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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.

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

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

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

$$< V >= \sum_{\mathbf{kk'}} V_{\mathbf{kk'}} F_{\mathbf{k}} F^*_{\mathbf{k'}}, \qquad F_{\mathbf{k}} \equiv u_{\mathbf{k}}\upsilon_{\mathbf{k}}. \tag{3}$$

$V_{\mathbf{kk'}} \equiv$ 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 $|00>_{\mathbf{k}}$ is an eigenstate of $n_{\mathbf{k}\sigma}$ with eigenvalue 0, and $|11>_{\mathbf{k}}$ with eigenvalue 1. Hence, taking into account the $\sum_\sigma$,

$< \hat{T} - \mu\hat{N} >= 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}|\upsilon_{\mathbf{k}}|^2$ (note: has finite negative energy in normal gas!)

and so:

$$< H >= 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}|\upsilon_{\mathbf{k}}|^2 + \sum_{\mathbf{kk'}} V_{\mathbf{kk'}}(u_{\mathbf{k}}\upsilon_{\mathbf{k}})(u_{\mathbf{k'}}\upsilon^*_{\mathbf{k'}}) \tag{5}$$

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

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

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

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

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

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)

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

($\sigma_{\mathbf{k}\perp} \equiv$ component of $\sigma_{\mathbf{k}}$ in xy= plane)
where pseudo-magnetic field $\mathcal{H}_{\mathbf{k}}$ given by

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

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

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

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

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

$$\theta_{\mathbf{k}} \to \pi - \theta_{\mathbf{k}}, \qquad \phi_{\mathbf{k}} \to \phi_{\mathbf{k}} + \pi \tag{11}$$

and up to an irrelevant overall phase factor this corresponds to

$$u'_{\mathbf{k}} = \sin\frac{\theta_{\mathbf{k}}}{2} \exp -i\phi_{\mathbf{k}} \equiv v^*_{\mathbf{k}} \tag{12}$$

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

i.e., the excited state so generated is

$$\Phi^{exc}_{\mathbf{k}} = v^*_{\mathbf{k}} |00> - u_{\mathbf{k}} |11> \tag{13}$$

which may be verified to be orthogonal to the GS $\Phi_{\mathbf{k}} = u_{\mathbf{k}}|00> + v_{\mathbf{k}}|11>$. (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 (*)

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\Delta_{\mathbf{k}'}/2E_{\mathbf{k}'} \tag{14}$$

or in terms of the complex quantity $\Delta_k \equiv \Delta_{kx} + i\Delta_{ky}$,

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

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 $\upsilon_{\mathbf{k}}$ by $\Delta_{\mathbf{k}}$ and $E_{\mathbf{k}} \equiv (\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2)^{1/2}$, as follows:

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

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

$$|u_{\mathbf{k}}|^2 = \frac{1}{2}(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}),\ |\upsilon_{\mathbf{k}}|^2 = \frac{1}{2}(1 - \frac{\upsilon_{\mathbf{k}}}{E_{\mathbf{k}}}),\ u_{\mathbf{k}}\upsilon_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \tag{17}$$

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

$$< H >= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}(1 - \epsilon_{\mathbf{k}}/E_{\mathbf{k}}) + \sum_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \frac{\Delta^*_{\mathbf{k}'}}{2E'_{\mathbf{k}}} \tag{18}$$

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

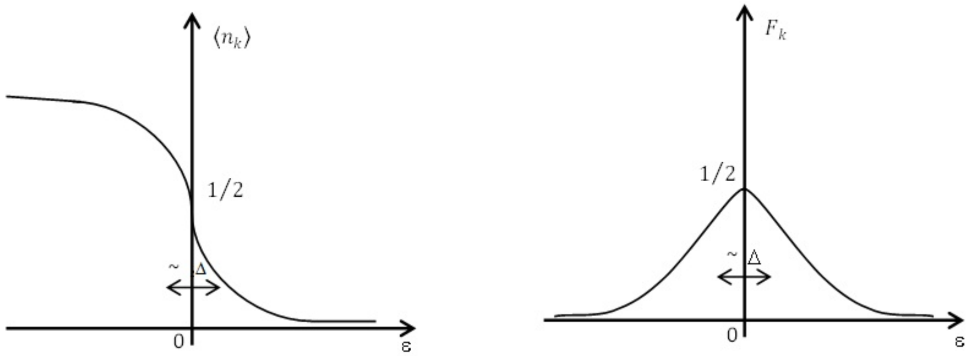
$$\frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2}(\Delta^*_{\mathbf{k}} - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta^*_{\mathbf{k}'}}{2E_{\mathbf{k}'}}) = 0 \tag{19}$$

