Quantitative Development of BCS Theory

Ref: AJL, Quantum Liquids, ch. 5, sections 4 and 5.

Recap: 'fully condensed' BCS state described by N-nonconserving wave function:

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

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

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.

$$\hat{H} = \hat{T} - \mu\hat{N} + \hat{V} \tag{2}$$

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:

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

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

Now consider the term

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

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

$$\langle\hat{T} - \mu\hat{N}\rangle = 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} |v_{\mathbf{k}}|^2$$

(note: has finite negative energy in normal gas!)

and so:

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

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

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

Then, apart from a constant,

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

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 $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$)

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

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

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

$$\mathcal{H}_{\mathbf{k}} \equiv -\epsilon_{\mathbf{k}} \hat{z} - \Delta_{\mathbf{k}} \tag{9}$$

$$\Delta_{\mathbf{k}} \equiv -\frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \sigma_{\mathbf{k}'\perp} \tag{10}$$

(− sign introduced for convenience)

Rather than representing $\Delta_{\mathbf{k}}$ and $\sigma_{\mathbf{k}\perp}$ as vectors, it is actually very convenient to represent them as complex numbers $\Delta_{\mathbf{k}} \equiv \Delta_{\mathbf{k}x} + i\Delta_{\mathbf{k}y}, \sigma_{\mathbf{k}\perp} \equiv \sigma_{\mathbf{k}z} + i\sigma_{\mathbf{k}y}$. Evidently the magnitude of the field $\mathcal{H}_{\mathbf{k}}$ is

$$|\mathcal{H}_{\mathbf{k}}| \equiv (\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2)^{1/2} \equiv E_{\mathbf{k}} \tag{11}$$

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

$$\theta_{\mathbf{k}} \to \pi - \theta_{\mathbf{k}}, \qquad \phi_{\mathbf{k}} \to \phi_{\mathbf{k}} + \pi \tag{12}$$

and up to an irrelevant overall phase factor this corresponds to

$$u'_{\mathbf{k}} = \sin \frac{\theta_{\mathbf{k}}}{2} \exp -i\phi_{\mathbf{k}} \equiv v_{\mathbf{k}}^* \tag{13}$$

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

i.e., the excited state so generated is

$$\Phi_{\mathbf{k}}^{\text{exc}} = v_{\mathbf{k}}^* |00\rangle - u_{\mathbf{k}} |11\rangle \tag{14}$$

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 $\Delta_{\mathbf{k}}$: since $\sigma_{\mathbf{k}'\perp} = -\Delta_{\mathbf{k}'}/E_{\mathbf{k}'}$, we have from (10)

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{k}'}/2E_{\mathbf{k}'} \tag{15}$$

or in terms of the complex quantity $\Delta_{\mathbf{k}} \equiv \Delta_{\mathbf{k}x} + i\Delta_{\mathbf{k}y}$,

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{k}'}/2E_{\mathbf{k}'} \quad \leftarrow \quad \text{BCS gap equation} \tag{16}$$

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:

$$v_\mathbf{k} \equiv \frac{\Delta_\mathbf{k}}{(|\Delta_\mathbf{k}|^2 + (E_\mathbf{k}+\epsilon_\mathbf{k})^2)^{1/2}} \qquad u_\mathbf{k} \equiv \frac{E_\mathbf{k}+\epsilon_\mathbf{k}}{(|\Delta_\mathbf{k}|^2 + (E_\mathbf{k}+\epsilon_\mathbf{k})^2)^{1/2}} \tag{17}$$

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

$$|u_\mathbf{k}|^2 = \frac{1}{2}\left[1 + \frac{\epsilon_\mathbf{k}}{E_\mathbf{k}}\right], \quad |v_\mathbf{k}|^2 = \frac{1}{2}\left[1 - \frac{\epsilon_\mathbf{k}}{E_\mathbf{k}}\right], \quad u_\mathbf{k}v_\mathbf{k} = \frac{\Delta_\mathbf{k}}{2E_\mathbf{k}} \tag{18}$$

