Problem 1: BCS Mean-Field Theory

The mean-field BCS Hamiltonian is

$$\overline{H}_{BCS} = \sum_{\mathbf{k}} \left\{ \epsilon_k \left(n_{\mathbf{k},\uparrow} + n_{-\mathbf{k},\downarrow} \right) + c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger \Delta + \Delta^* c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \right\}. \tag{1}$$

When the mean-field ansatz was made to write the Hamiltonian in terms of the gap energy Δ, it was necessary that Δ obey the consistency-condition

$$\Delta = \frac{U}{V} \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle, \tag{2}$$

where U is the effective attraction between unlike spins and V is the sample volume.

We are to determine all of the eigenenergies and eigenstates of this Hamiltonian, and study its properties at finite temperature. We will do this using the method introduced by Bogoliubov[1].

The key insight of Bogoliubov is that although the mean-field Hamiltonian (1) is clearly not diagonal in the space of states created by the operators $c_{\mathbf{k},\uparrow/\downarrow}^\dagger$, it may be diagonal in a basis of states created by operators related to these via a simple SU_2 transformation. Indeed, it may be the case that 'electrons' and 'holes' are the wrong degrees of freedom to consider; we should at least look to see if the Hamiltonian is simpler in terms of any collective degrees of freedom.

Along these lines, we define the rotated, 'collective' or 'Bogoliubov' creation and annihilation operators $b_{\mathbf{k},\uparrow/\downarrow}$ and $b_{\mathbf{k},\uparrow/\downarrow}^\dagger$ given by

$$b_{\mathbf{k},\uparrow} = A_k c_{\mathbf{k},\uparrow} + B_k c_{-\mathbf{k},\downarrow}^\dagger;$$
$$b_{-\mathbf{k},\downarrow} = A_k c_{-\mathbf{k},\downarrow} - B_k c_{\mathbf{k},\uparrow}^\dagger. \tag{3}$$

It is clear that we desire this to be an SU_2 transformation, which implies that $|A_k|^2 + |B_k|^2 = 1$. As an SU_2-related basis of fermionic operators, these Bogoliubov operators obey the normal anticommutation relations $\{b_j, b_k\} = \{b_j^\dagger, b_k^\dagger\} = 0$ and $\{b_j^\dagger, b_k\} = \delta_{jk}$.

To clarify, we merely propose the transformations (3) and hope that an appropriate choice of A_k and B_k will bring $\overline{H}_{BCS}$ into diagonal form. Therefore, the first thing we must do is re-cast the Hamiltonian in terms of 'Bogoliubons'—and to do this, the first thing we must do is invert the relationship (3).

Using the definitions (3) together with their Hermitian conjugates we obtain the system

$$
\begin{array}{rclcrcl}
c_{\mathbf{k},\uparrow} & = & \frac{1}{A_k} b_{\mathbf{k},\uparrow} - \frac{B_k}{A_k} c_{-\mathbf{k},\downarrow}^\dagger & & c_{-\mathbf{k},\downarrow}^\dagger & = & \frac{1}{B_k} b_{\mathbf{k},\uparrow} - \frac{A_k}{B_k} c_{\mathbf{k},\uparrow}^\dagger \\
c_{\mathbf{k},\uparrow} & = & -\frac{1}{B_k^*} b_{-\mathbf{k},\downarrow}^\dagger + \frac{A_k^*}{B_k^*} c_{-\mathbf{k},\downarrow}^\dagger & \text{and} & c_{-\mathbf{k},\downarrow}^\dagger & = & \frac{1}{A_k^*} b_{-\mathbf{k},\downarrow}^\dagger + \frac{B_k^*}{A_k^*} c_{\mathbf{k},\uparrow}^\dagger
\end{array}. \tag{4}
$$

