Lecture 7.3

BCS theory

"BCS" (Bardeen-Cooper-Schrieffer) theory is essentially just Hartree-Fock theory (Lec. 1.4X) for that case that "anomalous" operators (those which add or remove a pair of fermions: see Lec. 7.1), develop nonzero expectations; equivalently, fir metals whose ground state is a coherent superposition of terms with different numbers of pairs. ¹

I follow the Bogoliubov approach, 2 where you assume the expectations and derive the BCS wavefunction. As usual with Hartree-Fock, you get an effective noninteracting Hamiltonian (Sec. 7.3 A), whose ground state happens to be exactly $\Phi_{\rm BCS}$ (Sec. 7.3 C). In the process we obtain the formulas for the coefficients $u_{\bf k}$ and $v_{\bf k}$ in $\Phi_{\rm BCS}$, as well as the dispersion $E_{\bf k}$ of its fermionic elementary excitations – "Bogoliubov quasiparticles" (Sec. 7.3 B). Each is a superposition of an electron and a hole (!) and thus carries indefinite particle number (or does it? A closer examination [Sec. 7.3 X] indicates the true charge is zero, revealing that even plain BCS superconductors exhibit the exotic phenomenon "spin-charge separation".)

MOVE DOWN These are not to be confused with the Landau quasiparticles in a metal (Lec. 1.7) or with Laughlin quasiparticles in the fractional quantized Hall effect: a Bogoliubov quasiparticle is a linear combination of an electron and a hole excitation.

The keystone of the core BCS results is the gap equation (Sec. 7.3 D, a self-consistent formula for the gap parameter $\Delta_{\mathbf{k}}$ (and indirectly for $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, and $E_{\mathbf{k}}$.) The finite-temperature version of the gap equation tells the temperature dependence of all those quantities, and in particular gives the ordering temperature T_c .

With the quasiparticle operators in hand, all sorts of expectations are easy to compute. in particular, we obtain the self-consistent *gap equation* the Bogoliubov approach for this easily generalizes to nonzero temperatures (Sec. 7.3 E). Lec. 7.5 is devoted to further applications of the quasiparticles.

Finally, Sec. 7.3 Y develops the alternative to Bogoliubov's path: the original variational approach of BCS, where you first assume the wavefunction, and then derive the expectations. Once you recall that Hartree-Fock is variationally based (Lec. 1.4X), it is no surprise that these approaches are equivalent.

Although we imagined a Bose condensate of composite bosons made from tightly paired fermions in order to guess the BCS wavefunction (in Lec. 7.1), this is not necessary for the BSC state. Indeed, the BCS state is different from that state (although

 $^{^1}$ Although BCS originally had in mind s-wave singlet superconductors, with a phonon-mediated electron attraction, and they adopted a particular cartoon of this attraction, none of that is implicit in "BCS" as I use the term. However, weak coupling is implicit in this approximation.

²The fermionic Bogoliubov approach for superconductors was inspired by the bosonic Bogoliubov approach that models superfluid *Bose* gas. In that case, the elementary excitations were phonons.

Quantity	Formula
(BCS) Coherence length	$\xi = \hbar v_F / \pi \Delta$
BCS gap	$\Delta/T_c = 3.5$
Critical temperature	$T_c = (\ldots)\hbar\omega_0 \exp(-1/N(0)V_0)$
Quasiparticle dispersion	$E_k = \sqrt{ \epsilon(k) - \mu ^2 + \Delta(\mathbf{k}) ^2}$
(BCS coefficients)	$ u_{\mathbf{k}} ^2, v_{\mathbf{k}} ^2 = \frac{1}{2}(1 \pm (\epsilon(\mathbf{k}) - \mu)/E_{\mathbf{k}})$
	$u_{\mathbf{k}}v_{\mathbf{k}} = \Delta(\mathbf{k})/2E_{\mathbf{k}}$

they are adiabatically connected). The weak-coupling assumption hidden in the BCS derivation(s) implies that the gap (= pair binding) is much smaller than \mathcal{E}_F , whereas it is much larger than \mathcal{E}_F in the tight pair case.

Hamiltonian

Recall (from Lec. 7.0) our Hamiltonian is $\mathcal{H} = \mathcal{H}_{KE} + \mathcal{H}_V$ where the single-electron part is

$$\mathcal{H}_{KE} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \tag{7.3.1}$$

with $\epsilon_{\mathbf{k}}$ measured as usual from the chemical potential μ , the spin index σ runs over \uparrow, \downarrow . Sometimes we'll assume spherical symmetry, with $\epsilon_{\mathbf{k}} \approx \hbar v_F (k - k_F)$, and unbounded \mathbf{k} , but only where specifically noted. Otherwise, the calculation is valid for generic dispersions, and \mathbf{k} may be a crystal wavevector bounded to a Brillouin zone.

The general form of interaction potential is $\mathcal{H}_V = \mathcal{H}_V^{(0)} + \mathcal{H}_V^{(1)}$, broken up according to whether the electrons being scattered are in a singlet or triplet spin state, respectively ³.

$$\mathcal{H}_{V}^{(0)} = \sum_{\mathbf{p}\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{(0,\mathbf{p})} (c_{\mathbf{k}'+\mathbf{p}/2,\uparrow}^{\dagger} c_{-\mathbf{k}'+\mathbf{p}/2,\downarrow}^{\dagger} c_{-\mathbf{k}+\mathbf{p}/2,\downarrow} c_{\mathbf{k}+\mathbf{p}/2,\uparrow})$$
(7.3.2)

where $V_{{f k}{f k}'}^{(0,{f p})}=-V_{{f k},-{f k}'}^{(0,{f p})}$ ensures the singlet symmetry. The triplet term is

$$\mathcal{H}_{V}^{(1)} = \sum_{\mathbf{p}\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{(1,\mathbf{p})} \left(c_{\mathbf{k}'+\mathbf{p}/2,\sigma_{1}'}^{\dagger} \boldsymbol{\tau}_{\sigma_{1}',\sigma_{2}'} c_{-\mathbf{k}'+\mathbf{p}/2,\sigma_{2}'}^{\dagger} \right) \cdot \left(c_{-\mathbf{k}+\mathbf{p}/2,\sigma_{1}} \boldsymbol{\tau}_{\sigma_{1},\sigma_{2}} c_{\mathbf{k}+\mathbf{p}/2,\sigma_{2}} \right). \tag{7.3.3}$$

In the case of the phonon-mediated coupling (Lec. 7.6), the potential is the same for both channels. Which term enters the pairing Hamiltonian depends on the symmetry of the superconducting order. This unit emphasizes singlet superconductivity so, where it makes a difference, we'll assume the singlet interaction (7.3.2).

7.3 A Bogoliubov effective Hamiltonian

The only assumption used is that we have an expectation of the "anomalous" operator

$$\langle c_{-\mathbf{k}|} c_{\mathbf{k}\uparrow} \rangle \neq 0 \tag{7.3.4}$$

The relation of this to Bose condensation was given in Lec. 7.1.

We could have, instead, assumed the expectation was nonzero for pairs with a nonzero total momentum:

$$\langle c_{-\mathbf{k}+\mathbf{p}/2,\downarrow} c_{\mathbf{k}+\mathbf{p}/2,\uparrow} \rangle = 0?$$
 (7.3.5)

³A similar form was already exhibited in Sec. 7.0 C

It can be verified that the energy is lower when this is nonzero for *only* one choice of \mathbf{p} . The case $\mathbf{p} \neq 0$ actually corresponds to two physical situations (i) a nonzero current (see Lec. 7.8 [omitted]) (ii) an exotic ordering at nonzero wavevector, the "FFLO" superconductor. But let's specialize to $\mathbf{P} = \mathbf{0}$, since that normally has the lowest energy.

In view of (7.3.5) and (7.3.4), the only terms which contribute to the anomalous part of the Hartree-Fock effective Hamiltonian are the *pairing terms* 5 of the potential, defined as those with $\mathbf{p} = 0$:

$$\mathcal{H}^{\text{pair}} = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{(\mathbf{0})} c_{\mathbf{k}'\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$$
 (7.3.6)

In this story, we glossed over the large, non-anomalous ($c^{\dagger}c$ type) expectations. These same "Hartree" and "Fock" terms are encountered in the variational approach (Lec. 7.3 Y, but canceled there by an appeal to Fermi liquid theory. The right viewpoint is that we already dealt with this part of the interactions via the Landau quasiparticle construction (Lec. 1.7). Then our $c^{\dagger}_{\mathbf{k}}$ operators really make Fermi-liquid quasiparticles, and the dispersion $\epsilon_{\mathbf{k}}$ already incorporates the effects of interactions, as long as $\epsilon_{\mathbf{k}}$ is near the Fermi energy.

