

Quantitative Development of BCS Theory
 Ref: AJL, Quantum Liquids, ch. 5, sections 4 and 5.

Recap: “fully condensed” BCS state described by N-nonconserving w.f.

$$\Psi = \prod_{\mathbf{k}} \Phi_{\mathbf{k}}, \quad \Phi_{\mathbf{k}} \equiv u_{\mathbf{k}}|00\rangle_{\mathbf{k}} + v_{\mathbf{k}}|11\rangle_{\mathbf{k}} \quad (1)$$

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1.$$

We need to determine the values of $u_{\mathbf{k}}$ in the GS, i.e. the state which minimizes the total energy with the $-\mu\hat{N}$ subtraction, i.e.

$$\hat{H} = \hat{T} - \mu\hat{N} + \hat{V} \quad (2)$$

In the following, we ignore the Fock term in $\langle V \rangle$ until further notice (we already saw the Hartree term just contributes a constant, $\frac{1}{2}V_0 \langle N \rangle^2$.) Then $\langle V \rangle$ is just the pairing terms, see Lecture 5:

$$\langle V \rangle = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} F_{\mathbf{k}} F_{\mathbf{k}'}^*, \quad F_{\mathbf{k}} \equiv u_{\mathbf{k}} v_{\mathbf{k}}. \quad (3)$$

$V_{\mathbf{k}\mathbf{k}'} \equiv$ matrix element for $(\mathbf{k} \downarrow, -\mathbf{k} \uparrow) \rightarrow (\mathbf{k}' \uparrow, -\mathbf{k}' \downarrow)$

Now consider the term

$$\hat{T} - \mu\hat{N} = \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} (\xi_{\mathbf{k}} - \mu) \equiv \sum_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \quad (4)$$

It is clear that $|00\rangle_{\mathbf{k}}$ is an eigenstate of $n_{\mathbf{k}\sigma}$ with eigenvalue 0, and $|11\rangle_{\mathbf{k}}$ an eigenstate with eigenvalue 1. Hence, taking into account the \sum_{σ} ,

$$\langle \hat{T} - \mu\hat{N} \rangle = 2 \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2 \quad (\text{note: has finite negative energy in normal gas!})$$

and so:

$$\langle H \rangle = 2 \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2 + \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} (u_{\mathbf{k}} v_{\mathbf{k}}) (u_{\mathbf{k}'} v_{\mathbf{k}'}^*) \quad (5)$$

and this must be minimized subject to constraint $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$

One pretty way of visualizing problem: Anderson pseudospin representation: Put

$$u_{\mathbf{k}}(= \text{real}) = \cos \theta_{\mathbf{k}}/2, \quad v_{\mathbf{k}} = \sin(\theta_{\mathbf{k}}/2) \cdot \exp i\phi_{\mathbf{k}} \quad (6)$$

Then, apart from a constant ($\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$),

$$\langle H \rangle = \sum_{\mathbf{k}} (-\epsilon_{\mathbf{k}} \cos \theta_{\mathbf{k}}) + \frac{1}{4} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sin \theta_{\mathbf{k}} \sin \theta_{\mathbf{k}'} \cdot \cos(\phi_{\mathbf{k}} - \phi_{\mathbf{k}'}) \quad (7)$$

Anderson pseudospin representation of BCS Hamiltonian: use Pauli vectors $\sigma_{\mathbf{k}}$ such that (“classically”) $|\sigma_{\mathbf{k}}| = 1$ and take $\theta_{\mathbf{k}}, \phi_{\mathbf{k}}$ to be polar angles, then (up to a constant)

$$\langle H \rangle = - \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \sigma_{z\mathbf{k}} + \frac{1}{4} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sigma_{\mathbf{k}\perp} \cdot \sigma_{\mathbf{k}'\perp} = - \sum_{\mathbf{k}} \sigma_{\mathbf{k}} \cdot \mathcal{H}_{\mathbf{k}} \quad (8)$$