By subtracting the related identities, we find that

$$c_{\mathbf{k},\uparrow} = A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^\dagger;$$
$$c_{-\mathbf{k},\downarrow}^\dagger = B_k^* b_{\mathbf{k},\uparrow} + A_k b_{-\mathbf{k},\downarrow}^\dagger. \tag{5}$$

Now, writing the mean-field Hamiltonian in terms of the Bogoliubov operators, we encounter

$$\overline{H}_{BCS} = \sum_{\mathbf{k}} \left\{ \epsilon_k \left[\left(A_k b_{\mathbf{k},\uparrow}^\dagger - B_k^* b_{-\mathbf{k},\downarrow} \right) \left(A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^\dagger \right) + \left(B_k^* b_{\mathbf{k},\uparrow} + A_k b_{-\mathbf{k},\downarrow}^\dagger \right) \left(B_k b_{\mathbf{k},\uparrow}^\dagger + A_k^* b_{-\mathbf{k},\downarrow} \right) \right] \right.$$

$$\left. + \Delta \left(A_k b_{\mathbf{k},\uparrow}^\dagger - B_k^* b_{-\mathbf{k},\downarrow} \right) \left(B_k^* b_{\mathbf{k},\uparrow} + A_k b_{-\mathbf{k},\downarrow}^\dagger \right) + \Delta^* \left(B_k b_{\mathbf{k},\uparrow}^\dagger + A_k^* b_{-\mathbf{k},\downarrow} \right) \left(A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^\dagger \right) \right\},$$

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[1]This is the method discussed the course textbook, Tinkham's *Introduction to Superconductivity*. Our analysis will closely follow the discussion in that text.

which at first-sight appears horrendous to expand. Using anti-commutation relations to simplify things a bit,

$$\overline{H}_{BCS} = \sum_{\mathbf{k}} \left\{ \epsilon_k \left[\left(|A_k|^2 - |B_k|^2 \right) \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) + 2|B_k|^2 - 2A_k B_k b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger - 2A_k^* B_k^* b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} \right] \right.$$

$$+ \Delta \left[A_k B_k^* \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) - A_k B_k^* + A_k^2 b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger - B_k^{*2} b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} \right]$$

$$\left. + \Delta^* \left[A_k^* B_k \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) - A_k^* B_k + A_k^{*2} b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} - B_k^2 b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger \right] \right\}$$

$$= \sum_{\mathbf{k}} \left\{ 2\epsilon_k |B_k|^2 - 2\, \mathfrak{Re}\left(\Delta A_k B_k^* \right) + \left[\epsilon_k \left(|A_k|^2 - |B_k|^2 \right) + 2\, \mathfrak{Re}\left(\Delta A_k B_k^* \right) \right] \left(b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow} + b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow} \right) \right.$$

$$\left. + b_{\mathbf{k},\uparrow}^\dagger b_{-\mathbf{k},\downarrow}^\dagger \left(\Delta A_k^2 - \Delta^* B_k^2 - 2\epsilon_k A_k B_k \right) + b_{-\mathbf{k},\downarrow} b_{\mathbf{k},\uparrow} \left(\Delta^* A_k^{*2} - \Delta B_k^{*2} - 2\epsilon_k A_k^* B_k^* \right) \right\}. \quad (6)$$

Now, because we are free to choose A_k and B_k any way we'd like—so long as the transformation is SU_2—we would obviously like to define them so that the off-diagonal contributions to $\overline{H}_{BCS}$ vanish—these are the last two terms in (6). Now, the off-diagonal terms will vanish if the Bogoliubov coefficients are chosen to satisfy

$$\Delta A_k^2 - \Delta^* B_k^2 - 2\epsilon_k A_k B_k = 0. \quad (7)$$

This is a simple quadratic equation, the solution to which is simply[2]

$$A_k = \frac{B_k}{\Delta} \left(\epsilon_k \pm \sqrt{\epsilon_k^2 + |\Delta|^2} \right) \equiv \frac{B_k}{\Delta} \left(\epsilon_k \pm E_k \right). \quad (8)$$