The BCS GS energy can therefore be written in the form

$$\langle H \rangle = \sum_\mathbf{k} \epsilon_\mathbf{k}(1 - \epsilon_\mathbf{k}/E_\mathbf{k}) + \sum_{\mathbf{k}\mathbf{k}'} \frac{\Delta_\mathbf{k}}{2E_\mathbf{k}} \frac{\Delta_{\mathbf{k}'}^*}{2E_{\mathbf{k}'}} \tag{19}$$

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

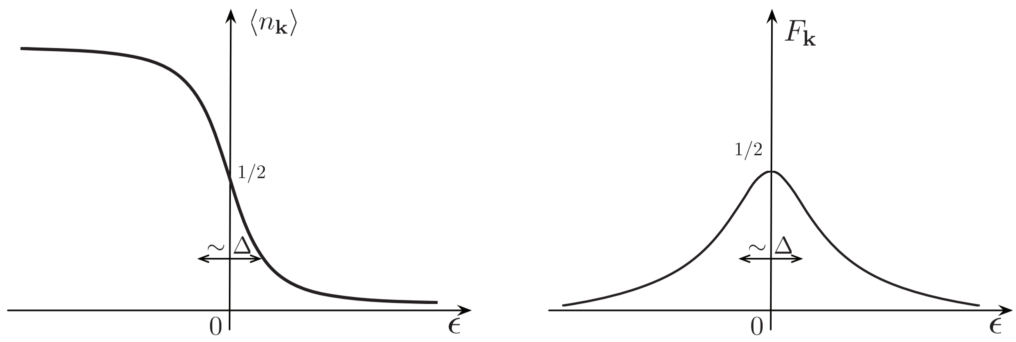
$$\frac{\epsilon_\mathbf{k}^2}{E_\mathbf{k}^3}\left[\Delta_\mathbf{k}^* - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}^*}{2E_{\mathbf{k}'}}\right] = 0 \tag{20}$$

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

[Assume s-state until further notice, i.e., $\Delta_\mathbf{k}$ = 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 $\sim$ const $\equiv \Delta$ over a range $\gg \Delta$ itself near the F.S. Then we have $\langle n_\mathbf{k}\rangle = |v_\mathbf{k}|^2 = \frac{1}{2}(1 - \frac{\epsilon_\mathbf{k}}{\sqrt{\epsilon_\mathbf{k}^2+|\Delta|^2}})$ 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-nonconserving GSWF: many body density matrix $\hat{\rho}$ is product over density matrices referring to occupation space of states $\mathbf{k}\uparrow$, $-\mathbf{k}\downarrow$:

$$\hat{\rho} = \prod_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} \tag{21}$$

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

$$\begin{aligned} \Phi_{\mathrm{GP}} &\equiv u_{\mathbf{k}}|00\rangle + v_{\mathbf{k}}|11\rangle, \text{ "ground pair"} \\ \Phi_{\mathrm{EP}} &\equiv v_{\mathbf{k}}^*|00\rangle - u_{\mathbf{k}}|11\rangle, \text{ "excited pair"} \\ \Phi_{\mathrm{BP}}^{(1)} &\equiv |10\rangle,\ \Phi_{\mathrm{BP}}^{(2)} \equiv |01\rangle, \text{ "broken pair"} \end{aligned} \tag{22}$$

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.

$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\langle\sigma_{\perp\mathbf{k}'}\rangle \tag{23}$$

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

$$\langle\sigma_{\perp\mathbf{k}'}\rangle = -(P_{\mathrm{GP}}^{(\mathbf{k}')} - P_{\mathrm{EP}}^{(\mathbf{k}')})\Delta_{\mathbf{k}'}/E_{\mathbf{k}'} \tag{24}$$

and thus the gap equation becomes

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}(P_{\mathrm{GP}}^{(\mathbf{k}')}) - P_{\mathrm{EP}}^{(\mathbf{k}')})\Delta_{\mathbf{k}'}/2E_{\mathbf{k}'} \tag{25}$$