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

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

Behavior of $< n_{\mathbf{k}} >$ 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 $< n_{\mathbf{k}} >= |\upsilon_{\mathbf{k}}|^2 = \frac{1}{2}(1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}})$ and $F_{\mathbf{k}} = u_{\mathbf{k}}\upsilon_{\mathbf{k}} = \frac{\Delta}{2E_{\mathbf{k}}}$



Thus, behavior of $< n_{\mathbf{k}} >$ 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 of states $\mathbf{k}\uparrow$, $-\mathbf{k}\downarrow$.

$$\hat{\rho} = \prod_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} \tag{20}$$

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

$$\begin{gathered} \Phi_{GP} \equiv u_{\mathbf{k}}|00> + v_{\mathbf{k}}|11>, \text{ “ground pair”} \\ \Phi_{EP} \equiv v^*_{\mathbf{k}}|00> - u_{\mathbf{k}}|11>, \text{ “excited pair”} \\ \Phi^{(1)}_{BP} \equiv |10>, \ \Phi^{(2)}_{BP} \equiv |01>, \text{ “broken pair”} \end{gathered} \tag{21}$$

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 $< V >$ and thus not to the effective field. Thus, we can go through the argument as above and derive the result.

$$\Delta_{\mathbf{k}} = -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} < \sigma\perp_{\mathbf{k}'} > \tag{22}$$

but the $< \sigma\perp_{\mathbf{k}'} >$ is now given by the expression

$$< \sigma_{\perp\mathbf{k}'} > = -(P^{(\mathbf{k}')}_{GP} - P^{(\mathbf{k}')}_{EP})\Delta_{\mathbf{k}'}/E_{\mathbf{k}'} \tag{23}$$

and thus the gap equation becomes

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

We therefore need to calculate the quantities $P_{GP}^{(\mathbf{k})}$, $P_{EP}^{(\mathbf{k})}$. (Since the states $|10>$ and $|01>$ 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,

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

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 $|01>$ or $|10>$ 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

$$\begin{aligned} E_{BP} - E_{GP} &= E_{\mathbf{k}} \\ E_{EP} - E_{GP} &= 2E_{\mathbf{k}} \end{aligned} \tag{26}$$

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

$$\alpha_{\mathbf{k}\uparrow}^{+} = u_{\mathbf{k}} a_{\mathbf{k}\uparrow}^{+} - \upsilon_{\mathbf{k}} a_{\mathbf{k}\downarrow} \tag{27}$$

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

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

and

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

[1]Note that in the normal state, where "GP" is simply $|11>$ for $\epsilon_{\mathbf{k}} < 0$ and $|00>$ 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:

$$\boxed{\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh \beta E_{\mathbf{k}'}/2} \tag{30}$$

[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 $< n_{\mathbf{k}} >$ and $F_{\mathbf{k}}$: $F_{\mathbf{k}}$ is simply reduced by factor $\tanh \beta E_{\mathbf{k}}/2$. $< n_{\mathbf{k}} >$ 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 $\alpha^+_{\mathbf{k}\sigma}$ defined by (*)

$$\alpha^+_{\mathbf{k}\sigma} \equiv u_{\mathbf{k}} a^+_{\mathbf{k}\sigma} - \sigma v^*_{\mathbf{k}} a_{-\mathbf{k},-\sigma}, \text{ and H.C.} \tag{31}$$

so that inverse transformation is:

$$a^+_{\mathbf{k}\sigma} \equiv u_{\mathbf{k}} \alpha^+_{\mathbf{k}\sigma} + \sigma v_{\mathbf{k}} \alpha_{-\mathbf{k},-\sigma} \tag{32}$$

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,

$$[\alpha_{\mathbf{k}\sigma}, \alpha^+_{\mathbf{k}'\sigma'}] = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'} \tag{33}$$