With this condition, the last line of (6) vanishes. But we actually have a bit more than that: the additional constraint $|A_k|^2 + |B_k|^2 = 1$ allows us to eliminate these coefficients all-together[3]. Notice that (8) implies that, after a bit of algebra,

$$|A_k|^2 = \frac{|B_k|^2}{|\Delta|^2} \left(\epsilon_k \pm E_k \right)^2 = \left(1 - |A_k|^2 \right) \frac{1}{|\Delta|^2} \left(\epsilon_k \pm E_k \right)^2 = \frac{\left(\epsilon_k \pm E_k \right)^2}{|\Delta|^2 + \left(\epsilon_k \pm E_k \right)^2} = \ldots = \frac{1}{2} \left(1 \pm \frac{\epsilon_k}{E_k} \right). \quad (9)$$

And, similarly,

$$|B_k|^2 = \frac{1}{2} \left(1 \mp \frac{\epsilon_k}{E_k} \right). \quad (10)$$

Notice also that $\Delta A_k B_k^*$ is manifestly real and specifically

$$\mathfrak{Re}\left(\Delta A_k B_k^* \right) = \Delta A_k B_k^* = |B_k|^2 \left(\epsilon_k \pm E_k \right). \quad (11)$$

Let us define the quasi-particle ('Bogoliubon') number operators $\tilde{n}_{\mathbf{k},\uparrow} \equiv b_{\mathbf{k},\uparrow}^\dagger b_{\mathbf{k},\uparrow}$ and $\tilde{n}_{-\mathbf{k},\downarrow} \equiv b_{-\mathbf{k},\downarrow}^\dagger b_{-\mathbf{k},\downarrow}$. Putting all of this together, we may re-express the BCS Hamiltonian completely in terms of the Bogoliubov operators.

$$\overline{H}_{BCS} = \sum_{\mathbf{k}} \left\{ 2\epsilon_k |B_k|^2 - 2|B_k|^2 \left(\epsilon_k \pm E_k \right) + \left[\epsilon_k \left(|A_k|^2 - |B_k|^2 \right) + 2|B_k|^2 \left(\epsilon_k \pm E_k \right) \right] \left(\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} \right) \right\},$$

$$= \sum_{\mathbf{k}} \left\{ \mp 2|B_k|^2 E_k + \left(\epsilon_k \pm 2|B_k|^2 E_k \right) \left(\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} \right) \right\},$$

$$= \sum_{\mathbf{k}} \left\{ \epsilon_k \mp E_k \pm E_k \left(\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} \right) \right\}.$$

The physical requirement that the total energy be bounded below demands that '$\pm$' $\mapsto$ '$+$': otherwise, the creation of Bogoliubons would lower the energy of the system without bound. Therefore, we have shown that in terms of the Bogoliubon quasi-particles,

$$\therefore \overline{H}_{BCS} = \sum_{\mathbf{k}} \left\{ \epsilon_k - E_k + E_k \left(\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} \right) \right\}. \quad (12)$$

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[2]We have not made use of the freedom to make A_k real—nor will we: it never is necessary.

[3]To be precise, there is still an arbitrary (unphysical) phase between A_k and B_k, and there is an insofar unspecified sign in A_k. This sign will be determined below—until then, however, we'll keep it unspecified.

Notice that the Hamiltonian is diagonal in terms of the quasi-particles—it manifestly commutes with the Bogoliubon number operators. Eigenstates are therefore labeled by their momenta $\mathbf{k}$ and quasi-particle numbers: for a given momentum, let $|\mathbf{k}\rangle$ be defined as that which is annihilated by both $b_{\mathbf{k},\uparrow}$ and $b_{-\mathbf{k},\downarrow}$; clearly, $|\mathbf{k}\rangle$ has both quasi-particle numbers 0. Because the quasi particles are fermions, there can be at most one of each kind at a given momentum. Therefore, the eigenstates of $\overline{H}_{BCS}$ for a given $\mathbf{k}$ are exactly