Now let's substitute (7.3.4) into (7.3.6) using the Lec. 1.4Xdecoupling rule: this produces an effective Hamiltonian, quadratic in electron operators:

$$\mathcal{H}_{\text{pair}}^{\text{eff}} = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{(\mathbf{0})} (\langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle c_{\mathbf{k}'\uparrow}^{\dagger} c_{-\mathbf{k}'\downarrow}^{\dagger}) - \text{const}_V$$
 (7.3.7)

We'll drop the constant "const $_V$ " from here on. ⁶

Eq. (7.3.7) invites a simplification by defining

$$\Delta_{\mathbf{k}} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{(0)} \langle c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \rangle \tag{7.3.8}$$

Having collected the terms from (7.3.7), we obtain the grand result of this section, the quadratic effective Hamiltonian

$$\mathcal{H}_{\text{pair}}^{\text{eff}} \approx -\sum_{\mathbf{k}} (\Delta_{\mathbf{k}}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger})$$
 (7.3.9)

This is weird, in that it does not conserve particle number: two fermions can be created from nothing, or annihilated. Actually, this is just like Bogoliubov's effective Hamiltonian for the (superfluid) dilute Bose gas from Lec. 7.2; we prefer to say the particles are coming from, or going into, the *condensate*, which functions as a reservoir.

A close analog of the present calculation is the Hubbard model Hartree-Fock calculations of Lec. 5.3X. In that case, however, an electron creation operator at \mathbf{k} merely got mixed with one at $\mathbf{k} + \mathbf{Q}$, whereas now it gets mixed with an annihilation operator.

⁴Details: If you have a **p** for which (7.3.5) is nonzero, that indicates you have ordering of pairs with a net center-of-mass momentum **p**. Certainly, to model a superconductor with a superflow, we should consider the case with ordering $\mathbf{p} \neq 0$ in place of the usual $\mathbf{p} = 0$ ordering of (7.3.4). We rule out the ordering with two wavevectors \mathbf{p}_1 and \mathbf{p}_2 , because we can show (variationally in Lec. 7.3 Y) that it has a higher energy. Roughly, it's like you are dividing up your superfluid density into two equal parts n_{s1} and n_{s2} , or making a a GL theory with two order parameters Ψ_1 and Ψ_2 . The condensation energy according to GL theory is something like $n_{s1}^2 + n_{s2}^2 \propto (1/2)^2 + (1/2)^2$ which is 1/2 as much. A similar argument is made in Lec. 8.2 for anisotropic order parameters.

⁵To shorten (7.3.6), one could have written it using the *BCS pair operator* $b_{\mathbf{k}}^{\dagger} \equiv c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}$ that creates a pair in momentum space.

 $^{^6}$ But "const_V" must be kept in order to compare total energy of the BCS state with a competing hypothetical state of the electron sea. For its value see Ex. 7.3.5.

7.3 B Bogoliubov quasiparticle operators

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We've beaten the Hamiltonian into a quadratic form,

$$\tilde{\mathcal{H}}_{\text{Bogo.}} \equiv \mathcal{H}_{KE} + \mathcal{H}_{\text{pair}}^{\text{eff}}.$$
 (7.3.10)

Any such quadratic form can be diagonalized, that is, put into the form

$$\tilde{\mathcal{H}}_{\text{Bogo.}} = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \gamma_{\mathbf{k}\sigma}^{\dagger} \gamma_{\mathbf{k}\sigma}$$
 (7.3.11)

The fermion operators $\{\gamma_{\mathbf{k}\sigma}^{\dagger}\}$ and $\{\gamma_{\mathbf{k}\sigma}\}$ create and annihilate the "Bogoliubov quasi-particles". They will be linear combinations of the creation and annihilation operators of the real electrons:

$$\gamma_{\mathbf{k}\uparrow} \equiv u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger}, \tag{7.3.12a}$$

$$\gamma_{\mathbf{k}\downarrow} \equiv u_{\mathbf{k}} c_{\mathbf{k}\downarrow} + v_{\mathbf{k}} c_{-\mathbf{k}\uparrow}^{\dagger}$$
 (7.3.12b)

while the creation operators are conjugates of these. We'll also write quasiparticle number operators

$$\hat{n}_{\mathbf{k}\sigma}^{\mathrm{qp}} \equiv \gamma_{\mathbf{k}\sigma}^{\dagger} \gamma_{\mathbf{k}\sigma} \tag{7.3.13}$$

In fact, all we need to do assume forms like (7.3.12), with $v_{\mathbf{k}\uparrow}$ and $v_{\mathbf{k}\downarrow}$ in general. Then force the commutators to work such that the γ anticommute, except with their conjugates, like properly diagonalized operators. In particular, $v_{\mathbf{k}\uparrow} = -v_{\mathbf{k}\downarrow}$ emerges. (For spin-pairing with an odd angular momentum, this would be a + sign: in effect the parity of the pair relative wavefunction.

Notice each quasiparticle operator carries a definite wavevector and spin. Thus in $\gamma_{\mathbf{k}\uparrow}^{\dagger}$, one operator $(c_{\mathbf{k}\uparrow}^{\dagger})$ creates an electron and the other operator $(c_{-\mathbf{k}\downarrow})$ creates a *hole* with the same quantum numbers (\mathbf{k},\uparrow) .

The arbitary overall phase in the definitions (7.3.12) is resolved by letting every $u_{\mathbf{k}}$ be real positive. Because there is a physical symmetry between \mathbf{k} and $-\mathbf{k}$, this implies

$$u_{\mathbf{k}} = u_{-\mathbf{k}} \tag{7.3.14}$$

As for $v_{\mathbf{k}}$: Though not obvious from what was written above, our assumption of a superconductor with spatial s-wave pairing implies that $v_{\mathbf{k}}$ in (7.3.12a) and (7.3.12b) may be taken real without loss of generality. More generally, the phase of $v_{\mathbf{k}}$ depends on the orientation of \mathbf{k} according to the angular momentum representation of the spatial pairing. Both of these facts were suggested by the construction in Lec. 7.1 that produced $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in terms of a pair wave function $\chi(\mathbf{r}_1 - \mathbf{r}_2)$.

Anticommutators, inverse, and symmetries

[Let's start on the details of making the Bogoliubov transformation work.] First, what are the necessary conditions for $\{\gamma_{\mathbf{k}\sigma}^{\dagger}\}$ and $\{\gamma_{\mathbf{k}\sigma}\}$ to have canonical fermion anti-commutation relations? The self-anticommutator gives a normalization condition:

$$1 = \{ \gamma_{\mathbf{k}\uparrow}^{\dagger}, \gamma_{\mathbf{k}\uparrow} \} = \{ u_{\mathbf{k}}^{*} c_{\mathbf{k}\uparrow}^{\dagger} - v_{\mathbf{k}}^{*} c_{-\mathbf{k}\downarrow}, u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^{\dagger} \} = u_{\mathbf{k}}^{2} + |v_{\mathbf{k}}|^{2}.$$
 (7.3.15)

 $^{^7}$ These are *not* the quasiparticles in the sense of Landau Fermi liquid theory (Lec. 1.7), since the superconducting ground state does not connect adiabatically to the Fermi sea state.