($\sigma_{\mathbf{k}\perp} \equiv$ component of $\sigma_{\mathbf{k}}$ in xy= plane)

where pseudo-magnetic field $\mathcal{H}_{\mathbf{k}}$ given by

$$\mathcal{H}_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} \hat{z} + \Delta_{\mathbf{k}} \quad (9)$$

$$\Delta_{\mathbf{k}} \equiv -\frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sigma_{\mathbf{k}'\perp} \quad (-\text{sign introduced for convenience}) \quad (9b)$$

Rather than representing $\Delta_{\mathbf{k}}$ and $\sigma_{\mathbf{k}\perp}$ as vectors in the xy-plane, it is actually very convenient to represent them as complex numbers $\Delta_{\mathbf{k}} \equiv \Delta_{kx} + i\Delta_{ky}, \sigma_{k\perp} \equiv \sigma_{kz} + i\sigma_{ky}$.

Evidently the magnitude of the field $\mathcal{H}_{\mathbf{k}}$ is

$$|\mathcal{H}_{\mathbf{k}}| \equiv (\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2)^{1/2} \equiv E_{\mathbf{k}} \quad (10)$$

and in the ground state the spin \mathbf{k} lies along the field $\mathcal{H}_{\mathbf{k}}$, giving an energy $-E_{\mathbf{k}}$. If spin is reversed, this costs $2E_{\mathbf{k}}$ (not $E_{\mathbf{k}}$!). This reversal corresponds to

$$\theta_{\mathbf{k}} \rightarrow \pi - \theta_{\mathbf{k}}, \quad \phi_{\mathbf{k}} \rightarrow \phi_{\mathbf{k}} + \pi \quad (11)$$

and up to an irrelevant overall phase factor this corresponds to

$$u'_{\mathbf{k}} = \sin \frac{\theta_{\mathbf{k}}}{2} \exp -i\phi_{\mathbf{k}} \equiv v_{\mathbf{k}}^* \quad (12)$$

$$v'_{\mathbf{k}} = -\cos \frac{\theta_{\mathbf{k}}}{2} \equiv -u_{\mathbf{k}}$$

i.e., the excited state so generated is

$$\Phi_{\mathbf{k}}^{exc} = v_{\mathbf{k}}^* |00\rangle - u_{\mathbf{k}} |11\rangle \quad (13)$$

which may be verified to be orthogonal to the GS $\Phi_{\mathbf{k}} = u_{\mathbf{k}}|00\rangle + v_{\mathbf{k}}|11\rangle$. (remember, we take $u_{\mathbf{k}}$ real)

Since in the GS each spin \mathbf{k} must point along the corresponding field, this gives a set of self-consistent conditions for the $\Delta_{\mathbf{k}}$'s: since $\sigma_{\mathbf{k}'\perp}$ is a unit vector, its in-plane component must be equal to that of the unit vector $\mathcal{H}_{\mathbf{k}}/|\mathcal{H}_{\mathbf{k}}|$ namely $\Delta_{\mathbf{k}}/E_{\mathbf{k}}$.

That is

$$\sigma_{\mathbf{k}'\perp} = \Delta_{\mathbf{k}'}/E_{\mathbf{k}'} \quad (14)$$

and so from eqn. (9b)

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{k}'}/2E_{\mathbf{k}'} \leftarrow \text{BCS gap equation.} \quad (15)$$

Note derivation is quite general, in particular never assumes s-state (though does assume spin singlet pairing)

Alternative derivation of BCS gap equation: Simply parametrize $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ by $\Delta_{\mathbf{k}}$ and $E_{\mathbf{k}} \equiv (\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2)^{1/2}$, as follows:

$$v_{\mathbf{k}} \equiv \frac{\Delta_{\mathbf{k}}}{(|\Delta_{\mathbf{k}}|^2 + (E_{\mathbf{k}} + \epsilon_{\mathbf{k}})^2)^{1/2}} \quad u_{\mathbf{k}} \equiv \frac{E_{\mathbf{k}} + \epsilon_{\mathbf{k}}}{(|\Delta_{\mathbf{k}}|^2 + (E_{\mathbf{k}} + \epsilon_{\mathbf{k}})^2)^{1/2}} \quad (16)$$

This clearly satisfies the normalization condition: $|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$, and gives

$$|u_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad |v_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad u_{\mathbf{k}}v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \quad (17)$$