$$|\mathbf{k}\rangle, \qquad b_{\mathbf{k},\uparrow}^{\dagger}|\mathbf{k}\rangle, \qquad b_{-\mathbf{k},\downarrow}^{\dagger}|k\rangle, \quad \text{and} \quad b_{\mathbf{k},\uparrow}^{\dagger}b_{-\mathbf{k},\downarrow}^{\dagger}|\mathbf{k}\rangle, \tag{13}$$

with eigenenergies, respectively,

$$\epsilon_k - E_k, \qquad \epsilon_k, \qquad \epsilon_k, \quad \text{and} \quad \epsilon_k + E_k. \tag{14}$$

Now, recall that the consistency of the mean-field Hamiltonian requires that

$$\Delta = \frac{U}{V}\sum_{\mathbf{k}}\langle c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow}\rangle.$$

To find the expectation value of the operator $c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow}$ at a given momentum $\mathbf{k}$, we'll need the partition function

$$\mathcal{Z} = \sum_{\text{states}} e^{-\beta H} = e^{-b(\epsilon_k - E_k)} + 2e^{-\beta\epsilon_k} + e^{-\beta(\epsilon_k + E_k)} = 2e^{-\beta\epsilon_k}\left(1 + \cosh(\beta E_k)\right). \tag{15}$$

Now, we should express the operator $(c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow})$ in terms of the Bogoliubov operators,

$$c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow} = \left(B_k b_{\mathbf{k},\uparrow}^{\dagger} + A_k^* b_{-\mathbf{k},\downarrow}\right)\left(A_k^* b_{\mathbf{k},\uparrow} - B_k b_{-\mathbf{k},\downarrow}^{\dagger}\right),$$
$$= A_k^* B_k\left(\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} - 1\right) + A_k^{*2}b_{-\mathbf{k},\downarrow}b_{\mathbf{k},\uparrow} - B_k^2 b_{\mathbf{k},\uparrow}^{\dagger}b_{-\mathbf{k},\downarrow}^{\dagger}.$$

Because the last two terms do not commute with the Hamiltonian, they will not contribute anything to the expectation value $\langle c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow}\rangle$. Therefore[4],

$$\langle c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow}\rangle = \frac{1}{\mathcal{Z}}\sum_{|\psi\rangle}A_k^* B_k\langle\psi|\left(\tilde{n}_{\mathbf{k},\uparrow} + \tilde{n}_{-\mathbf{k},\downarrow} - 1\right)e^{-\beta H}|\psi\rangle,$$

$$= \frac{\Delta e^{\beta\epsilon_k}}{4E_k(1 - \cosh(\beta E_k))}\left\{-e^{-\beta(\epsilon_k - E_k)} + e^{-\beta(\epsilon_k + E_k)}\right\},$$

$$= -\frac{\Delta\sinh(\beta E_k)}{2E_k(1 - \cosh(\beta E_k))},$$

$$= -\frac{\Delta}{2}\frac{\tanh\left(\beta E_k/2\right)}{E_k}.$$

So in the large-volume limit, the consistency demands that

$$-\Delta\frac{V}{U} = \Delta\frac{1}{2}\int_{\substack{\text{fermi}\\\text{surface}}}\frac{\tanh\left(\frac{\beta}{2}\sqrt{\epsilon_k^2 + |\Delta|^2}\right)}{\sqrt{\epsilon_k^2 + |\Delta|^2}}d\epsilon_k \qquad \Longrightarrow \qquad \Delta = 0 \quad \text{or} \quad -\frac{V}{U} = \int_0^{\hbar\omega_c}\frac{\tanh\left(\frac{\beta}{2}\sqrt{\epsilon_k^2 + |\Delta|^2}\right)}{\sqrt{\epsilon_k^2 + |\Delta|^2}}d\epsilon_k. \tag{16}$$

We were asked to argue that for low enough temperature, $\Delta > 0$ is consistent, but for high enough temperatures only $\Delta = 0$ is possible. We will actually do a bit more and determine the critical temperate, T_c, above which $\Delta = 0$ is required for consistency. However, before we do that calculation, let us argue generally to understand the results qualitatively.