Otherwise, anticommutator of any pairs of Bogoliubov operators must give zero. The only case where this cancellation is not obvious is the pair $\gamma_{\mathbf{k}\uparrow}$ and $\gamma_{-\mathbf{k}\downarrow}$, since the c operators included in the former operator are the conjugates (with different coefficients) of the c operators in the latter operator. We are demanding

$$0 = \{\gamma_{\mathbf{k}\uparrow}, \gamma_{-\mathbf{k}\downarrow}\} = \{u_{\mathbf{k}}c_{\mathbf{k}\uparrow} - v_{\mathbf{k}}c_{-\mathbf{k}\downarrow}^{\dagger}, u_{-\mathbf{k}}c_{-\mathbf{k}\downarrow} + v_{-\mathbf{k}}c_{\mathbf{k}\uparrow}^{\dagger}\} = u_{\mathbf{k}}v_{-\mathbf{k}} - v_{\mathbf{k}}u_{-\mathbf{k}}. \quad (7.3.16)$$

This is satisfied, in light of (7.3.14), if and only if we require

$$v_{\mathbf{k}} = v_{-\mathbf{k}} \tag{7.3.17}$$

Note: the physical symmetry between ${\bf k}$ and $-{\bf k}$ merely implied $|v_{-{\bf k}}| = |v_{\bf k}|$. The phase relationship in (7.3.17) is specific to pairing with an even angular momentum (which implies the the pair wavefunction is even under spatial inversion.) Since fermions are antisymmetric under exchange, that happens if and only if the spin symmetry of the pairing is antisymmetric – as in the spin singlet we are assuming here. If it is strictly s-wave symmetry, then $v_{\bf k}/u_{\bf k}$ is independent of the direction of ${\bf k}$, i.e. $u_{\bf k}$ and $|v_{\bf k}|$ are functions only of $|{\bf k}|$. [However, by a slight abuse of language, the term s-wave symmetry is normally used whenever the actual symmetry coincides with s-wave symmetry under rotations which belong to the point group describing the material's symmetry.] For antisymmetric (e.g. p-wave) spatial pairing, $v_{-{\bf k}}=-v_{\bf k}$ instead; that normally entails a multi-component order parameter, so is discussed among the exotic kinds of pairing in Lec. 8.1 [2007] and Lec. 8.2.

Note the arbitariness of the phase of $v_{\bf k}$ in (7.3.17). (even after we fixed $u_{\bf k}$ to be real). If we wrote $v_{\bf k} = |v_{\bf k}| e^{i\theta_{\bf k}}$, we'll find that the only solution of the self-consistent equations (below) has the same phase $\theta_{\bf k} \equiv \theta$, for all $\bf k$. This phase factor $e^{i\theta}$ turns out to be the same one appearing in the BCS wavefunction; and, as shown by Ex. [7.1.4(c)], physical expectations don't depend on θ . Hence θ is a symmetry as was already stated in Lec. 7.1. We will normally adopt the gauge $\theta=0$.

With these conditions, (7.3.12a) and (7.3.12b) define a canonical (unitary) transformation, which (lucky for us) breaks up into 2×2 blocks. The inverse transformation reads:

$$c_{\mathbf{k}\uparrow} = u_{\mathbf{k}}^* \gamma_{\mathbf{k}\uparrow} + v_{\mathbf{k}}^* \gamma_{-\mathbf{k}\downarrow}^{\dagger}$$
 (7.3.18a)

$$c_{\mathbf{k}\downarrow} = u_{\mathbf{k}}^* \gamma_{\mathbf{k}\downarrow} - v_{\mathbf{k}}^* \gamma_{-\mathbf{k}\uparrow}^{\dagger}$$
 (7.3.18b)

where of course $u_{\mathbf{k}}^* = u_{\mathbf{k}}$ by our convention.

Physical picture: pairs and Bogoliubov quasiparticles

Loosely, the Bogoliubov quasiparticle would appear to be a mixture of electron and hole, and we are tempted to call it a resonance between them. But on closer inspection, if we launch an unpaired electron on top of the condensate, (7.3.9) does nothing to it: every term in (7.3.9) involving the unpaired wavevectors annihilates the state.

Let's visualize the physical meaning of (7.3.9). The Hilbert (sub)space involving $|\mathbf{k}\uparrow\rangle$ and $|-\mathbf{k},\downarrow\rangle$ – which has room for two fermions – resonates between being empty or occupied by a pair; the scattering between these states is accomplished by the omnipresent condensate. [Really the pair gets scattered into another pair, but within our mean-field approximation, it doesn't matter which pair: the condensate acts as a reservoir to supply or absorb pairs whenever needed.] Within this subspace, (7.3.9) describes a two-state system. The asymmetry – bare difference between the energy of one state and the average of both – is $\pm \epsilon_{\mathbf{k}}$; the mixing amplitude is $\Delta_{\mathbf{k}}$ (or its conjugate). Thus,

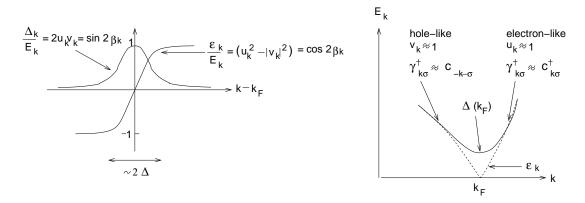


Figure 7.3.1: (Left). Functions of wavevector \mathbf{k} (or energy), related to angle parameter $\beta_{\mathbf{k}}$. [It has been implicitly assumed that Δ is nearly constant near the Fermi energy.]

the ground state energy is $-E_{\mathbf{k}} = -\sqrt{\epsilon_k^2 + |\Delta_{\mathbf{k}}|^2}$. As with any other two-level system, resonance is most important when the bare asymmetry is zero, in this case when $|\mathbf{k}| = k_F$. From this viewpoint, the BCS gap is much like an avoided level crossing.

In the unpaired situation, when the occupation of this little subspace is just one, (7.3.9) gives zero, so these states have energy zero. They are none other than the Bogoliubov quasiparticles; in other words, when either of the terms in $\gamma_{\bf k}^{\dagger}$ actually hits the BCS state, it makes the *same* state.

7.3 C Bogoliubov coefficients and BCS wavefunction

Our next aim is the algebra and parametrization of the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in terms of the gap function $\Delta_{\mathbf{k}}$.

Coefficients in Bogoliubov diagonalization

To solve efficiently for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ we substitute Eqs. (7.3.12) into (7.3.11), collect terms, and demand that the result reproduces the two terms of (7.3.10). The square terms, compared with (7.3.1), give

$$E_{\mathbf{k}}(u_{\mathbf{k}}^2 - |v_{\mathbf{k}}|^2) = \epsilon_{\mathbf{k}} \tag{7.3.19a}$$

while the anomalous terms, compared with (7.3.9), give

$$2u_{\mathbf{k}}v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}}. (7.3.19b)$$

The phase factor $e^{i\theta}$ is hiding in $\Delta_{\mathbf{k}}$ and in $v_{\mathbf{k}}$ in these equations.

If we add the absolute squares of (7.3.19a) and (7.3.19b), we get $E_{\mathbf{k}}^2(u_{\mathbf{k}}^2 + |v_{\mathbf{k}}|^2)^2 = \epsilon_k^2 + |\Delta_{\mathbf{k}}|^2$; in view of (7.3.15), this reduces to the first big result, the dispersion relation of Bogoliubov quasiparticles:

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}. (7.3.20)$$

This dispersion relation is plotted in Fig. 7.3.2.

Figure 7.3.2: (Right) Dispersion relations of quasiparticles: Dashed: Landau quasiparticles in normal state (=Fermi liquid); Solid: Bogoliubov quasiparticles in paired superconductor.

Combining (7.3.19a) and (7.3.15) gives the second big result, the magnitudes of the coefficients themselves:

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right) \tag{7.3.21a}$$

$$|v_{\mathbf{k}}|^2 = \frac{1}{2} \left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}} \right) \tag{7.3.21b}$$

The $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the key parameters in this lecture; Sorry, they should have been plotted in Lec. 7.1? see Fig. 7.3.1, in any case. The gap, of course, has a small effect on the nature of quasiparticles, except right near k_F . For $\epsilon_{\mathbf{k}} \gg \Delta(k_F)$, in (7.3.12a) and (7.3.12b), $u_{\mathbf{k}} \approx 1$, so the Bogoliubov quasiparticle is essentially an electron, as in the normal state (Fig. 7.3.2), while for $\epsilon_{\mathbf{k}} \ll -\Delta(k_F)$, $v_{\mathbf{k}} \approx 1$ and it is essentially a hole.

Note: it's sometimes handy to use trigonometric functions to parametrize the coefficients: let

$$u_{\mathbf{k}} = \sin \beta_{\mathbf{k}} \tag{7.3.22a}$$

$$v_{\mathbf{k}} = e^{i\theta} \cos \beta_{\mathbf{k}} \tag{7.3.22b}$$

The phase factor should really be $e^{i\theta_{\mathbf{k}}}$, and we should really assume that, but it can (will) be shown that all $\theta_{\mathbf{k}}$ must be the same.

Ground state wavefunction is the BCS wavefunction

Let $|\Phi_0\rangle$ be the "vacuum" of the quasiparticles, i.e., the state which is annihilated by any of the operators $\{\gamma_{\mathbf{k}}\}$. We can construct it as

$$|\Phi_0\rangle \propto \prod_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma} |0\rangle$$
 (7.3.23)

where $|0\rangle$, as usual, denotes the bare vacuum – the state which is annihilated by any of $\{c_{\mathbf{k}\sigma}\}$. Manifestly $\gamma_{\mathbf{k}\sigma}|\Phi_0\rangle = 0$ is indeed satisfied for any (\mathbf{k},σ) , since $(\gamma_{\mathbf{k}\sigma})^2 = 0$.