The BCS energy (5) can therefore be written in the form

$$\langle H \rangle = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}(1 - \epsilon_{\mathbf{k}}/E_{\mathbf{k}}) + \sum_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \frac{\Delta_{\mathbf{k}'}^*}{2E_{\mathbf{k}'}} \quad (18)$$

The various $\Delta_{\mathbf{k}}$ are independent variational parameters: varying them to minimize $\langle H \rangle$ and using $\partial E_{\mathbf{k}}/\partial \Delta_{\mathbf{k}} = \Delta_{\mathbf{k}}^*/E_{\mathbf{k}}$, we find an equation which can be written

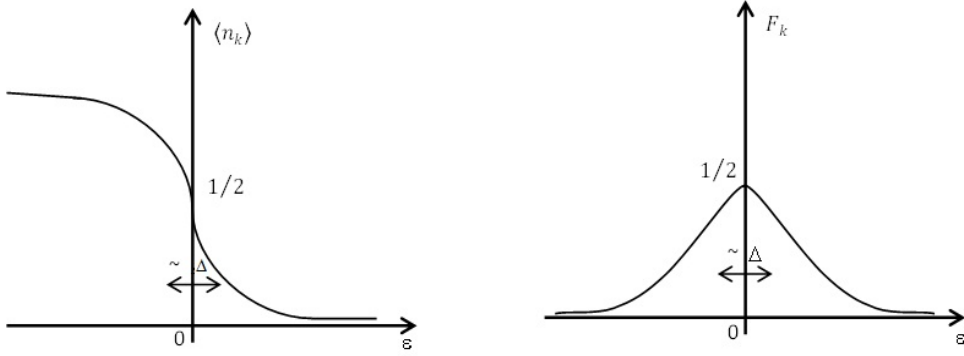
$$\frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} (\Delta_{\mathbf{k}}^* - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}) = 0 \quad (19)$$

Cancelling the prefactor and taking the complex conjugate gives back the standard gap equation.

[Assume s-state until further notice, i.e., $\Delta_{\mathbf{k}} = \text{function of only } |\mathbf{k}|$.]

Behavior of $\langle n_{\mathbf{k}} \rangle$ and $F_{\mathbf{k}}$ in groundstate

Let's anticipate the result that in most cases of interest, $\Delta_{\mathbf{k}}$ will turn out to be $\sim \text{const}$ $\equiv \Delta$ over a range $\gg \Delta$ itself near the F.S. Then we have $\langle n_{\mathbf{k}} \rangle = |v_{\mathbf{k}}|^2 = \frac{1}{2} \left(1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}} \right)$ and $F_{\mathbf{k}} = u_{\mathbf{k}} v_{\mathbf{k}} = \frac{\Delta}{2E_{\mathbf{k}}}$



Thus, behavior of $\langle n_{\mathbf{k}} \rangle$ qualitatively similar to normal-state behavior at finite T (but falls off very slowly, $\sim \epsilon^{-2}$ rather than exponentially). $F_{\mathbf{k}}$ falls off as $|\epsilon|^{-1}$ for large ϵ . [$F(\mathbf{r})$ in coordinate space: see below, lecture 7.]

BCS theory at finite T

Obvious generalization of N -conserving GSWF: many body density matrix $\hat{\rho}$ is product of density matrices referring to occupation space (call it \mathbf{k}) of states $\mathbf{k} \uparrow, -\mathbf{k} \downarrow$.

$$\hat{\rho} = \prod_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} \quad (20)$$

The space \mathbf{k} is 4-dimensional, and can be spanned by states of the forms

$$\begin{aligned} \Phi_{GP} &\equiv u_{\mathbf{k}}|00\rangle + v_{\mathbf{k}}|11\rangle, \text{ "ground pair"} \\ \Phi_{EP} &\equiv v_{\mathbf{k}}^*|00\rangle - u_{\mathbf{k}}|11\rangle, \text{ "excited pair"} \\ \Phi_{BP}^{(1)} &\equiv |10\rangle, \Phi_{BP}^{(2)} \equiv |01\rangle, \text{ "broken pair"} \end{aligned} \quad (21)$$

As regards the first two, they can again be parametrized by the Anderson variables $\theta_{\mathbf{k}}, \phi_{\mathbf{k}}$: the difference, now, is that there is a finite probability that a given "spin" \mathbf{k} will be reversed, i.e., the pair is in state Φ_{EP} rather than Φ_{GP} . There is also finite probability that the pair in question will be a broken-pair state, in which case it clearly will not contribute to $\langle V \rangle$ and thus not to the effective field. Thus, we can go through the argument as above and derive the result.