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

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 $\exp -\beta E_n$ ($\beta \equiv 1/k_{\mathrm{B}}T$) where E_n is the energy of the state. Thus,

$$P_{\mathrm{GP}}^{(\mathbf{k})} : P_{\mathrm{BP}}^{(\mathbf{k})} : P_{\mathrm{EP}}^{(\mathbf{k})} = \exp -\beta E_{\mathrm{GP}} : \exp -\beta E_{\mathrm{BP}} : \exp -\beta E_{\mathrm{EP}} \tag{26}$$

we already know that $E_{\mathrm{EP}} - E_{\mathrm{GP}} = 2E_{\mathbf{k}}$, (but $E_{\mathbf{k}} = E_{\mathbf{k}}(T)$!). What is $E_{\mathrm{BP}} - E_{\mathrm{GP}}$? Here care is needed in accounting. If all (MB) energies are taken relative to the normal-state Fermi 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 Fermi sea is not $-E_{\mathbf{k}}$ but $\epsilon_{\mathbf{k}} - E_{\mathbf{k}}$. Hence, we have

$$\begin{aligned} E_{\text{BP}} - E_{\text{GP}} &= E_{\mathbf{k}} \\ E_{\text{EP}} - E_{\text{GP}} &= 2E_{\mathbf{k}} \end{aligned} \tag{27}$$

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 a 2 "quasiparticles." (Formalized in Bogoliubov transformation:

$$\alpha^\dagger_{\mathbf{k}\uparrow} = u_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} - v_{\mathbf{k}} a_{-\mathbf{k}\downarrow} \tag{28}$$

etc. Return to this below)
Anyway, this gives[1]

$$P^{(\mathbf{k})}_{\text{GP}} : P^{(\mathbf{k})}_{\text{BP}} : P^{(\mathbf{k})}_{\text{EP}} = 1 : \exp -\beta E_{\mathbf{k}} : \exp -2\beta E_{\mathbf{k}} \tag{29}$$

and

$$P^{(\mathbf{k})}_{\text{GP}} - P^{(\mathbf{k})}_{\text{EP}} = \frac{1 - e^{-2\beta E_{\mathbf{k}}}}{1 + 2e^{-\beta E_{\mathbf{k}}} + e^{-2\beta E_{\mathbf{k}}}} = \tanh(\beta E_{\mathbf{k}}/2) \tag{30}$$

Therefore, the finite-T BCS gap equation is:

$$\boxed{\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh \beta E_{\mathbf{k}'}/2} \tag{31}$$

[Note: Also possible to derive by brute-force minimization of free energy as $F(\Delta_{\mathbf{k}})$, see e.g. AJL QL 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 $\Delta \to 0$, T finite.

Alternative approach in terms of Bogoliubov quasiparticle operators.
Consider the operators $\alpha^\dagger_{\mathbf{k}\sigma}$ defined by (28)

$$\alpha^\dagger_{\mathbf{k}\sigma} \equiv u_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma} - \sigma v^*_{\mathbf{k}} a_{-\mathbf{k},-\sigma}, \text{ and H.C.} \tag{32}$$

so that inverse transformation is:

$$a^\dagger_{\mathbf{k}\sigma} \equiv u_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}\sigma} + \sigma v_{\mathbf{k}} \alpha_{-\mathbf{k},-\sigma} \tag{33}$$

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

$$[\alpha_{\mathbf{k}\sigma}, \alpha^\dagger_{\mathbf{k}'\sigma'}]_+ = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \tag{34}$$

[1] Note 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 $\epsilon_{\mathbf{k}} > 0$ $\langle n_{\mathbf{k}} \rangle = 2(P_{\text{EP}} + P_{\text{BP}}) = 2/(e^{\beta\epsilon_{\mathbf{k}}} + 1)$, and similarly for $\epsilon_{\mathbf{k}} < 0$, i.e. the correct single-particle Fermi statistics.