This $|\Phi_0\rangle$ must be the *ground state* of $\tilde{\mathcal{H}}_{\mathrm{Bogo.}}$, since it has zero quasiparticles, and each quasiparticle costs a nonvanishing energy $E_{\mathbf{k}}$. This fact is the key step for future manipulations: we now know how to figure out the ground state expectations of any string of γ and γ^{\dagger} operators. It is the same as the expectation of the corresponding string of c and c^{\dagger} operators in the vacuum of ordinary electrons (not the Fermi sea!).

Furthermore, if you substitute the definitions of $\gamma_{\mathbf{k}\sigma}$ into (7.3.23), it just reduces to the BCS wavefunction (modulo a normalization factor):

$$|\Phi_{\rm BCS}\rangle \propto |\Phi_0\rangle$$
 (7.3.24)

where $|\Phi_0\rangle$ was defined in (7.3.23). The (few) steps are left as an exercise, Ex. 7.3.3.

7.3 D The gap equation

The quantity $\Delta_{\mathbf{k}}$ is known as the *gap function* because its most obvious effect is the gap Δ_{k_F} in the Bogoliubov excitation spectrum, but it is actually a function defined

for **k** far away from the Fermi surface. It is a central object in BCS theory, as $E_{\mathbf{k}}$ and the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ [Eqs. (7.3.21)] that enter all pysical expectations depend on $\Delta_{\mathbf{k}}$. In this section, we'll obtain the self-consistent equation for $\Delta_{\mathbf{k}}$, and see how the Bogoliubov approach extends to T > 0.

Gap equation

We still need to solve for $\Delta_{\mathbf{k}}$. We just need to evaluate the factor $\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle$ in (7.3.8), is now easy to do using Eqs. (7.3.18) to convert electron into quasiparticle operators:

$$\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle = u_{\mathbf{k}}v_{\mathbf{k}}(\langle \gamma_{-\mathbf{k}\downarrow}\gamma_{-\mathbf{k}\downarrow}^{\dagger}\rangle - \langle \gamma_{\mathbf{k}\uparrow}^{\dagger}\gamma_{\mathbf{k}\uparrow}\rangle). \tag{7.3.25}$$

The terms of form $\gamma\gamma$ or $\gamma^{\dagger}\gamma^{\dagger}$ had zero expectation [in $|\Phi_{BCS}\rangle$, which we now know to be the vacuum of the Bogoliubov operators.] Using (7.3.19b) we get

$$\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle = \frac{1}{2} \left(\frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}} \right) \left(1 - \langle \hat{n}_{\mathbf{k}\uparrow}^{\mathrm{qp}} \rangle - \langle \hat{n}_{\mathbf{k}\downarrow}^{\mathrm{qp}} \rangle \right)$$
(7.3.26)

in terms of the number expectation defined in (7.3.13). At T=0, we have $\langle \hat{n}_{\mathbf{k}\sigma}^{\mathrm{qp}} \rangle \equiv 0$. So substituting (7.3.26) back into (7.3.8), we obtain the gap equation

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k'}} V_{\mathbf{k}\mathbf{k'}}^{(\mathbf{0})} \frac{\Delta_{\mathbf{k'}}}{\sqrt{|\epsilon_{\mathbf{k'}}|^2 + |\Delta_{\mathbf{k'}}|^2}}$$
(7.3.27)

This is a nonlinear integral equation for a whole unknown function $\Delta_{\mathbf{k}}$, which in general could only be solved by numeric integration. [You would guess the function $\Delta_{\mathbf{k}}$, insert it in the right-hand side of (7.3.27) which provides a new set of values for $\Delta_{\mathbf{k}}$, and keep iterating until it converges.]

Cooper approximation

CARTOON of "true" $V_{\mathbf{k}\mathbf{k}'}$ versus the Cooper pot.?

We can solve the gap function analytically. if the pairing potential $V_{\mathbf{k}\mathbf{k}'}^{(\mathbf{0})}$ is "separable", i.e. equal to $VA(\mathbf{k}')A(\mathbf{k})$ for some function $A(\mathbf{k})$. Then $A(\mathbf{k})$ factors out of the gap equation, and the rest is independent of \mathbf{k} , so we know $\Delta(\mathbf{k}) = \Delta_0 A(\mathbf{k})$.

As it happens, for the case of phonon-mediated coupling (but *not* necessarily for other mechanisms), the actual pairing potential is hardly dependent on wavevectors at all: the electrons at \mathbf{k} and $\mathbf{k'}$ (see Lec. 7.6) feel an attraction of about the same size, provided only that $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k'}}| < \hbar \omega D$, the Debye energy (energy scale of the phonons responsible for pairing). So Cooper took a separable toy potential $V_{\mathbf{k'k}}^{(0)} \to V_{\mathbf{k'k}}^{\text{Cooper}}$, where

$$V_{\mathbf{k}'\mathbf{k}}^{\text{Cooper}} = \begin{cases} -\frac{V_0}{N} & \text{when } |\epsilon_{\mathbf{k}}|, |\epsilon'_{\mathbf{k}}| < \hbar\omega_c; \\ 0 & \text{otherwise.} \end{cases}$$
 (7.3.28)

The cutoff frequency ω_c is roughly the Debye frequency.

Hence $\Delta_{\mathbf{k}} = \Delta$, up to the cutoff $|\mathbf{k}|$, beyond which $\Delta_{\mathbf{k}} = 0$. So we factor Δ out of the sum in (7.3.27), and divide it from both sides of (7.3.29) obtaining

$$1 = +\frac{1}{2} \frac{V_0}{N} \sum_{|\epsilon_{\mathbf{k}'}| < \hbar \omega_c} \frac{1}{\sqrt{|\epsilon_{\mathbf{k}'}|^2 + |\Delta_{\mathbf{k}'}|^2}}$$
 (7.3.29)

Since Cooper's toy potential is just a constant, all that matters here is the energies $\epsilon_{\mathbf{k}}$, not \mathbf{k} itself.

Obviously, if $-V_0 > 0$ (potential is repulsive in Fourier space), no solution is possible. ⁸

Solution of the BCS gap equation

Let $\mathcal{N}(\epsilon)$ be the density of electron states for one spin state only, per site. [The standard convention takes $\mathcal{N}(\epsilon)$ to be the DOS per unit volume, and takes V_0 to have units [energy][volume]. The conversion factor to that convention would be v_{cell} , the volume of a unit cell.]

We obtain

$$1 = +\frac{1}{2}V_0 \int_{-\hbar\omega_c}^{+\hbar\omega_c} d\epsilon \mathcal{N}(\epsilon) \frac{1}{\sqrt{\epsilon^2 + |\Delta|^2}}.$$
 (7.3.30)

Notice $\mathcal{N}(\epsilon) \approx \mathcal{N}(0)$ since $\hbar\omega_c \ll \epsilon_{\rm band}$, the bandwidth. Further assume $\Delta \ll \hbar\omega_c$; otherwise, and the Cooper potential is no longer such a good approximation. The integral (7.3.30) may be done exactly, but is better understood by "a poor man's" approximation. The integrand is approximately $\int d\epsilon/\epsilon$ over most of the range, which is log divergent both at $\epsilon \to 0$ and $\epsilon \to \infty$. The actual integrand stops diverging and levels off once $|\epsilon| < |\Delta|$ upper cutoff is $\hbar\omega_c$. Thus, the "poor man's" approximation of the integral is

$$\approx \left(\int_{\Delta}^{\hbar\omega_c} + \int_{\hbar\omega_c}^{\Delta} \right) \frac{d\epsilon}{\epsilon}. \tag{7.3.31}$$

The gap equation says

$$1 \approx \mathcal{N}(0)V_0 \left[\ln \left(\frac{\hbar \omega_c}{\Delta} \right) + \text{const} \right]$$
 (7.3.32)

Inverting this function, you obtain the grand formula $\Delta \approx (\text{const})\hbar\omega_c \exp[-1/\mathcal{N}(0)V_0]$. From the exact integral of (7.3.30) we get the same grand result for the BCS gap formula, but with the correct prefactor:

$$\Delta = \frac{\hbar\omega_c}{\sinh(1/\mathcal{N}(0)V_0)} \approx 2\hbar\omega_c e^{-1/\mathcal{N}(0)V_0}$$
 (7.3.33)

The exponential result is reliable only in the weak-coupling regime, $\mathcal{N}(0)V_0 \ll 1$. [Lec. 7.7 [omitted 2007]outlines the strong-coupling regime of the pairing theory.]