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle \sigma_{\perp\mathbf{k}'} \rangle \quad (22)$$

but the $\langle \sigma_{\perp\mathbf{k}'} \rangle$ is now given by the expression

$$\langle \sigma_{\perp\mathbf{k}'} \rangle = -(P_{GP}^{(\mathbf{k}')} - P_{EP}^{(\mathbf{k}')}) \Delta_{\mathbf{k}'} / E_{\mathbf{k}'} \quad (23)$$

and thus the gap equation becomes

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} (P_{GP}^{(\mathbf{k}')} - P_{EP}^{(\mathbf{k}')}) \Delta_{\mathbf{k}'} / 2E_{\mathbf{k}'} \quad (24)$$

We therefore need to calculate the quantities $P_{GP}^{(\mathbf{k})}$, $P_{EP}^{(\mathbf{k})}$. (Since the states $|10\rangle$ and $|01\rangle$ are fairly obviously degenerate, we clearly must have $P_{GP}^{(\mathbf{k})} + P_{EP}^{(\mathbf{k})} + 2P_{BP}^{(\mathbf{k})} = 1$).

Since we are talking about different occupation states, there is no question of Fermi or Bose statistics, and the probability of occupation of a given state is simply proportional to $\exp -\beta E_n$ ($\beta \equiv 1/k_B T$) where E_n is the energy of the state.

Thus,

$$P_{GP}^{(\mathbf{k})} : P_{BP}^{(\mathbf{k})} : P_{EP}^{(\mathbf{k})} = \exp -\beta E_{GP} : \exp -\beta E_{BP} : \exp -\beta E_{EP} \quad (25)$$

we already know that $E_{EP} - E_{GP} = 2E_{\mathbf{k}}$, (but $E_{\mathbf{k}} = E_{\mathbf{k}}(T)$!). What is $E_{BP} - E_{GP}$? Here care is needed in accounting. If all (MB) energies are taken relative to the normal-state F . sea, then evidently the energy of the “broken pair” states $|01\rangle$ or $|10\rangle$ is $\epsilon_{\mathbf{k}}$ (which can be negative!). In writing down the Anderson pseudospin Hamiltonian, however, we omitted the constant term $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$. Hence the energy of the GP state relative to the normal F . sea is not $-E_{\mathbf{k}}$ but $\epsilon_{\mathbf{k}} - E_{\mathbf{k}}$. Hence, we have

$$E_{BP} - E_{GP} = E_{\mathbf{k}} \quad (26)$$

$$E_{EP} - E_{GP} = 2E_{\mathbf{k}}$$

Hence tempting to think of BP states $|10\rangle$ and $|01\rangle$ as excitations of a “quasi-particle” and the EP state as involving excitations of 2 “quasiparticles.” (Formalized in Bogoliubov transformation:

$$\alpha_{\mathbf{k}\uparrow}^+ = u_{\mathbf{k}} a_{\mathbf{k}\uparrow}^+ - v_{\mathbf{k}} a_{\mathbf{k}\downarrow} \quad (27)$$

etc. Return to this below)

Anyway, this gives¹

$$P_{GP}^{(\mathbf{k})} : P_{BP}^{(\mathbf{k})} : P_{EP}^{(\mathbf{k})} = 1 : \exp -\beta E_{\mathbf{k}} : \exp -2\beta E_{\mathbf{k}} \quad (28)$$

and

$$P_{GP}^{(\mathbf{k})} - P_{EP}^{(\mathbf{k})} = \frac{1 - e^{-2\beta E_{\mathbf{k}}}}{1 + 2e^{-\beta E_{\mathbf{k}}} + e^{-2\beta E_{\mathbf{k}}}} = \tanh(\beta E_{\mathbf{k}}/2) \quad (29)$$