It is also straightforward to verify that[2]

$$\alpha_{\mathbf{k}\sigma}|\mathrm{GP}\rangle \equiv 0, \quad \alpha^\dagger_{\mathbf{k}\uparrow}|\mathrm{GP}\rangle = |10\rangle, \quad \alpha^\dagger_{-\mathbf{k}\downarrow}|\mathrm{GP}\rangle = |01\rangle$$
$$\alpha^\dagger_{\mathbf{k}\uparrow}\alpha^\dagger_{-\mathbf{k}\downarrow}|\mathrm{GP}\rangle = |\mathrm{EP}\rangle \tag{35}$$

Hence the $\alpha^\dagger_{\mathbf{k}}$'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 $E_{\mathrm{BP}} - E_{\mathrm{GP}} = E_{\mathbf{k}}$ and $E_{\mathrm{EP}} - E_{\mathrm{GP}} = 2E_{\mathbf{k}}$, we can write the Hamiltonian in the form

$$\hat{H} = \text{const} + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma} \tag{36}$$

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

$$n_{\mathrm{QP}}(\mathbf{k}) = (\exp\beta E_{\mathbf{k}} + 1)^{-1} \tag{37}$$

We see that the quantity $F^*_{-\mathbf{k}} = F^*_{\mathbf{k}} \equiv \langle a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow}\rangle$ is given by

$$\begin{aligned}\langle a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow}\rangle &= u_{\mathbf{k}}v^*_{\mathbf{k}}\langle\alpha^\dagger_{\mathbf{k}\uparrow}\alpha_{\mathbf{k}\uparrow} - \alpha_{\mathbf{k}\downarrow}\alpha^\dagger_{-\mathbf{k}\downarrow}\rangle + \text{terms with no e.v.} \\ &= u_{\mathbf{k}}v^*_{\mathbf{k}}(n_{\mathbf{k}\uparrow} - (1 - n_{-\mathbf{k}\downarrow})) = u_{\mathbf{k}}v^*_{\mathbf{k}}(1 - 2n_{\mathbf{k}}) \\ &= u_{\mathbf{k}}v^*_{\mathbf{k}}\tanh\beta E_{\mathbf{k}}/2, \quad \text{as previously.}\end{aligned} \tag{38}$$

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

Note: a Bogoliubov quasiparticle doesn't carry unit particle number, because of the fact that $(\sum_\sigma\langle a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}\rangle = \epsilon_{\mathbf{k}}/E_{\mathbf{k}})$, but does carry unit spin $(\sum_\sigma\langle\sigma a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}\rangle = 1)$.

Properties of BCS gap equation

(1) Independently of form of $V_{\mathbf{k}\mathbf{k}'}$, equation always has trivial solution $\Delta_{\mathbf{k}} = 0$ (N state)

(2) If all $V_{\mathbf{k}\mathbf{k}'}$ positive, no solutions.

(3) for $T \to \infty$, no solution.

[reduces to $-\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\Delta'_{\mathbf{k}} = k_{\mathrm{B}}T\Delta_{\mathbf{k}}$, 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 form ($V_{\mathbf{k}\mathbf{k}'} \cong -V_0 = $ 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

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

BCS form]. If so, define $\epsilon_c \gg \Delta, T$ so that for $\epsilon_{\mathbf{k}}$ within ϵ_c $V_{\mathbf{kk'}} \cong$ independent of $\epsilon_{\mathbf{k}}$, and write BCS equation in symbolic matrix form

$$\Delta = -\hat{V}\hat{Q}\Delta \equiv -\hat{V}(\hat{P}_1 + \hat{P}_2)\hat{Q}\Delta \tag{39}$$

where

$$\hat{Q} \equiv \delta_{\mathbf{kk'}} \cdot (\tanh \beta E_{\mathbf{k'}}/2)/2E_{\mathbf{k'}} \tag{40}$$

P_1 projects out states $|\epsilon_{\mathbf{k}}| > \epsilon_c$, and P_2 states $< \epsilon_c$, (so $\hat{P}_1 + \hat{P}_2 = \hat{1}$). (39) can be rearranged to give

$$\Delta = -\frac{\hat{V}\hat{P}_2\hat{Q}\Delta}{(1 + \hat{P}_1\hat{Q}\hat{V})} \equiv -\hat{t}\hat{P}_2\hat{Q}\Delta, \qquad \hat{t} = \frac{\hat{V}}{1 + \hat{P}_1\hat{Q}\hat{V}} \tag{41}$$