Remarks on gap formula

Rather like the charge-density-wave (CDW) gap of Lec. 3.4, this formula combines three parameters: one $(\mathcal{N}(0))$ characterizing the free-electron energy scale, another $(\hbar\omega_c)$ characterizing the phonon energy scale, and a third (V_0) related to the interaction term. In contrast to the CDW case, the third parameter is not directly the electron-phonon coupling strength g, but is a function of it since $V_0 = O(g^2/\hbar\omega_c)$. The dependence of Δ on V_0 is non-analytic, indeed it is exactly the function $\exp(-1/z)$ that is the cautionary example of analytic function theory. [Its Taylor series is zero term-by-term.]

It is now evident, in (7.3.33), why the gap Δ was small compared even to $\hbar\omega_c$. So is T_c , which (we'll shortly see) is essential the same quantity as Δ within BCS theory. So

⁸Still, it's possible to have an instantaneous potential $V(\mathbf{R}) > 0$ for all electron separations \mathbf{R} in real space, yet $V_{\mathbf{k}\mathbf{k}'}^{(0)} < 0$ in Fourier space for the wavevectors that dominate scatterings near the Fermi suface. Then the gap equation has a solution and superconductivity is expected.

(7.3.33) would would imply that (provided $V_0 > 0$), every metal goes superconducting at a sufficiently low temperature. In reality, if the predicted T_c is too small, the system will be unstable first to some competing kind of correlated electron state, so as to gain some energy from the interaction terms.

We are now equipped to compute, e.g., expectations of the $order\ parameter$ operator introduced in Lec. 7.1,

$$\langle \Psi(\mathbf{r}) \rangle \equiv \langle c \downarrow(\mathbf{r}) c_{\uparrow}(\mathbf{r}) \rangle = \frac{1}{N} \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle$$
 (7.3.34)

(See Ex. 7.3.4).

7.3 E Nonzero temperatures

I SHOULD SHOW SOME EXPERIMENTAL RESULT HERE...

What happens at T > 0? An obvious idea is simply to generalize the quantum expectations appearing in the decoupling (which were taken with respect to the ground state of particles) to the *thermal* expectations, for an ensemble in which quasiparticle states are occupied as independent fermions. This turns out to be correct. ⁹ If we return to (7.3.26), then we need simply set

$$\langle \hat{n}_{\mathbf{k}\sigma}^{\mathrm{qp}} \rangle_T = f_T(E_{\mathbf{k}}) = \frac{1}{1 + e^{E_{\mathbf{k}}/T}}$$
 (7.3.35)

the Fermi function. The chemical potential μ_{γ} of quasiparticles is equal to zero.

It's a somewhat subtle point why μ_{γ} is pinned to zero. Let's first review the chemical potential μ of ordinary electrons (which, I note, has no relation to μ_{γ} .) This is not pinned to zero physically. [Indeed it varies with temperature in both normal and superconducting states.] We merely shifted our energy scale to measure from μ . A general way to see that μ must be included in the Fermi distribution of electrons is that, since the electron number is conserved, there is no way to induce a transition that adds an electron at wavevector \mathbf{p} : thus $\epsilon_{\mathbf{p}}$ by itself is not an separation of two possible energy levels of the same system, which is the only physically meaningful energy difference. It is only when we append a reservoir (at chemical potential μ) to our system that we make that addition. The difference of energy levels is now $\epsilon_{\mathbf{p}} - \mu$, and the distribution function must be a function of this physically well-defined quantity.

On the other hand, $\mu_{\gamma} \equiv 0$ because the number of quasiparticles is *not* conserved – there are processes that create or annihilate a pair of quasiparticles. Whenever total particle number is non-conserved, the chemical potential is pinned at zero, as is familiar in the Bose-Einstein distributions for phonons or photons.

Since $v_{\mathbf{k}}^2 - u_{\mathbf{k}}^2 \equiv \epsilon_{\mathbf{k}}/E_{\mathbf{k}}$ is antisymmetric, as elaborated in Lec. 7.5, to lowest order you get zero net change in the filling of real electrons if you change μ_{γ} . This might make a good T.Q.

Temperature-dependent gap and value of T_c

The new gap equation looks like (7.3.27) except that a factor $\tanh(E_{\mathbf{k'}}/2T)$ is inserted in the right-hand side. If we adopt Cooper's toy potential, we get

$$1 = \frac{1}{2N} V_0 \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2T}\right)$$
 (7.3.36)

⁹I have not shown that this is the correct generalization, and it would be difficult to do so here, given my choice of an ad-hoc justification of the decoupling.

Is there a wrong factor, compare with (7.3.27)? As we raise T, the tanh factor gradually takes over the job of suppressing the logarithmic divergence, which was handled by Δ in $E_{\mathbf{k}} \equiv \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}$ in the denominator. Correspondingly, the value of Δ will decrease.

By definition, T_c is the temperature where $\Delta = 0$ and thus $E_{\mathbf{k}} = |\epsilon_{\mathbf{k}}|$. At the critical $\beta_c \equiv 1/T_c$, we get

$$1 = \frac{1}{2N} V_0 \sum_{\mathbf{k}} \frac{1}{|\epsilon_{\mathbf{k}}|} \tanh(\frac{1}{2}\beta_c |\epsilon_{\mathbf{k}}|) = \frac{1}{2} \mathcal{N}(0) V_0 \int_{\hbar\omega_c}^{+\hbar\omega_c} d\epsilon \frac{1}{|\epsilon|} \tanh\frac{1}{2}\beta_c |\epsilon|$$
 (7.3.37)

using the same approximations as in Sec. 7.3 D. Let's estimate this integral by the "poor man's approximation" as in Sec. 7.3 D. The upper cutoff is $\hbar\omega_c$ again, while the lower cutoff is roughly $\epsilon_{\bf k} \approx T_c$, since that is where the tanh function in (7.3.37) crosses over from unity to a linear behavior that cancels the $1/|\epsilon|$ divergence. Thus T_c is playing the same role in (7.3.37) that Δ played in the gap equation in Sec. 7.3 D; as you might anticipate, we have $1 \approx \mathcal{N}(0)V_0[\ln(\hbar\omega_c/T_c) + \text{const.}$ and $T_c \sim \Delta(0)$. In fact you can solve (7.3.37) exactly too, which gives the BCS result

$$T_c = 1.14 \, \hbar \omega_c \, e^{1/\mathcal{N}(0)V_0};$$
 (7.3.38)

comparing with (7.3.33), we get the ratio

$$\frac{2\Delta(0)}{T_c} = 2\pi e^{-C} \approx 3.50,\tag{7.3.39}$$

where C = 0.577 is Euler's constant.

A different anomalous quantity is the BCS order parameter Ψ , as noted in Lec. 7.0. But its expectation (including phase factor) is proportional to Δ within BCS theory. Consequently, Δ is often used as the order parameter – for both temperature and spatial dependences. Commonly Δ is called the "gap" even where it is being used as an order parameter and the excitation gap is not in mind. See Sec. 7.4 E(?) about the BdG equations.

Notice that even at T > 0, $\Delta(T)$, is the excitation gap of a quasiparticle. It is temperature dependent, somewhat like a semiconductor's bandgap is, but stronger since it vanishes at T_c .

Coherence length?

The BCS coherence length is

$$\xi(T) = \frac{\hbar v_F}{\pi \Delta(T)} \tag{7.3.40}$$

This is, in fact, the correlation length of the order parameter,

$$C_{\Psi}(R) \sim e^{-R/\xi(T)}$$
. (7.3.41)

I believe this is computed in an exercise. I should also mention the Green's functions $\langle c(\mathbf{r})c(\mathbf{r}')\rangle$.

The scaling with $\hbar v_F$ in (7.3.40) should be familiar, since length scales and energy scales always have this relation in a Fermi sea. ¹⁰

The T=0 coherence length has a special name, $\xi_0=\xi(0)$, and this is roughly the analog of the lattice constant in a spin model, in that the microscopic degrees of freedom and their interactions are localized to this length scale.

 $^{^{10}}$ Compare how the electron-density correlation length ξ_T scales with temperature T in the noninteracting Fermi sea (Ex. 1.3.5x), or the Kondo length scale as a function of the Kondo energy (Lec. 4.5).