¹Note that in the normal state, where “GP” is simply $|11\rangle$ for $\epsilon_{\mathbf{k}} < 0$ and $|00\rangle$ for $\epsilon_{\mathbf{k}} > 0$, this gives for $\epsilon_{\mathbf{k}} > 0 < n_{\mathbf{k}} > = 2(P_{EP} + P_{BP}) = 2/(e^{\beta \epsilon_{\mathbf{k}}} + 1)$, and similarly for $\epsilon_{\mathbf{k}} < 0$, i.e. the correct single-particle Fermi statistics.

Therefore, the finite-T BCS gap equation is:

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh \beta E_{\mathbf{k}'}/2 \quad (30)$$

[Note: Also possible to derive by brute-force minimization of free energy as $F(\Delta_{\mathbf{k}})$, see e.g. AJL app. 5D] This may or may not have (one or more) nontrivial solutions, depending on form of $V_{\mathbf{k}\mathbf{k}'}$ and value of T , see below.

Finite-T values of $\langle n_{\mathbf{k}} \rangle$ and $F_{\mathbf{k}} : F_{\mathbf{k}}$ is simply reduced by factor $\tanh \beta E_{\mathbf{k}}/2$. $\langle n_{\mathbf{k}} \rangle$ is given by a more complicated expression which correctly reduces to the Fermi distribution for $\Delta \rightarrow 0$, T finite.

Alternative approach in terms of Bogoliubov quasiparticle operators:

Consider the operators $\alpha_{\mathbf{k}\sigma}^+$ defined by (*)

$$\alpha_{\mathbf{k}\sigma}^+ \equiv u_{\mathbf{k}} a_{\mathbf{k}\sigma}^+ - \sigma v_{\mathbf{k}}^* a_{-\mathbf{k},-\sigma}, \text{ and H.C.} \quad (31)$$

so that inverse transformation is:

$$a_{\mathbf{k}\sigma}^+ \equiv u_{\mathbf{k}} \alpha_{\mathbf{k}\sigma}^+ + \sigma v_{\mathbf{k}} \alpha_{-\mathbf{k},-\sigma} \quad (32)$$

It may be easily verified that the operators $\alpha_{\mathbf{k}\sigma}$ satisfy the same fermion A.C. relations as the $a_{\mathbf{k}\sigma}$, namely,

$$[\alpha_{\mathbf{k}\sigma}, \alpha_{\mathbf{k}'\sigma'}^+] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \quad (33)$$

It is also straightforward to verify that²

$$\begin{aligned} \alpha_{\mathbf{k}\sigma} |GP \rangle &\equiv 0, \alpha_{\mathbf{k}\uparrow}^+ |GP \rangle = |10 \rangle, \alpha_{\mathbf{k}\downarrow}^+ |GP \rangle = |01 \rangle \\ \alpha_{\mathbf{k}\uparrow}^+ \alpha_{-\mathbf{k}\downarrow}^+ |GP \rangle &= |EP \rangle \end{aligned} \quad (34)$$

Hence the $\alpha_{\mathbf{k}}^+$'s effectively create independent quasiparticles—EP states can be regarded as two independent excited quasiparticles corresponding to $\mathbf{k} \uparrow$ and $-\mathbf{k} \downarrow$.

Since $E_{BP} - E_{GP} = E_{\mathbf{k}}$ and $E_{EP} - E_{GP} = 2E_{\mathbf{k}}$, we can write the Hamiltonian in the form

$$\hat{H} = \text{const} + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \alpha_{\mathbf{k}\sigma}^+ \alpha_{\mathbf{k}\sigma} \quad (35)$$

At finite T the QP's will satisfy the standard Fermi distribution (but with $\mu = 0$, since they can be created and destroyed):

$$n_{QP}(\mathbf{k}) = (\exp \beta E_{\mathbf{k}} + 1)^{-1} \quad (36)$$

²Here it is essential to remember that $|11 \rangle$ is defined as $a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+ |00 \rangle$, not $a_{-\mathbf{k}\downarrow}^+ a_{\mathbf{k}\uparrow}^+ |00 \rangle$ [sign change].