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 $\delta_{\mathbf{kk'}}/2|\epsilon_{\mathbf{k'}}|$ and 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, $t_{\mathbf{kk'}}$ is practically constant, $\sim t_0$, within shell. Hence gap equation becomes (putting $t_0 \equiv -V_0$)

$$\Delta_{\mathbf{k}} = -V_0 \sum_{\mathbf{k'}, |E_{\mathbf{k'}}| < \epsilon_c} \Delta_{\mathbf{k'}} \frac{\tanh \beta E_{\mathbf{k'}}/2}{2E_{\mathbf{k'}}} \tag{42}$$

This is exactly the equation originally obtained by BCS, who assumed $V_{\mathbf{kk'}} =$ 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:

Rewrite using $\sum_{\mathbf{k}} \to N(0) \int d\epsilon \qquad N(0) \equiv \frac{1}{2}(\frac{dn}{d\epsilon})$

$$\lambda^{-1} = \int_0^{\epsilon_c} \frac{\tanh \beta E/2}{E} d\epsilon, \qquad \lambda \equiv= -N(0)V_0 \equiv -\frac{1}{2}\left(\frac{dn}{d\epsilon}\right) V(0) \tag{43}$$

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

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

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

$$\lambda^{-1} = \int_0^{\epsilon_c} \frac{\tanh(\beta_c \epsilon/2)}{\epsilon} d\epsilon = \ln(1.14\beta_c\epsilon_c) \tag{44}$$

$$\Rightarrow k_{\mathrm{B}}T_c = 1.14\epsilon_c \exp -\lambda^{-1} \equiv 1.14\epsilon_c \exp -1/N(0)|V_0|$$

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

Zero-T solution:

$$\lambda^{-1} = \int_0^{\epsilon_c} \frac{d\epsilon}{\sqrt{\epsilon^2 + |\Delta(0)|^2}} = \sinh^{-1}(\epsilon_c/\Delta(0)) \cong \ln(2\epsilon_c/\Delta(0)) \tag{45}$$

$$\Rightarrow \Delta(0) = 2\epsilon_c \exp -1/\lambda = 1.75 T_c \qquad (1.75 = 2/1.14)$$

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/ω_c not very small, $\Delta(0)/k_\mathrm{B}T_c$ usually somewhat > 1.75.

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

$$\int_0^{\epsilon_c} \{\tanh \beta E(T)/E(T) - \tanh \beta_c \epsilon/\epsilon\}\, d\epsilon = 0 \tag{46}$$

and $\int$ extended to ∞ (since it converges) $\Rightarrow \Delta(T)$ is of form

$$\Delta(T)/\Delta(0) = f(T/T_c) \tag{47}$$

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

$$\Delta(T)/\Delta(0) = (1 - (T/T_c)^4)^{1/2}, \tag{48}$$

Near T_c exact results obtainable, cf. below:

$$\frac{\Delta(T)}{\Delta(0)} \sim 1.74(1 - T/T_c)^{1/2} \quad \text{or} \quad \Delta(T)/k_\mathrm{B}T_c \sim 3.06(1 - T/T_c)^{1/2} \tag{49}$$

(6) Back to the question of the Fock term

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

$$\langle H - \mu N\rangle_{\mathrm{Fock}} = -\frac{1}{2}\sum_{\mathbf{k}\mathbf{k}'\sigma} V_{\mathbf{k}\mathbf{k}'}\langle n_{\mathbf{k}\sigma}\rangle\langle n_{\mathbf{k}'\sigma}\rangle \tag{50}$$

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

$$\epsilon_\mathbf{k} \to \epsilon_\mathbf{k} - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\langle n_{\mathbf{k}'}\rangle \ \text{(assuming } \langle n_{\mathbf{k}\sigma}\rangle \text{ independent of } \sigma) \tag{51}$$

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 surface[3]. Thus, if $V_{\mathbf{k}\mathbf{k}'}$ is approximate 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.

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

(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 to "naive" BCS. (e.g. ratio $\Delta(0)/k_{\mathrm{B}}T_c$, 1.75 in naive BCS, can be as large as 2.4 (Hg, Pb)).