Critical exponents and special-heat jump

BCS theory is just a kind of mean-field theory, so it gives the same critical exponents as the Ginzburg-Landau (GL) theory did. See Lec. 6.1 . I have mentioned the GINZBURG CRITERION there, which explains the regime of validity for mean-field theory in terms of $T-T_c$ and the G-L coefficients.

In particular, if we solve (7.3.36) near T_c , we find

$$\Delta(T) \sim (T_c - T)^{1/2}$$
 (7.3.42)

which implies (via (7.3.40)) that

$$\xi(T) \sim |T_c - T|^{-1/2}$$
. (7.3.43)

The specific heat has a jump at T_c , as in GL theory (or mean-field theory in general). The exact ratio (for a weak-coupling, s-wave superconductor) of the superconducting and normal state specific heats at T_c is ¹¹

$$\frac{C_s(T_c)}{C_n(T_c)} = 1 + \frac{12}{7\zeta(3)} = 2.43. \tag{7.3.44}$$

The specific heat ratio (7.3.44), and especially the gap/ T_c ratio (7.3.39), are diagnostic of weak coupling superconductors, well approximated by BCS theory. In strong-coupling superconductors (see Lec. 7.7 [omitted 2007]) (7.3.39) is larger.

Also, the T=0 condensation energy is $-E_{\rm cond}=\langle\mathcal{H}\rangle_{|\Phi_{\rm BCS}\rangle}-\langle\mathcal{H}\rangle_{|\Phi_F\rangle}$. The result is

$$-F_{cond}(0) \approx -\frac{1}{2}\mathcal{N}(0)\Delta^2 + \frac{1}{8}\mathcal{N}(0)\frac{\Delta^4}{(\hbar\omega_c)^2}$$
 (7.3.45)

within BCS theory using the Cooper potential. [Compare this with the GL result!]

7.3 X Charge of a quasiparticle

A quasiparticle is strange superposition of an electron and a hole. Since it carries an indefinite electron number, it carries an indefinite charge, but it's obvious from inspection that the *expectation* of its charge

$$Q_{\rm qp}(\mathbf{k}) \equiv (-e) \left(|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 \right) = (-e) \frac{\epsilon(\mathbf{k})}{E_{\mathbf{k}}}$$
 (7.3.46)

Basically, the fraction of time the quasiparticle spends as an hole or an electron is $u_{\mathbf{k}}^2$ or $|\mathbf{v}_{\mathbf{k}}|^2$, respectively (Ex. 7.3.7). The electron number is the odd function graphed in Fig. 7.3.1. Thus the effective charge $Q_{\rm qp}(\mathbf{k})$ ranges from +e, for $\epsilon \ll -\Delta$; to exactly zero, at the Fermi level where the quasiparticle is an equal mixture of electron and hole; to -e, for $\epsilon \gg +\Delta$.

Is this an example of fractional charge? Certainly in other kinds of many-body wavefunctions, elementary excitations are fractionally charged at some particular rational multiple of the electron charge, such as the fractional quantized Hall effect. But actually, the real charge of a Bogoliubov quasiparticle is exactly zero. ¹² If you inject an electron into a superconductor, indeed you can create a quasiparticle that travels

 $^{^{11}\}mathrm{See}$ Landau and Lifshitz, $Statistical\ Physics\ Part\ 2,\ \mathrm{Sec.}\ 40.$

¹²S. A. Kivelson and D. S. Rokhsar, Phys. Rev. B 41, 11693 (1990). For further discussion, see: Q. Si, Phys Rev. Lett. 78, 1767 (1997); H. L. Zhao and S. Hershfield, Phys. Rev. B 52, 3632 (1995).

through the bulk. But as it travels, it carries no charge; the actual charge is carried around the surface as a screening current (of the condensate of Cooper pairs.)

from Jörn 2005: surface current is carried by electrons in Cooper pairs.

In the BCS approximation, it sure looks like the quasiparticle is carrying a net current. But this is, I think, an artifact of omitting the long-range Coulomb interaction from our Hamiltonian. A superconductor excludes magnetic fields from its bulk, which means it must exclude any current that could make a magnetic field, which it does by making an equal and opposite screening current. [This "counterflow" of the condensate adjacent to the quasiparticle somewhat resembles the counterflow in a classical fluid with a hard sphere moving through it.] At the other side of the superconductor, the charge can recombine with quasiparticles to reconstitute electrons.

In exotic, non-pairing theories of superconductivity, elementary excitations called "spinons" appeared which are spin-1/2 chargeless fermions. It is amusing to find there is really no line separating the (comparatively) prosaic Bogoliubov quasiparticles – having spin (as a good quantum number) but zero charge – from the spinons.

I am slightly worried that one could assign physical meaning to the charge of the quasiparticle within the bulk, by the Aharonov-Bohm interference effects it experiences whenever it goes around some flux. It appears to me that that could be computed using the Bogoliubov-de Gennes equations (Sec. 7.4 E(?)) in which each quasiparticle is explicitly divided into particle and hole components. The flux acts differently on the electron and the hole parts, so it tends to break up the quasiparticle. This was very relevant, at least in the late 1990s, to understanding the thermal transport behavior in the vortex lattice of a d-wave superconductor, which was measured by experiments on the magnetic field effects on the thermal conductivity.

7.3 Y Variational derivation of BCS parameters

This derivation is spread across the next two sections. It mostly follows the original BCS path. 13 14

Sorry, parts of this are redundant with the earlier notes; other parts are skipped.

In this approach, unlike the Bogoliubov way, we assume the BCS wavefunction; as a justification, it could be shown this is the most general product form that has anomalous expectations only at zero wavevector.

We assume a BCS wavefunction, evaluate the energy expectation, and minimize with respect to the parameters $u_{\mathbf{k}}$, $v_{\mathbf{k}}$. To get a clean formula for the energy, though, we need to throw away all terms except the "pairing" terms – those which scatter one Fourier-space pair into another Fourier-space pair. We discover the "gap parameter" $\Delta_{\mathbf{k}}$ as the sum of a whole bunch of terms which all multiply the same combination $u_{\mathbf{k}}v_k$. Then, it is convenient to reparametrize $(u_{\mathbf{k}}, v_k)$ as the cosine and sine of some angle $\beta_{\mathbf{k}}$, which builds in the normalization.

Out of this we get a self-consistent "gap equation". It looks pretty horrible – if you have N discrete wavevectors, it is a nonlinear equation in N unknowns (or in the $N \to \infty$ limit, an integral equation.) To get an analytic answer, we use Cooper's approximation, that all electron states within a range $\hbar\omega_c$ of \mathcal{E}_F interact equally. For the

¹³ For another way to motivate the BCS guess, see R. P. Feynman, chapter 10 in *Statistical Mechanics* (Addison-Wesley, 1972), as well as the BCS paper itself.

¹⁴For a general introduction to the variational derivation, see (i) "Microscopic quantum interference effects in superconductivity" L. Cooper, Nobel Lecture, 1972 (reprinted in *Superconductivity* by J. R. Schrieffer); (ii) Chapter 4, "The superconducting ground state" (esp. Sec. 4.2), in G. Rickayzen, *Theory of Superconductivity* (Wiley, 1965).

phonon-mediated coupling, think of the cutoff ω_c as being the Debye frequency.¹⁵ With this approximation, $\Delta_{\bf k}$ is independent of $\bf k$ so the gap equation becomes an equation for a single unknown. In fact Δ enters the equation as the cutoff of an otherwise logarithmically divergent integral, so common when we have a Fermi surface. It looks a lot like the CDW gap equation (Lec. 3.4). The exponential dependence of Δ on the parameters explains the sensitivity of T_c to details.

Actually, it isn't so hard to solve the full gap equation numerically by iteration (compare the Eliashberg and McMillan equations in Lec. 7.7 [omitted 2007]). They still use one simplification: the gap function depends only on $\epsilon_{\mathbf{k}}$, so the integral equations involve one dimensional integrals over energies rather than three-dimensional integrals over wavevector.

The variational approach incorporates the same physical ideas as the Bogoliubov approach of Secs. 7.3 A ff and gives exactly the same results. ¹⁶

Hamiltonian

The Hamiltonian is assumed to be $\mathcal{H} = \mathcal{H}_{KE} + \mathcal{H}_{V}^{(0)}$, with

$$\mathcal{H}_{KE} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \equiv \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{n}_{\mathbf{k}\sigma}$$
 (7.3.47)

where $\hat{n}_{\mathbf{k}\sigma}$ is the number of fermions in that state. To be most precise, we are trying to minimize $\mathcal{H} - \mu \hat{N}$ where \hat{N} is the total number and μ is chemical potential. However, our convention is that the energy scale has been shifted so that $\mu = 0$; equivalently we are measuring $\epsilon_{\mathbf{k}}$ from the chemical potential (= Fermi energy, at T = 0).