It is also straightforward to verify that[2]

$$\alpha_{\mathbf{k}\sigma}|GP> \equiv 0,\ \alpha^+_{\mathbf{k}\uparrow}|GP> = |10>,\ \alpha^+_{\mathbf{k}\downarrow}|GP> = |01> \tag{34}$$
$$\alpha^+_{\mathbf{k}\uparrow}\alpha^+_{-\mathbf{k}\downarrow}|GP> = |EP>$$

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

$$\hat{H} = \text{const} + \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \alpha^+_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma} \tag{35}$$

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

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

[2] Here it is essential to remember that $|11>$ is defined as $a^+_{\mathbf{k}\uparrow}a^+_{-\mathbf{k}\downarrow}|00>$, not $a^+_{-\mathbf{k}\downarrow}a^+_{\mathbf{k}\uparrow}|00>$ [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

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

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

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

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

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

(2) If $V_{\mathbf{kk}'} = V_o > 0$, no (nontrivial) solution (cf. below).

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

[reduces to $-\sum_{\mathbf{k}'} V_{\mathbf{kk}'}\Delta'_{\mathbf{k}} = k_B T \Delta_{\mathbf{k}}$, and $-V_{\mathbf{kk}'}$ 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[3] ($V_{\mathbf{kk}'} \cong -V_0 =$ const with cutoff).

Possible if and only if typical energy range over which $V_{\mathbf{kk}'}$ 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 $V_{\mathbf{kk}'} \cong$ independent of $\epsilon_{\mathbf{k}}$, and write BCS equation in symbolic matrix form

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

where

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

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

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

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 $\delta_{\mathbf{kk}'}/2|\epsilon_{\mathbf{k}'}|$ and

[3]The ensuing argument implicitly assumes that $V_{\mathbf{kk}'}$ is not a strong function of the directions of $\mathbf{kk}'$. 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, $t_{\mathbf{kk'}}$ is practically constant, $\sim t_0$, within shell. Hence gap equation becomes (putting $t_0 \equiv -V_0$)

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

This is exactly the equation originally obtained by BCS, who assumed $V_{\mathbf{kk'}} = \text{const} = V_0$ 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)<u>Solution of BCS model:</u> (eqn. (41))

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

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

[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 $E \to |\epsilon|$:

$$\lambda^{-1} = \int_0^{\epsilon_c} \frac{\tanh(\beta_c \epsilon/2)}{\epsilon} d\epsilon = \ln(1.14\beta_c\epsilon_c) \tag{43}$$

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

This expression is insensitive to arbitrary cutoff energy ϵ_c since $|V_0| \sim$ const + lnϵ_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:

$$\lambda^{-1} = \int_0^{\epsilon_c} \frac{d\epsilon}{\sqrt{\epsilon^2 + |\Delta(0)|^2}} = \sinh^{-1}(\epsilon_c/\Delta(0)) \cong \ln(2\epsilon_c/\Delta(0)) \tag{44}$$

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

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/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

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

and $\int$ extended to ∞ (since it converges)

$$\Rightarrow \Delta(T) \text{ is of form} \tag{46}$$
$$\Delta(T)/\Delta(0) = f(T/T_c)$$

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

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

Near T_c exact results obtainable, cf. below:
$\frac{\Delta(T)}{\Delta(0)} \sim 1.74(1 - T/T_c)^{1/2}$ *or* $\Delta(T)/k_\epsilon T_c \sim 3 \cdot 06(1 - T/T_c)^{1/2}$

(6)Back to the question of the Fock term

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

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

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

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

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 surface[4]. 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 $\to$ Bloch: $\Rightarrow \Delta$ may be $f(\hat{\mathbf{n}})$, but qualitatively unchanged.

(b) Landau Fermi-liquid: to the extent, $\sum_{|\mathbf{k}|} < n_{\mathbf{k}} >$ unchanged on going from N to S, the "polarizations" which bring the molecular field terms into play do not occur $\Rightarrow$ only effect is $m \to m*$: 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 $\Delta/\omega_D \to 0$. (e.g. approximation of constant renormalized V not exact). Need much more complicated treatment(Eliashberg). Generally speaking, this treatment provides only fairly small corrections

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

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)).