We see that the quantity $\langle a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+ \rangle \equiv \langle a_{-k\downarrow} a_{k\uparrow} \rangle^* \equiv F_k^*$ is given by

$$\begin{aligned} \langle a_{\mathbf{k}\uparrow}^+ a_{-\mathbf{k}\downarrow}^+ \rangle &= u_{\mathbf{k}} v_{\mathbf{k}}^* \langle \alpha_{\mathbf{k}\uparrow}^+ \alpha_{\mathbf{k}\uparrow} - \alpha_{\mathbf{k}\downarrow} \alpha_{-\mathbf{k}\downarrow}^+ \rangle + \text{terms with no e.v.} \\ &= u_{\mathbf{k}} v_{\mathbf{k}}^* (n_{\mathbf{k}\uparrow} - (1 - n_{-\mathbf{k}\downarrow})) = u_{\mathbf{k}} v_{\mathbf{k}}^* (1 - 2n_{\mathbf{k}}) \\ &= u_{\mathbf{k}} v_{\mathbf{k}}^* \tanh \beta E_{\mathbf{k}}/2, \text{ as previously.} \end{aligned} \quad (37)$$

[cf. p. 5.6, foot, for sign +c.c.!]

Note: a Bogoliubov quasiparticle doesn't carry unit particle number, since $[\hat{N}, \alpha_{k\sigma}^+] \neq \text{const. } \alpha_{k\sigma}^+$, but does carry unit spin ($[\hat{S}, \alpha_{k\sigma}^+] = \sigma \alpha_{k\sigma}^+$).

Properties of BCS gap equation (eqn. (30))

- (1) Independently of form of $V_{\mathbf{k}\mathbf{k}'}$, equation always has trivial solution $\Delta_{\mathbf{k}} = 0$ (N state)
- (2) If $V_{\mathbf{k}\mathbf{k}'} = V_o > 0$, no (nontrivial) solution (cf. below).
- (3) for $T \rightarrow \infty$, no nontrivial solution.

[reduces to $-\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \Delta'_{\mathbf{k}} = k_B T \Delta_{\mathbf{k}}$, and $-V_{\mathbf{k}\mathbf{k}'}$ must have maximum eigenvalue.]

Hence, if \exists nontrivial solution at $T = 0$, must \exists critical temperature T_c at which this solution vanishes.

- (4) Reduction to BCS form³ ($V_{\mathbf{k}\mathbf{k}'} \cong -V_0 = \text{const}$ with cutoff).

Possible if and only if typical energy range over which $V_{\mathbf{k}\mathbf{k}'}$ changes appreciably is $\gg \Delta(0)$, which as we can verify, is $\geq T$ for $T \leq T_c$ [self-consistent solution using BCS form]. If so, define $\epsilon_c \gg \Delta, T$ so that for $\epsilon_{\mathbf{k}}$ within ϵ_c $V_{\mathbf{k}\mathbf{k}'} \cong$ independent of $\epsilon_{\mathbf{k}}$, and write BCS equation in symbolic matrix form

$$\Delta = -\hat{V} \hat{Q} \Delta \equiv -\hat{V} (\hat{P}_1 + \hat{P}_2) \hat{Q} \Delta \quad (+) \quad (38)$$

where

$$\hat{Q} \equiv \delta_{\mathbf{k}\mathbf{k}'} \cdot (\tanh \beta E_{\mathbf{k}'}/2) / 2E_{\mathbf{k}'} \quad (39)$$

P_1 projects out states $|\epsilon_{\mathbf{k}}| > \epsilon_c$, and P_2 states $< \epsilon_c$, (so $\hat{P}_1 + \hat{P}_2 = \hat{1}$). (+) can be rearranged to give

$$\Delta = -\frac{\hat{V} \hat{P}_2 \hat{Q} \Delta}{(1 + \hat{P}_1 \hat{Q} \hat{V})} \equiv -\hat{t} \hat{P}_2 \hat{Q} \Delta, \quad \hat{t} = \frac{\hat{V}}{1 + \hat{P}_1 \hat{Q} \hat{V}} \quad (40)$$

i.e. \hat{t} sums over multiple scatterings outside "shell". Crucial point: since all states outside shell by hypothesis have $|\epsilon_{\mathbf{k}}| \gg \Delta, T$ the factor Q occurring in \hat{t} is essentially $\delta_{\mathbf{k}\mathbf{k}'}/2|\epsilon_{\mathbf{k}'}|$ and

