Lecture 1. Reminders Re BCS Theory

References: Kuper, Schrieffer, Tinkham, De Gennes, articles in Parks. AJL RMP **47**, 331 (1975); AJL Quantum Liquids ch. 5, sections 3-4.

Notations: ξ_k = absolute value of kinetic energy for free gas, i.e., $\hbar^2 k^2/2m$,
$\varepsilon_k \equiv \xi_k - \mu(T)$
E_k reserved for something special to BCS theory.
$N(0) \equiv \frac{1}{2}\left(\frac{dn}{d\varepsilon}\right)_{\varepsilon_F}$ = density of states of one spin at Fermi surface,
v_F = Fermi velocity.

1. BCS model

N (= even) spin –1/2 fermions in free space (=Sommerfeld model) with <u>weak</u> attraction.

2. BCS wave function

Fundamental assumption: GSWF ground state wave function in class

$$\Psi(\mathbf{r}_1\sigma_1 \ldots \mathbf{r}_N\sigma_N) = \mathcal{A}\left[\phi(\mathbf{r}_1\sigma_1;\mathbf{r}_2\sigma_2)\phi(\mathbf{r}_3\sigma_3;\mathbf{r}_4\sigma_4)\ldots\phi(\mathbf{r}_{N-1}\sigma_{N-1};\mathbf{r}_N\sigma_N)\right]$$

Antisymmetrizer.

Note all pairs have the *same* ϕ.

Specialize to

(a) spin singlet pairing;

(b) orbital *s*-wave state;

(c) center of mass at rest.

Then

$$\phi(\mathbf{r}_1\sigma_1;\mathbf{r}_2\sigma_2) = 2^{-1/2}\left(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2\right) \times \phi(\mathbf{r}_1 - \mathbf{r}_2)$$

ϕ even in $\mathbf{r}_1 - \mathbf{r}_2$. F.T.:

$$\phi(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} \chi(\mathbf{k}) e^{i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)}, \quad \chi(\mathbf{k}) = \chi(|\mathbf{k}|), \text{ so that } \chi(-\mathbf{k}) = \chi(\mathbf{k})$$

Then

$$\phi(\mathbf{r}_1\sigma_1; \mathbf{r}_2\sigma_2) = \frac{1}{\sqrt{2}} (\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2) \sum_{\mathbf{k}} \chi(\mathbf{k}) e^{i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)} \equiv$$

$$\sum_{\mathbf{k}} \frac{1}{\sqrt{2}} \chi(\mathbf{k}) \left(\uparrow_1\downarrow_2 e^{i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)} - \downarrow_1\uparrow_2 e^{i\mathbf{k}(\mathbf{r}_1 - \mathbf{r}_2)} \right) =$$

$$= (\mathbf{k} \to -\mathbf{k} \text{ in the second term}) =$$

$$\frac{1}{\sqrt{2}} \sum_{\mathbf{k}} \chi(\mathbf{k}) \left((\mathbf{k}\uparrow)_1 (-\mathbf{k}\downarrow)_2 - (-\mathbf{k}\downarrow)_1 (\mathbf{k}\uparrow)_2 \right)$$

$$\equiv \sum_{\mathbf{k}} \chi(\mathbf{k}) a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} |\text{vac}\rangle \equiv \Omega^\dagger |\text{vac}\rangle$$

The N-body wave function above is just

$$\Psi_N = (\Omega^\dagger)^{N/2} |\text{vac}\rangle \equiv \left(\sum_k \chi(k) a^+_{k\uparrow} a^+_{-k\downarrow} \right)^{N/2} |\text{vac}$$

Note: automatically eigenstate of N.
Note: normal ground state is special case! since

$$\Psi_N^{\text{norm}} = \prod_{k<k_F} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} |\text{vac}\rangle \overset{\text{Fermi statistics}}{=} \left(\sum_{k<k_F} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow} \right)^{N/2} |\text{vac}\rangle$$

which is special case with $\chi(\mathbf{k}) = \theta(k_F - |\mathbf{k}|)$.