The interaction energy can be written, quite generally, as

$$\mathcal{H}_{V}^{(0)} = \sum_{\mathbf{pkk'}} V_{\mathbf{kk'}}^{(\mathbf{p})} \sum_{\sigma_{1},\sigma_{2}} (c_{\mathbf{k'+p/2},\sigma_{1}}^{\dagger} c_{-\mathbf{k'+p/2},\sigma_{2}}^{\dagger} c_{-\mathbf{k+p/2},\sigma_{2}} c_{\mathbf{k+p/2},\sigma_{1}}$$
(7.3.48)

I've assumed just two things: translational symmetry (so the total wavevector of each term is zero, taking creation minus annihilation operators); and no spin dependence in the interaction. I also assumed the $V_{\mathbf{k}\mathbf{k}'}^{\mathbf{p}}$ was real...

(Later on we'll use Cooper's toy potential.)

7.3 Z Energy expectation

The next step is simply to find $\langle \mathcal{H} \rangle_{|\Phi_{\rm BCS}\rangle}$. Some of the inputs were exercises in Lec. 7.1. The noninteracting term is trivial: we already noted that $\langle \hat{n}_{\mathbf{k}\sigma} \rangle = |v_{\mathbf{k}}|^2$, thus

$$\langle \mathcal{H}_{KE} \rangle = \sum_{\mathbf{k}} 2\epsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2$$
 (7.3.49)

(the 2 is for spin).

 $^{^{15}}$ See Lec. 7.6). The real phonon-mediated coupling could be well approximated by saying all electron states within $\hbar\omega_c$ interact equally. But electron states that are farther away from \mathcal{E}_F than $hbar\omega_c$ are not very important and we can get away with omitting their interaction.

¹⁶ "Random-phase approximation in the Theory of Superconductivity" by P. W. Anderson, Phys. Rev. 112, 1900 (1958), discusses the equivalence of the BCS variational approach and the Bogoliubov-Valatin approach.

Why the "pairing" terms?

Let's first consider the plain Fermi sea $|\Psi_F\rangle$, which is actually just the special case of $|\Phi_{\rm BCS}\rangle$ with $u_{\bf k}=0, v_{\bf k}=1$ for $\epsilon_{\bf k}<\mathcal{E}_F$, but $u_{\bf k}=1, v_{\bf k}=0$ for for $\epsilon_{\bf k}>\mathcal{E}_F$. For a term in \mathcal{H}_V to have a nonzero expectation in $|\Psi_F\rangle$ (or any other state with definite occupation numbers), each creation operator must be paired with the annihilation operator of the same state. As usual, there are two ways to do this.

First, the "Hartree" term has the final state of the two interacting electrons identical to the initial state, $|\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2\rangle \rightarrow |\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2\rangle$. This corresponds to $\mathbf{k}'=\mathbf{k}$ and the result is simply

$$\langle \mathcal{H}_V^{(0)} \rangle_{\text{Hartree}} = \sum_{\mathbf{pk}} V_{\mathbf{kk}}^{(\mathbf{p})} n_{\mathbf{k}+\mathbf{p}/2} n_{-\mathbf{k}+\mathbf{p}/2}$$
 (7.3.50)

where $n_{\mathbf{k}} \equiv \sum_{\sigma} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$.

Secondly, the "Fock" (= "exchange") term is given by $\mathbf{k}' = -\mathbf{k}$ and $\sigma_1 = \sigma_2$; again the outgoing state is identical to the incoming one, but now the scattering is such as to permute electrons 1 and 2.

$$\langle \mathcal{H}_V^{(0)} \rangle_{\text{Fock}} = -\sum_{\mathbf{pk}} V_{\mathbf{k},-\mathbf{k}}^{(\mathbf{p})} \sum_{\sigma} n_{\mathbf{k}+\mathbf{p}/2,\sigma} n_{-\mathbf{k}+\mathbf{p}/2,\sigma}$$
 (7.3.51)

(I NEED TO VERIFY THE - SIGN) These terms are large – of order eV per electron. ¹⁷ Those expectations are coming from the entire Fermi sea and not just the portion around the Fermi energy.

Now, expectations (7.3.50) and (7.3.51) have just exactly the form assumed in Fermi liquid theory, which they inspired. The spirit of Fermi liquid theory suggests we ought to cancel these terms by making the unsual transformation to Fermi-liquid quasiparticles (Lec. 1.7). After all, superconductivity will only involve the states close in energy to \mathcal{E}_F , exactly those for which Fermi liquid theory is valid.

So, although we will continue to call $\{c_{\mathbf{k}}\}$ "electron" operators, they are really quasiparticle operators. The main consequences, for our purposes here, are (i) the value of v_F will be renormalized because of the interactions (ii) we can assume the Hartree and Fock terms have already been accounted for in $\epsilon_{\mathbf{k}}$ (iii) the coefficients $V_{\mathbf{k}\mathbf{k}'}^{(\mathbf{p})}$ will be changed in the transformation.

We've argued away the large energies that will (however) not differ much between the normal and superconducting phases. To explain the latter's stability, we must turn to the small energies which depend on the superconducting correlations.

Pairing terms

Taking $\langle \mathcal{H}_V^{(0)} \rangle$ in $|\Phi_{\rm BCS}\rangle$, one obtains the same terms as before, and a third type of expectation, those of the *pairing terms*. ¹⁸ That means any term with $\mathbf{p} = 0.19$

$$\mathcal{H}^{\text{pair}} = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{(\mathbf{0})} b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}}$$
 (7.3.52)

¹⁷See Ashcroft and Mermin, chapter 17.

¹⁸The original BCS paper made their derivation more straightforward by simply assuming an interaction of form $\mathcal{H}^{\text{pair}}$. Notice that $|\Phi_{\text{BCS}}\rangle$ is not necessarily an eigenstate of $\mathcal{H}^{\text{pair}}$, but at least $\mathcal{H}^{\text{pair}}$ preserves its paired nature (of having occupation always 0 or 2 for the two single-electron states which were paired.

¹⁹Here $\mathbf{p} = \mathbf{0}$ plays a special role because it did so in $|\Phi_{BCS}\rangle$. You could instead have paired states with $\mathbf{k} + \mathbf{k}' = \mathbf{p}$ and then you would have to make the same change in the definition of $b_{\mathbf{k}}$.

Possibly should exclude $\mathbf{k} = \mathbf{k}'$ in this sum? In this case, we get a nonzero expectation by (say) selecting the $u_{\mathbf{k}}$ term in $\langle \Phi_{\mathrm{BCS}} |$ and the $va_{\mathbf{k}}$ term in $|\Phi_{\mathrm{BCS}}\rangle$ in $\langle \Phi_{\mathrm{BCS}} | \mathcal{H}_V^{(0)} | \Phi_{\mathrm{BCS}} \rangle$. So let's compute the expectation of a term in $\mathcal{H}^{\mathrm{pair}}$. We get

$$\langle b_{\mathbf{k}'}^{\dagger}, b_{\mathbf{k}} \rangle_{|\Phi_{\mathrm{BCS}}\rangle} = \langle 0 | (u_{\mathbf{k}'}^* + \underline{v_{\mathbf{k}'}^*} b_{\mathbf{k}}') (\underline{u_{\mathbf{k}}^*} + v_{\mathbf{k}}^* b_{\mathbf{k}}) b_{\mathbf{k}'}^{\dagger} \underline{b_{\mathbf{k}}} (u_{\mathbf{k}} + v_{\mathbf{k}} b_{\mathbf{k}}^{\dagger}) (\underline{u_{\mathbf{k}'}} + v_{\mathbf{k}'} b_{\mathbf{k}'}^{\dagger}) | 0 \rangle \quad (7.3.53)$$

In (7.3.53), the terms which give nonzero expectations are underlined. The factors inside (...) all came from the $\langle \Phi_{\rm BCS} |$ and $|\Phi_{\rm BCS} \rangle$ factors. All the other factors in the BCS wavefunction (with \mathbf{k}'' different from \mathbf{k} or \mathbf{k}') simply gave factors of $|u_{\mathbf{k}''}|^2 + |v_{\mathbf{k}''}|^2$.