³The ensuing argument implicitly assumes that $V_{\mathbf{k}\mathbf{k}'}$ is not a strong function of the directions of $\mathbf{k}\mathbf{k}'$. If it is, non-s-wave solutions may be possible (cf. part 2 of course).

hence \hat{t} depends neither on Δ nor on T , but is just some fixed operator which is a sort of “effective potential within shell.” Moreover, by hypothesis, $t_{\mathbf{k}\mathbf{k}'}$ is practically constant, $\sim t_0$, within shell. Hence gap equation becomes (putting $t_0 \equiv -V_0$)

$$\Delta_{\mathbf{k}} = -V_0 \sum_{\mathbf{k}', |E_{\mathbf{k}'}| < \epsilon_c} \Delta_{\mathbf{k}'} \frac{\tanh \beta E_{\mathbf{k}'}/2}{2E_{\mathbf{k}'}} \quad (41)$$

This is exactly the equation originally obtained by BCS, who assumed $V_{\mathbf{k}\mathbf{k}'} = \text{const} = V_0$ within shell $|\epsilon_{\mathbf{k}}|, |\epsilon_{\mathbf{k}'}| < \epsilon_c$, otherwise zero. Note one can show that solution of equation doesn't depend on arbitrary cutoff energy ϵ_c (V_0 scales so as to cancel this).

(5) Solution of BCS model: (eqn. (41))

Rewrite using $\sum_{\mathbf{k}} \rightarrow N(0) \int d\epsilon$ $N(0) \equiv \frac{1}{2} \left(\frac{dn}{d\epsilon} \right)$ and put $\Delta_{\mathbf{k}} = \text{const.} \equiv \Delta$

$$\lambda^{-1} = \int_0^{\epsilon_c} \frac{\tanh \beta E/2}{E} d\epsilon, \quad \lambda \equiv -N(0)V_0 \left(\equiv -1/2 \left(\frac{dn}{d\epsilon} V(0) \right) \right), \quad E \equiv (\epsilon^2 + |\Delta|^2)^{1/2} \quad (42)$$

[Factor of 2 cancelled by $\int_{-\epsilon_c}^{\epsilon_c} d\epsilon \rightarrow 2 \int_0^{\epsilon_c} d\epsilon$]

Obvious that no solution exists for $V_0 > 0$. For $V_0 < 0$:

Critical temperature: put $\beta = \beta_c$, $\Delta \rightarrow 0$, hence $E \rightarrow |\epsilon|$:

$$\begin{aligned} \lambda^{-1} &= \int_0^{\epsilon_c} \frac{\tanh(\beta_c \epsilon/2)}{\epsilon} d\epsilon = \ln(1.14\beta_c \epsilon_c) \\ \Rightarrow k_B T_c &= 1.14\epsilon_c \exp -\lambda^{-1} \equiv 1.14\epsilon_c \exp -1/N(0)|V_0| \end{aligned} \quad (43)$$

This expression is insensitive to arbitrary cutoff energy ϵ_c since $|V_0| \sim \text{const} + \ln \epsilon_c$, i.e. cancels dependence. So, plausible to take value $\epsilon_c \sim \omega_D$, (as in original BCS paper): since $\omega_D \sim M^{-1/2}$, predicts $T_c \sim M^{-1/2}$ and helps to explain isotope effect. Also, assures self-consistency since experimentally, $T_c \ll \epsilon_c$.