3. BCS method

Relax particle number conservation and minimize not $\hat{H}$ but $\hat{H}-\mu\hat{N}$ (Bogoliubov, 1948). One obvious way:

$$\left(\Omega^\dagger\right)^{N/2} \to \exp \Omega^\dagger \equiv \sum_{N/2=0}^{\infty} \left(\Omega^\dagger\right)^{N/2}/(N/2)!$$

Thus up to normalization,

$$\Psi = \exp\left\{\sum_{\mathbf{k}} \chi(\mathbf{k}) a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\right\}|\mathrm{vac}\rangle \equiv \prod_{\mathbf{k}} \exp\left\{\chi(\mathbf{k}) a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\right\}|\mathrm{vac}\rangle$$

or since $(a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow})^2 = 0$,

$$\Psi = \prod_{\mathbf{k}} \left(1 + \chi(\mathbf{k}) a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\right)|\mathrm{vac}\rangle$$

Go over to representation in terms of occupation spaces of k, -k: $|00>_k$, $|10>_k$, $|01>_k$, $|11>_k$ Then

$$\Psi = \prod_{\mathbf{k}} \Phi_{\mathbf{k}}, \quad \Phi_{\mathbf{k}} \equiv |00\rangle_{\mathbf{k}} + \chi_{\mathbf{k}}|11\rangle_{\mathbf{k}}$$

To normalize multiply by $(1 + |\chi_k|^2)^{-1/2}$

$$\Phi_{\mathbf{k}} = u_{\mathbf{k}}|00\rangle_{\mathbf{k}} + v_{\mathbf{k}}|11\rangle_{\mathbf{k}}, \quad |u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1, \quad v_{\mathbf{k}}/u_{\mathbf{k}} = \chi_{\mathbf{k}} \quad (\text{i.e. } v_{\mathbf{k}} = \chi_{\mathbf{k}}/\sqrt{1+|\chi_{\mathbf{k}}|^2})$$

Normal GS is special case with $u_{\mathbf{k}} = 0$ and $v_{\mathbf{k}} = 1$ for $k<k_F$ and $u_{\mathbf{k}} = 1$, $v_{\mathbf{k}} = 0$ for $k > k_F$. Thus, general form of N-nonconserving BCS wave function is,

$$\Psi_{\mathrm{BCS}} = \prod_{k} \left(u_{\mathbf{k}}|00\rangle_{\mathbf{k}} + v_{\mathbf{k}}|11\rangle_{\mathbf{k}}\right) = \boxed{\prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} a^\dagger_{\mathbf{k}\uparrow} a^\dagger_{-\mathbf{k}\downarrow}\right)|\mathrm{vac}\rangle}$$

Notes:

a) very general (for spin singlet pairing), e. g. $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ can be $f(\hat{\boldsymbol{k}})$.

b) $u_{\mathbf{k}} \rightarrow v_{\mathbf{k}} \exp i\varphi_k$, $v_{\mathbf{k}} \rightarrow v_{\mathbf{k}} \exp i\varphi_k$ has no physical effect $\Rightarrow$ choose all $v_{\mathbf{k}}$ to be real.

c) $v_{\mathbf{k}} \rightarrow v_{\mathbf{k}} \exp i\psi$ no physical effect

↑ same for all $\boldsymbol{k}$

d) hence, to obtain N-conserving MBWF,

$$\Psi_N = \frac{1}{2\pi} \int_0^{2\pi} d\phi \, \Psi_{\mathrm{BCS}}(\phi) \exp -iN\phi /2$$

where

$$\Psi_{\mathrm{BCS}}(\phi) \equiv \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + (v_{\mathbf{k}} \exp i\phi) a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow}\right) |\mathrm{vac}\rangle$$

4. The 'pair wave function'

Role of the relative wave function of a Cooper pair played at T=0, by

$$F_{\mathbf{k}} \equiv u_{\mathbf{k}} v_{\mathbf{k}}$$

or its Fourier transform $F(\mathbf{r}) = \Sigma_{\mathbf{k}} F_{\mathbf{k}} \exp i\mathbf{kr}$.

E.g. e.v. of potential energy $\langle V \rangle$ given by

$$\langle V \rangle = \frac{1}{2} \sum_{\substack{\mathbf{pp'q} \\ \sigma\sigma'}} V_{\mathbf{pp'q}} \langle a^{\dagger}_{\mathbf{p+q}/2,\sigma} a^{\dagger}_{\mathbf{p'-q}/2,\sigma'} a_{\mathbf{p'+q}/2,\sigma'} a_{\mathbf{p-q}/2,\sigma} \rangle$$

For BCS w.f. only 3 types of term contribute:

(1) Hartree terms: ($\mathbf{q} = 0$).