The result is

$$\langle \mathcal{H}^{\text{pair}} = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}^{(\mathbf{0})}(u_{\mathbf{k}}^* v_{\mathbf{k}})(u_{\mathbf{k}'} v_{\mathbf{k}'}^*)$$
(7.3.54)

It is a bit tedious, but BCS also (i) could extract the excitation spectrum, which has a gap equal to the minimum value of $\Delta(\mathbf{k})$ for \mathbf{k} on the Fermi surface (ii) could generalize the theory to T > 0 and thus extract T_c .

Rest of these notes

Sorry, I didn't manage to convert the rest of these notes. As noted earlier, to a fair extent it duplicates the Bogoliubov approach, so you can take your pick. However, there are certain handy identities for our parametrization of the BCS theory (the angles $\beta_{\mathbf{k}}$) which are summarized in the next section, and I think *not* included in the Bogoliubov notes.

Exercises

General advice for these exercises

The questions here are mostly about the BCS wavefunction and could have been asked in Lec. 7.1, but they can be answered more efficiently using the machinery introduced in this section. In many instances, one needs to evaluate the expectation of a string of $c_{\mathbf{k}\sigma}$'s and $c_{\mathbf{k}\sigma}^{\dagger}$'s. One workable method is direct substitution into the BCS formula. A second method is possible after Lec. 7.5: rewrite $c_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}\sigma}^{\dagger}$ in terms of the Bogoliubov quasiparticle operators $\gamma_{\mathbf{k}\sigma}$ and $\gamma_{\mathbf{k}\sigma}^{\dagger}$. Then note that $|\Phi_{\rm BCS}\rangle$ is the "vacuum" for quasiparticles, i.e. $\gamma_{\mathbf{k}\sigma}|\Phi_{\rm BCS}\rangle\equiv 0$. The second approach is a bit less messy algebraically, at the price of demanding a bit more sophistication.

More hints – In general, for the exercises involving Bogoliubov manipulations, the most convenient method seems to be writing $\{c_{\mathbf{k}\sigma}\}$ and $\{c_{\mathbf{k}\sigma}^{\dagger}\}$ in terms of $\{\gamma_{\mathbf{k}\sigma}\}$ and $\{\gamma_{\mathbf{k}\sigma}^{\dagger}\}$. In every case, first give the result in terms of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. You can then reexpress it in terms of $\epsilon_{\mathbf{k}}$, Δ and (for convenience) $E_{\mathbf{k}}$. As in lecture, I personally find it convenient to use trigonometric functions: defining an angle $\beta_{\mathbf{k}}$ by $\epsilon_{\mathbf{k}} = -\Delta \cot 2\beta_{\mathbf{k}}$. Thus

$$u_{\mathbf{k}} = \sin \beta_{\mathbf{k}}; \qquad v_{\mathbf{k}} = \cos \beta_{\mathbf{k}}$$
 (7.3.55)

You may leave results in terms of $\beta_{\mathbf{k}}$ if you find it tedious to put them in terms of $\epsilon_{\mathbf{k}}$ and Δ .

Ex. 7.3.1 Electron occupation in BCS I (T)

The Fermi distribution function decays with \mathbf{k} as $f_T(\mathbf{k}) \sim e^{-\epsilon_{\mathbf{k}}/T}$ for $\epsilon_{\mathbf{k}} - \mu \gg T$, where $\epsilon_{\mathbf{k}}$ is the electron dispersion relation. What about the function $f_{BCS}(\mathbf{k}) \equiv |v_{\mathbf{k}}|^2$ from the BCS wavefunction: how does it decay with k for $\epsilon_{\mathbf{k}} - \mu \gg \Delta$?

Ex. 7.3.2 Electron occupation in BCS II (T)

- (a) If $|v_{\mathbf{k}}|^2 \sim (\Delta/2\epsilon_{\mathbf{k}})^2 \sim 1/|k-k_F|^2$ at large k in Fourier space, what power-law behavior does this imply for the pair wavefunction at small R in real space?
 - (b)(OPTIONAL) Over what range of distances R is the power-law valid?

Ex. 7.3.3 BCS wavefunction as the Bogoliubov "vacuum"

(a). Let's start with a wavefunction containing just two factors from (7.3.23). Show that

$$\gamma_{\mathbf{k}\uparrow}\gamma_{-\mathbf{k}\downarrow}|0\rangle = v_{\mathbf{k}}(u_k + v_{\mathbf{k}}c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger})|0\rangle \tag{7.3.56}$$

by substituting from (7.3.12a) and (7.3.12b).

(b). Argue that

$$\prod_{\mathbf{k}} (\gamma_{\mathbf{k}\uparrow} \gamma_{-\mathbf{k}\downarrow}) |0\rangle \propto \prod_{\mathbf{k}} (u_k + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}) |0\rangle$$
 (7.3.57)

This verifies (7.3.24) (it should be obvious why the products of γ operators are the same).

Hints: The key step is to show the *only* way to keep an annihilation operator factor in (7.3.57) from making its term be zero, is to pair it with a creation operator (on its right) from the factor $\gamma_{\mathbf{k}\downarrow}$ within the same parenthesis in the left-hand side of (7.3.57).

Ex. 7.3.4 Order parameter expectation

This problem continues the warm-up exercises of Lec. 7.1 by computing expectations and correlation functions of the order parameter operator $\Psi(\mathbf{r})$ defined there.

- (a). Find $\langle \Psi(\mathbf{r}) \rangle$, as an integral over **k** with integrand depending on Δ and $\epsilon(\mathbf{k})$.
- (b). You may need to adopt the "Cooper approximation" (that Δ is a constant). Then use the gap equation to simplify the above result and show $\langle \Psi(\mathbf{r}) \rangle = \Delta/V_0$.

Ex. 7.3.5 Constant term in BCS energy

Show the constant term in (7.3.7) is $\operatorname{const}_V = |\langle \Psi \rangle|^2$, where Ψ is given by (7.3.34) (see Ex. 7.3.4).

WORRY: are factors of N right, here?

Ex. 7.3.6 "Off-diagonal long-range order:" Correlation functions in BCS ground state

- (a). For T=0 find $C_{\Psi}^{\rm un}({\bf r})\equiv \langle \Psi^{\dagger}({\bf 0})\Psi({\bf r})\rangle$ as defined in Lec. 7.1 , written as an integral over ${\bf k}$ as in Ex. Ex. 7.3.4.
- (b). From the results of (a), calculate $\delta C(\mathbf{r}) = C_{\Psi}^{\mathrm{un}}(\mathbf{r}) \lim_{\mathbf{r} \to \infty} C_{\Psi}^{\mathrm{un}}(\mathbf{r})$ as defined in Lec. 7.1 . Show that this result can be written as a Fourier transform $|\tilde{f}_{BCS}(\mathbf{r})|^2$, where $f_{BCS}(\mathbf{k}) \equiv \langle n_{\mathbf{k}} \rangle$ is the analog for the BCS state of the Fermi function. (The function f_{BCS} can of course be written in terms of Δ and $\epsilon_{\mathbf{k}}$).

This correlation function is very similar to the correlation function of the ordinary electron density in the normal Fermi gas, which was computed in Sec. 1.2 C. Although f_{BCS} at T_0 has a slightly different shape from the Fermi function at T_c , the difference

is very small (Tinkham, Fig. 2-1); in either case, the key point is that the sharp Fermi surface has been smeared out.

There is a correlation length ξ_{ee} such that this correlation function decays as $e^{-r/\xi_{ee}}$.

(c). As a fudge, replace the function $f_{BCS}(\mathbf{k})$ by the Fermi function $f_T(\mathbf{k})$ with $T = T_c$. Then, assuming the result of Ex. 1.3.5x, find how ξ_{ee} depends on Δ and v_F (ignoring dimensionless prefactors!). How does this compare to the *order parameter* correlation length ξ defined in Lec. 7.1 C?

Ex. 7.3.7 Quasiparticle parameters for transport

In each part, sketch the behavior as a function of $\epsilon_{\mathbf{k}}/\Delta$; be sure to indicate the values at $\epsilon_{k}/\Delta = -\infty, 0, +\infty$.

- (a). What is the group velocity of the quasiparticles? (trivial).
- (b). Check the value asserted in Sec. 7.3 X for the mean charge $Q_{\rm qp}({\bf k})$ carried by a quasiparticle of wavevector ${\bf k}$.

Hint: write the electron number $\hat{N} = \sum_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma}^{\dagger} c_{\mathbf{p}\sigma}$ in terms of quasiparticle operators, and recall $|\Phi_{\mathrm{BCS}}\rangle$ is the vacuum of the latter.