and may eventually be shown to influence each other only weakly. To find the structure of an isolated vortex is a straightforward but tedious exercise in minimizing the GL free energy, and in fact can only be done numerically in full detail. But let's exploit the fact that we are interested primarily in strongly type-II systems, and therefore go back to the London equation we solved to find the penetration depth in the half-space geometry for weak fields, allow n_s to vary spatially, and look for vortex-like solutions. For example, equation (75) may be written

$$-\lambda^2 \nabla \times \nabla \times \vec{B} = \vec{B}. \qquad (133)$$

Let's integrate this equation over a surface perpendicular to the field $\vec{B} = \vec{B}(x, y)\hat{z}$ spanning one cell of the vortex lattice:

$$-\lambda^2 \int \nabla \times (\nabla \times \vec{B}) \cdot d\vec{S} \;=\; \int \vec{B} \cdot d\vec{S}, \qquad (134)$$

$$-\lambda^2 \frac{4\pi}{c} \oint \vec{j}_s \cdot d\vec{\ell} \;=\; \Phi_0. \qquad (135)$$

But we have already argued that $\vec{j}_s \cdot d\vec{\ell}$ should be zero on the boundary of a cell, so the left side is zero and there is a contradiction. What is wrong? The equation came from assuming a two-fluid hydrodynamics for the superconductor, with a nonzero n_s everywhere. We derived it, in fact, from BCS theory, but *only for the case where n_s was constant.* Clearly there must be another term in the equation when a vortex-type solution is present, one which can only contribute over the region where the superfluid density is strongly varying in space, i.e. the coherence length-sized region in the middle of the vortex where the order parameter goes to zero (vortex "core"). Let's simply add a term which enables us to get the right amount of flux to Eq. (133). In general we should probably assume something like

$$\lambda^2 \nabla \times \nabla \times \vec{B} + \vec{B} = \Phi_0 g(\vec{r})\hat{z} \qquad (136)$$

where $g(r)$ is some function which is only nonzero in the core. The flux will then come out right if we demand $\int d^3r g(\vec{r}) =$

1. But let's simplify things even further, by using the fact that $\xi \ll \lambda$: let's treat the core as having negligible size, which means it is just a *line singularity*. We therefore put $g(\vec{r}) = \delta(\vec{r})$. Then the modified London equation with line singularity acting as an inhomogeneous "source term" reads

$$-\lambda^2\nabla^2\vec{B} + \vec{B} = \Phi_0\delta^2(\vec{r})\hat{z} \tag{137}$$

$$-\lambda^2\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial B_z}{\partial\rho}) + B_z = \Phi_0\delta^2(\vec{r}), \tag{138}$$

where ρ is the radial cylindrical coordinate. Equation (91) has the form of a modified Bessel's equation with solution:

$$B_z = \frac{\Phi_0}{2\pi\lambda^2}K_0(\frac{\rho}{\lambda}). \tag{139}$$

The other components of $\vec{B}$ vanish. If you go to Abramowitz & Stegun you can look up the asymptotic limits:

$$B_z = \frac{\Phi_0}{2\pi\lambda^2}[\log(\frac{\lambda}{\rho}) + 0.116], \quad \xi < \rho \ll \lambda \tag{140}$$

$$B_z = \frac{\Phi_0}{2\pi\lambda^2}\sqrt{\frac{\pi\lambda}{2\rho}}e^{-\rho/\lambda}, \quad \rho \gg \lambda. \tag{141}$$

Note the form (93) is actually the correct asymptotic solution to (91) all the way down to $\rho = 0$, but the fact that the solution diverges logarithmically merely reflects the fact that we didn't minimize the free energy properly, and allow the order parameter to relax as it liked within the core. So the domain of validity of the solution is only down to roughly the core size, $\rho \simeq \xi$, as stated. In Figure 5 I show schematically the structure of the magnetic and order parameter profiles in an isolated vortex. The solution may now be inserted into the

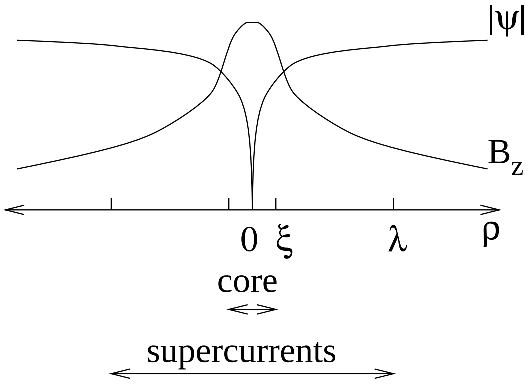

Figure 13: Isolated vortex

free energy and the spatial integrals performed, with some interesting results:

$$F = L_z \frac{\Phi_0^2}{16\pi^2\lambda^2}\log(\kappa). \tag{142}$$

It is easy to get an intuitive feel for what this means, since if we assume the field is uniform and just ask what is the magnetic energy, we get roughly

$$\begin{aligned} F_v &= \frac{1}{8\pi} \times \text{vortex volume} \times B^2 && (143)\\ &\simeq \frac{1}{8\pi} \times (\pi\lambda^2 L_z) \times (\Phi_0/\pi\lambda^2)^2 && (144)\\ &= L_z \frac{\Phi_0^2}{8\pi^2\lambda^2}, && (145) \end{aligned}$$

the same result up to a slowly varying factor. Now the *lower critical field* H_{c1} is determined by requiring the Gibbs free energies of the Meissner phase with no vortex be equal to the Gibbs free energy of the phase with a vortex.[20] G differs from

[20]We haven't talked about the Gibbs vs. Helmholtz free energy, but recall the Gibbs is the appropriate potential to use when the external field H is held fixed, which is the situation we always have, with a generator supplying work to maintain H.

F through a term $-\int BH/4\pi$. In the Meissner state $G = F$, so we may put

$$\begin{aligned} F &= F + E_{line}L_z - \frac{1}{4\pi}H_{c1}\int Bd^3r && (146) \\ &= F + E_{line}L_z - \frac{1}{4\pi}\Phi_0 L_z, && (147) \end{aligned}$$

where E_{line} is the free energy per unit length of the vortex itself. Therefore

$$H_{c1} = \frac{4\pi E_{line}}{\Phi_0} \tag{148}$$

is the upper critical field. But the line energy is given precisely by Eq. (95), $E_{line} = \frac{\Phi_0^2}{16\pi^2\lambda^2}\log(\kappa)$, so

$$H_{c1}(T) = \frac{\Phi_0}{4\pi\lambda^2}\log(\kappa). \tag{149}$$

6.5 Josephson Effect