At zero temperature, $\tanh(\beta E_k/2) \to 1$ so that a non-zero Δ would be determined by the equation

$$-\frac{V}{U} = \int_0^{\hbar\omega_c}\frac{dx}{\sqrt{x^2 + |\Delta|^2}} = \log\left(\hbar\omega_c\left(1 + \sqrt{1 + \frac{|\Delta|^2}{(\hbar\omega_c)^2}}\right)\right) - \log(\Delta) \approx \log\left(\frac{2\hbar\omega_c}{|\Delta|}\right). \tag{17}$$

Solving for $\Delta(T = 0)$ we find

$$|\Delta(T = 0)| \approx 2\hbar\omega_c e^{V/U}. \tag{18}$$

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[4]On the borderline of triviality, we recall the identities $\sinh(\xi) = 2\sinh(\xi/2)\cosh(\xi/2)$ and $1 + \cosh(\xi) = 2\cosh^2(\xi/2)$.

Therefore, we know that for small enough temperature, $\Delta \neq 0$ is consistent. However, for temperatures greater than about $kT > \frac{1}{2}\sqrt{(\hbar\omega_c)^2 + |\Delta|^2}$, we may Taylor-expand the integrand of the consistency equation, yielding

$$-\Delta\frac{U}{V} = \Delta \int\limits_0^{\hbar\omega_c} d\epsilon_k \frac{1}{E_k}\left(\frac{\beta}{2}E_k - \frac{\beta^3}{24}E_k^3 + \frac{\beta^5}{240}E_k^5 - \ldots\right). \tag{19}$$

Parametrically, if we suppose that $\Delta \neq 0$ then the constraint equation becomes a polynomial linear in β and with a leading Δ term of order $\beta^3\Delta^2$. Regardless of the details of integration, the general solution to a polynomial equation of the form $c_1\Delta^2\beta^3 + c_2\beta = c_3$ has Δ parametrically of the form $\Delta \sim 1/\beta^{3/2}$. But as β becomes small, Δ must therefore grow very large to compensate, immediately in contradiction with the hypothesis that $kT > \frac{1}{2}\sqrt{(\hbar\omega_c)^2 + |\Delta|^2}$.   —✕—

Therefore, we know that at sufficiently high temperatures the only consistent mean-field Hamiltonian is one for which $\Delta = 0$. But we have shown also that at zero temperature, $\Delta > 0$ is consistent and given by the expression above. Let us find the temperature T_c where Δ first vanishes.

When $\Delta \to 0$, $E_k \to \epsilon_k$ so that the consistency equation becomes

$$-\frac{V}{U} = \int\limits_0^{\beta_c\hbar\omega_c/2} \frac{\tanh(x)dx}{x} = \log\left(2e^{\gamma_E}\pi\beta_c\hbar\omega_c\right); \tag{20}$$

the integral was evaluated using a computer algebra package, and γ_E is Leonhard Euler's constant[5]. Combining this with the above, we find

$$\therefore kT_c = e^{\gamma_E}\pi\Delta(0). \tag{21}$$

$$\overset{\text{\'{o}}}{o}\pi\epsilon\rho\ \overset{\text{\`{e}}}{\epsilon}\delta\epsilon\iota\ \pi o\iota\widehat{\eta}\sigma\alpha\iota$$

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[5]For fun, $\gamma_E = \lim_{n\to\infty}\left[\frac{\Gamma(\frac{1}{n})\Gamma(n+1)n^{1+1/n}}{\Gamma(2+n+\frac{1}{n})} - \frac{n^2}{n+1}\right].$