$$\langle V \rangle_{\text{Hartree}} = \frac{1}{2} \sum_{\substack{\mathbf{pp'} \\ \sigma\sigma'}} V_{\mathbf{pp'}0} \; \langle n_{\mathbf{p}\sigma} n_{\mathbf{p'}\sigma'} \rangle \left(= \frac{1}{2} V_o \langle N^2 \rangle \text{ For } V = V(\boldsymbol{r}) \right)$$

(2) Fock terms, corresponding to $\sigma = \sigma'$, p – p'. These give

$$\langle V \rangle_{\text{Fock}} = -\frac{1}{2} \sum_{\mathbf{pq}\sigma} V_{\mathbf{ppq}} \; \langle n_{\mathbf{p+q}/2\sigma} n_{\mathbf{p-q}/2\sigma} \rangle$$

Because of the uncorrelated nature of the BCS wave function we can replace the right hand side by

$$-\frac{1}{2} \sum_{\mathbf{pq}\sigma} V_{\mathbf{ppq}} \; \langle n_{\mathbf{p+q}/2\sigma} n_{\mathbf{p-q}/2\sigma} \rangle = -\frac{1}{2} \sum_{\mathbf{pq}\sigma} V_{\mathbf{ppq}} \; |v_{\mathbf{p+q}/2}|^2 |v_{\mathbf{p-q}/2}|^2$$

(3) The pairing terms: p + q/2 = – (p' – q/2), σ' = – σ. Writing for convenience: p + q/2 = k ', p-q/2 = k, we have

$$\langle V\rangle = \frac{1}{2}\sum_{\mathbf{k}\mathbf{k}'\sigma} V_{\mathbf{k}\mathbf{k}'}\ \langle a^\dagger_{\mathbf{k}'\sigma}a^\dagger_{-\mathbf{k}'-\sigma}a_{-\mathbf{k}-\sigma}a_{\mathbf{k}\sigma}\rangle$$

where $V_{\mathbf{k}\mathbf{k}'} \equiv V_{\mathbf{k}+\mathbf{q}/2,\mathbf{k}'-\mathbf{q}/2,\mathbf{k}-\mathbf{k}'}$: for a local potential $V(\mathbf{r})$ this is just $V(\mathbf{k}-\mathbf{k}')$ where $V(\mathbf{k})$ is just the Fourier transform of $V(\mathbf{r})$. Note this expression is N-conserving!

Because of the factorizable nature of the BCS wave function this reduces (except for the $\mathcal{O}(N^{-1})$ case of $\mathbf{k}=\mathbf{k}'$) to the expression

$$\langle V\rangle_{\text{pair}} = \frac{1}{2}\sum_{\mathbf{k}\mathbf{k}'\sigma} V_{\mathbf{k}\mathbf{k}'}\ \langle a^\dagger_{\mathbf{k}'\sigma}a^\dagger_{-\mathbf{k}'-\sigma}\rangle\langle a_{-\mathbf{k}-\sigma}a_{\mathbf{k}\sigma}\rangle$$

or using the spin singlet nature of the wave function

$$\langle V\rangle_{\text{pair}} = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\ \langle a^\dagger_{\mathbf{k}'\uparrow}a^\dagger_{-\mathbf{k}'\downarrow}\rangle\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\rangle$$

It remains to evaluate the quantity

$$\begin{aligned}\langle a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}\rangle &\equiv \langle\Psi_{\text{BCS}}|a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}|\Psi_{\text{BCS}}\rangle \\ &= \langle\phi_{\mathbf{k}}|a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}|\phi_{\mathbf{k}}\rangle = u^*_{\mathbf{k}}v_{\mathbf{k}}\langle 00|a_{-\mathbf{k}\downarrow}a_{\mathbf{k}\uparrow}|11\rangle = u^*_{\mathbf{k}}v_{\mathbf{k}} = u_{\mathbf{k}}v_{\mathbf{k}}\end{aligned}$$

since $u_{\mathbf{k}}$ taken real, and similarly $\langle a^\dagger_{\mathbf{k}'\uparrow}a^\dagger_{-\mathbf{k}'\downarrow}\rangle = u_{\mathbf{k}'}v^*_{\mathbf{k}'}$. Hence

$$\boxed{\langle V\rangle_{\text{pair}} = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}F_{\mathbf{k}}F^*_{\mathbf{k}'}}\ ,\quad \boxed{F_{\mathbf{k}} \equiv u_{\mathbf{k}}v_{\mathbf{k}}}$$