Zero-T solution:

$$\begin{aligned} \lambda^{-1} &= \int_0^{\epsilon_c} \frac{d\epsilon}{\sqrt{\epsilon^2 + |\Delta(0)|^2}} = \sinh^{-1}(\epsilon_c/\Delta(0)) \cong \ln(2\epsilon_c/\Delta(0)) \\ \Rightarrow \Delta(0) &= 2\epsilon_c \exp -1/\lambda = 1.75T_c \quad (1.75 = 2/1.14) \end{aligned} \quad (44)$$

Since $\Delta(0)$ measured in tunneling experiments (Lecture 7), can compare with experiment. Usually works quite well, but for “strong-coupling” superconductors where T_c/ϵ_c not very small, $\Delta(0)/k_B T_c$ usually somewhat > 1.75 .

At finite temperature, $T < T_c$, gap equation can be written

$$\int_0^{\epsilon_c} \{ \tanh \beta E(T)/E(T) - \tanh \beta_c \epsilon/\epsilon \} d\epsilon = 0 \quad (45)$$

and \int extended to ∞ (since it converges)

$$\Rightarrow \Delta(T) \text{ is of form} \quad (46)$$

$$\Delta(T)/\Delta(0) = f(T/T_c)$$

(Or equivalently $\Delta(T) = kT_c \tilde{f}(T/T_c)$). Roughly,

$$\Delta(T)/\Delta(0) = (1 - (T/T_c)^4)^{1/2}, \quad (47)$$

Near T_c exact results obtainable, cf. below:

$$\frac{\Delta(T)}{\Delta(0)} \sim 1.74(1 - T/T_c)^{1/2} \quad \text{or} \quad \Delta(T)/k_c T_c \sim 3 \cdot 06(1 - T/T_c)^{1/2}$$

(6) Back to the question of the Fock term

We earlier neglected the Fock term in the energy, namely,

$$H - \mu N >_{Fock} = -\frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\sigma} V_{\mathbf{k}\mathbf{k}'} \langle n_{\mathbf{k}\sigma} \rangle \langle n_{\mathbf{k}'\sigma} \rangle \quad (48)$$

This is equivalent to a shift in the single particle energy:

$$\epsilon_{\mathbf{k}} \rightarrow \epsilon_{\mathbf{k}} - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle n_{\mathbf{k}'} \rangle \quad (\text{assuming } \langle n_{\mathbf{k}\sigma} \rangle \text{ independent of } \sigma) \quad (49)$$

and in general this depends on Δ . We have seen that crudely speaking, $\langle n_{\mathbf{k}} \rangle$ is smeared out away from its N-state value in the S state over an order $\sim \Delta$, and moreover the smearing is symmetric around the Fermi surface⁴. Thus, if $V_{\mathbf{k}\mathbf{k}'}$ is approximately constant over $\epsilon_{\mathbf{k}} \gg \Delta$, the renormalization of $\epsilon_{\mathbf{k}}$ is the same in the N and S states and has no effect on the energetics of the transition.

(7) Generalizations of BCS

(a) Sommerfeld \rightarrow Bloch: $\Rightarrow \Delta$ may be $f(\hat{\mathbf{n}})$, but qualitatively unchanged.

(b) Landau Fermi-liquid: to the extent, $\sum_{|\mathbf{k}|} \langle n_{\mathbf{k}} \rangle$ unchanged on going from N to S, the “polarizations” which bring the molecular field terms into play do not occur \Rightarrow only effect is $m \rightarrow m^*$: molecular-field terms do not affect the gap equation. But they do affect the responses, just as in the normal state. (cf. Lecture 8.)

(c) Coulomb long-range terms: have no effect on gap equation, do affect the responses.

(d) Strong coupling: crudely speaking, effects which vanish for $\Delta/\omega_D \rightarrow 0$. (e.g. approximation of constant renormalized V not exact). Need much more complicated treatment (Eliashberg). Generally speaking, this treatment provides only fairly small corrections

⁴Argument may fail in presence of severe particle-hole asymmetry: even if Δ itself is constant, may lead to $\sum_{|\mathbf{k}|} \langle n_{\mathbf{k}} \rangle = f(\hat{\mathbf{n}})$

to “naive” BCS. (e.g. ratio $(\Delta(0)/k_B T_c)$, 1.75 in naive BCS, can be as large as 2.4 (Hg, Pb)).