In the case of a local potential $V(\mathbf{r})$, we can write this in terms of the Fourier transform $F(\mathbf{r}) = \sum_{\mathbf{k}} \exp i\mathbf{k}\mathbf{r}\, F_{\mathbf{k}}$:

$$\langle V\rangle_{\text{pair}} = \int d\mathbf{r}\, V(\mathbf{r})|F(\mathbf{r})|^2$$

Compare for 2 particles in free space$V(r) = \int dr\, V(r)\, |\psi(r)|^2$.
Thus, for the paired degenerate Fermi system, *F*(r) essentially plays the role of the relative wave function ψ(r). (at least for the purpose of calculating 2-particle quantities). It is a much simpler quantity to deal with than the quantity φ (r) which appears in the N-conserving formalism. [Note however, that F(r) is not normalized.]

We do not yet know the specific form of *u*'s and *v*'s in the ground state, hence cannot calculate the form of $F(\mathbf{r})$, but we can anticipate the result that it will be bound in relative space and that we will be able to define a 'pair radius' as by the quantity $\xi \equiv (\int \mathbf{r}^2 |F|^2 d\mathbf{r} / \int |F|^2\, d\mathbf{r})^{1/2}$.

Emphasize: everything above very general, true independently of whether or not state we are considering is actually ground state.

5. 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:

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

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

We need to determine the values of $u_{\mathbf{k}}, u_{\mathbf{h}}$ in the GS, i.e. the state which minimizes

$$\langle H \rangle = \langle T - \mu N + V \rangle$$

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

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

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

Now consider the term

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

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 GS!)

and so:

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

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

One pretty way of visualizing problem:

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

Then, apart from a constant,

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

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

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

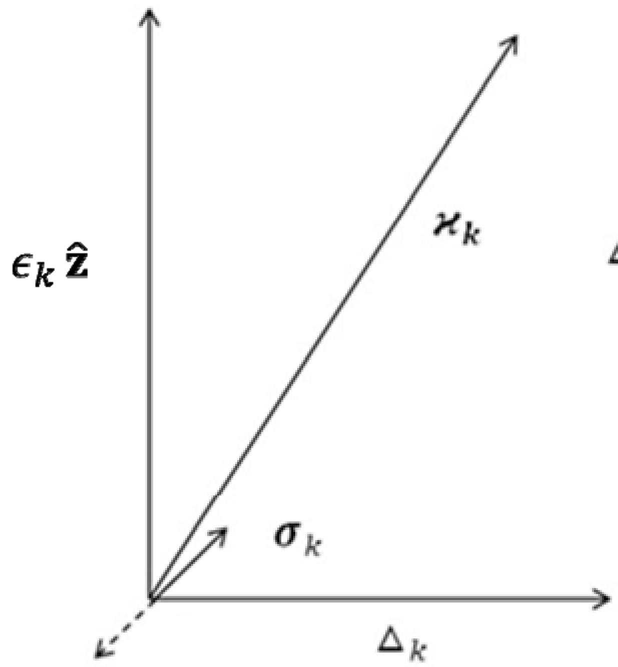
($\sigma_{\mathbf{k}\perp} \equiv$ component of $\sigma_{\mathbf{k}}$ in xy= plane)

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

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

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

(– sign introduced for convenience)



$$\Delta_k \equiv -\frac{1}{2} \sum_{k'} V_{kk'} \sigma_{k'\perp}$$

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

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

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

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

and up to an irrelevant overall phase factor this corresponds to

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

i.e., the excited state so generated is

$$\Phi_{\mathbf{k}}^{\mathrm{exc}} = v^*_{\mathbf{k}}|00\rangle - u_{\mathbf{k}}|11\rangle$$

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

$$\boxed{\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{k}'}/2E_{\mathbf{k}'}} \quad \leftarrow \text{BCS gap eqn.}$$

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:

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

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

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

The BCS GS energy can therefore be written in the form

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

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

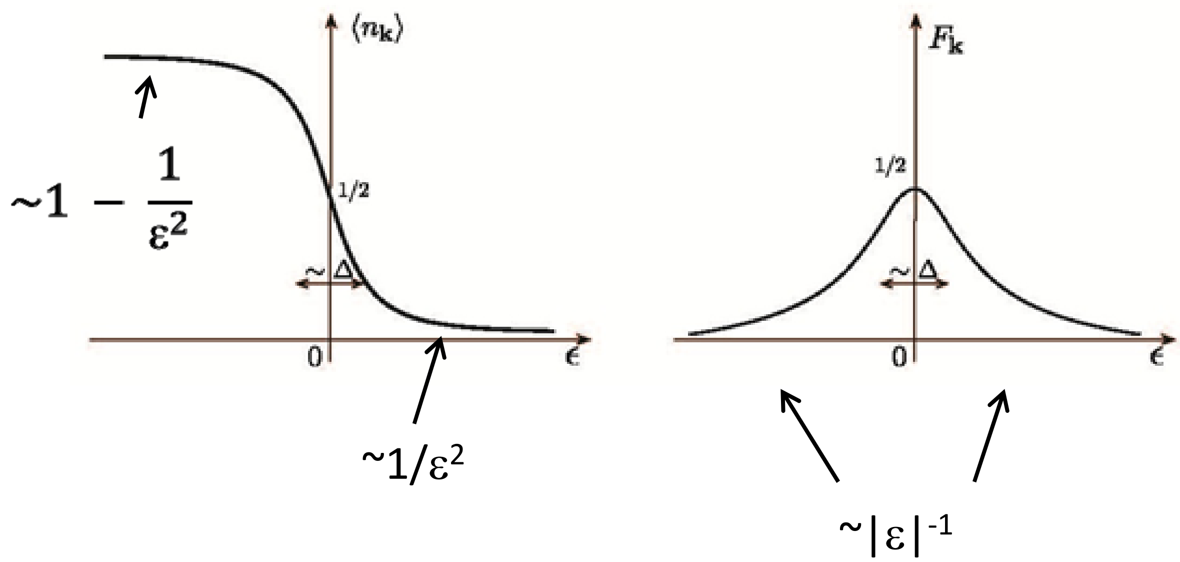
$$\frac{\epsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^3}\left[\Delta_{\mathbf{k}}^* - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}^*}{2E_{\mathbf{k}'}}\right] = 0$$

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 $\equiv$ Δ 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 $F_{\mathbf{k}} = u_{\mathbf{k}} v_{\mathbf{k}} = \frac{\Delta}{2E_{\mathbf{k}}}$.



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 $\mathbf{k}\uparrow$, $-\mathbf{k}\downarrow$:

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

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

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

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.

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

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

$$\langle\sigma_{\perp\mathbf{k}'}\rangle = -(P_{\text{GP}}^{(\mathbf{k}')} - P_{\text{EP}}^{(\mathbf{k}')})\Delta_{\mathbf{k}'}/\,2\,E_{\mathbf{k}'}$$

and thus the gap equation becomes

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

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

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,

$$P^{(\mathbf{k})}_{\mathrm{GP}} : P^{(\mathbf{k})}_{\mathrm{BP}} : P^{(\mathbf{k})}_{\mathrm{EP}} = \exp -\beta E_{\mathrm{GP}} : \exp -\beta E_{\mathrm{BP}} : \exp -\beta E_{\mathrm{EP}}$$

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

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

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 a 2 "quasiparticles."

Anyway, this gives[1]

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

and

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

Therefore, the finite-T BCS gap equation is:

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

[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 $F_\mathbf{k}$: $F_\mathbf{k}$ ($\equiv \langle \sigma_{\perp\mathbf{k}}\rangle$) 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 non zero

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

Properties of BCS gap equation

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

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

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

[reduces to $-\sum_{\mathbf{k}'} V_{\mathbf{kk}'}\Delta'_{\mathbf{k}} = k_{\mathrm{B}}T\Delta_{\mathbf{k}}$, 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) <u>Reduction to BCS form</u> ($V_{\mathbf{kk}'} \cong -V_0 =$ const with cutoff); see AJL, QL, appendix 5F

(5) <u>Solution of BCS model:</u>

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

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

[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 $E \to |\epsilon|$:

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

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

This expression is insensitive to arbitrary cutoff energy ϵ_c since $|V_0| \sim \text{const} + \ln \epsilon_c$, i.e. cancels dependence. So, plausible to take value $\epsilon_c \sim \omega_D$, (as in original BCS paper): since $\omega_c \sim M^{-1/2}$, 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:

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

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

Since $\Delta(0)$ measured in tunneling experiments, 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

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

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

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

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

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

Near T_c exact results obtainable, cf. below:

$$\frac{\Delta(T)}{\Delta(0)} \sim 1.74(1 - T/T_c)^{1/2} \quad \text{or} \quad \Delta(T)/k_B T_c \sim 3.06(1 - T/T_c)^{1/2}$$

(6) Back to the question of the Fock term

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

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

equivalent to a shift in the single particle energy:

$$\epsilon_{\mathbf{k}} \to \quad \epsilon_{\mathbf{k}} - \sum_{\mathbf{k'}} V_{\mathbf{kk'}} \langle n_{\mathbf{k'}} \rangle \equiv \tilde{\varepsilon}_{\mathbf{k}}$$

$\Rightarrow$ to extent V_{hh}, approx. constant over ε » Δ, $\tilde{\varepsilon}_k$ same in S as in N state

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

(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 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)).

The pair wave function

Most important expectation value characterizing the S phase is the 'pair wave function'
$F(\mathbf{r}) \equiv \langle \psi_\downarrow(\mathbf{r})\psi_\uparrow(0)\rangle \equiv \sum_{\mathbf{k}} F_{\mathbf{k}} \exp i\mathbf{kr}$, $F_{\mathbf{k}} \equiv \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow}\rangle$.

We saw that

$$F_{\mathbf{k}} = u_{\mathbf{k}} v_{\mathbf{k}} \tanh \beta E_{\mathbf{k}}/2 = (\Delta_{\mathbf{k}}/2E_{\mathbf{k}}) \tanh \beta E_{\mathbf{k}}/2$$

and so

$$F(\mathbf{r}) = \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \tanh(\beta E_{\mathbf{k}}/2) \exp i\mathbf{kr}$$

In the case of s-wave pairing, $\Delta_{\mathbf{k}}$ is not a function of $\hat{\mathbf{k}}$ and we can write

$$\sum_{\mathbf{k}} \exp i\mathbf{kr} = N(0) \int d\epsilon_{\mathbf{k}} \int \frac{d\Omega_{\mathbf{k}}}{4\pi} \exp i\mathbf{kr} = N(0) \int d\epsilon_{\mathbf{k}} \frac{\sin kr}{kr}$$

so

$$F(\mathbf{r}) \equiv F(r) = N(0) \int d\epsilon_{\mathbf{k}} \frac{\sin kr}{kr} \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} \tanh(\beta E_{\mathbf{k}}/2)$$

For the moment, no restrictions on $\int d\epsilon_{\mathbf{k}}$ (though lower limit cannot be $< \mu$!). We will assume in what follows

$$T_c \ll \epsilon_{\mathrm{F}}$$

and hence $k_{\mathrm{F}}\xi' \gg 1$ where $\xi' \sim \hbar v_{\mathrm{F}}/\Delta(0)$ (see below), as found experimentally.

Normalization: Consider the quantity:

$$N \equiv \int |F(\mathbf{r})|^2 d\mathbf{r} = \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}^2}{4E_{\mathbf{k}}^2} \tanh^2(\beta E_{\mathbf{k}}/2)$$

It is clear that the main contribution comes from $|\epsilon| < \Delta(T), k_{\mathrm{B}}T_c$, where we can approximate $\Delta(T) \sim \Delta(0)$. Thus $N = |\Delta(T)|^2 N(0) \int_0^\infty (d\epsilon/4E^2) \tanh^2 \beta E/2$. For $T \to 0$, this is $\sim N(0)\Delta(0)$ $\sim N\Delta(0)/E_F$; for $T \to T_c$, it is $\sim N(0)|\Delta(T)|^2/T$ $\sim N|\Delta(T)|^2/T_c E_F$ (Interpretation as 'number of Cooper pairs').

General behavior of F(**r**)

A. For r $\lesssim k_F^{-1}$, some of above approximations break down, but clear that F(r) ∝ φ(r), relative wf of 2 interacting electrons in free space with E~E_F.
B. For k_F^{-1} « r « $\hbar v_F / \Delta(o)$, can evaluate explicitly, F(r) ∝ φ_{free}(r). (w.f. of two freely moving particles w. zero com mom. at Fermi energy)
C. For r $\gtrsim \hbar v_F/\Delta(o)$, F(r) falls off exponentially, F(r) ∝ $e^{-r/\xi}$ with $\xi \sim \hbar v_F/\Delta(o)$ and only weakly T-dependent.

The bottom line:

1. Cooper pair radius always ~ $\hbar v_F/\Delta(o)$, ind. of T
2. "number" of Cooper pairs ~ N(Δ(o)/E_F) at T = 0, → 0 as T → T_c.