Fundamental Ideas of 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: will use ξ_k for absolute value of kinetic energy for free gas, i.e., $\hbar^2 k^2/2m$, and when necessary also for Bloch or Bloch-Landau energies. $\epsilon_k \equiv \xi_k - \mu$ is single particle energy in relation to chemical potential (which we may usually take $=\epsilon_F$), E_k reserved for something special to BCS theory. $N(0) \equiv \frac{1}{2}\left(\frac{dn}{d\epsilon}\right)_{\varepsilon_F}$ is the density of states of one spin at Fermi surface, v_F is Fermi velocity.

1 General nature of BCS state[*]

In a 'generic' BCS-type state (not necessary ground state), the N electrons, or a finite fraction of them, are bound into Cooper pairs, such that wave function of pairs is bounded in the relative coordinate, and moreover the Cooper pairs are Bose-condensed, i.e. all in the same state with respect to both relative and center-of-mass coordinate.

Formally, (for $N = 2N_{\mathrm{pair}} =$ even), the topological structure of many body wave function is of the general form:

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

where all ϕ's are the same ('generalized' BCS). ($\mathcal{N} \equiv$ normalizer, $\mathcal{A} \equiv$ antisymmetrizer) Description certainly adequate for classic superconductors, probably also including high temperature superconductors. Differences with a simple BEC of diatomic molecules (liquid D_2?); 'size' of Cooper pair $\ll$ mean distance between particles (e.g. for Al $\sim 10^4$ Å vs. 2–3 Å).

Why should system form such a state? At $T = 0$, evidently to lower energy; simplest case is attractive potential, then intuitively advantageous to localize particles relative to one another. However, for 2-particle problem in free space not every attractive potential gives rise to bound state! Here, Fermi statistics makes all the difference, as shown by Cooper (1956).

2 Cooper instability

L.N. Cooper, Phys. Rev. 104, 1189 (1956)

Consider two particles of spin 1/2 interacting in free space via spin-independent potential $V(|\mathbf{r}_1 - \mathbf{r}_2|)$. We can choose energy eigenstates to be spin singlet or triplet corresponding to orbital wave function being symmetric or antisymmetric respectively: for definiteness, consider singlet case. Choose reference frame so that center of mass is at rest, then orbital wave function has form:

$$\Psi = \psi(\mathbf{r}_1 - \mathbf{r}_2) \equiv \sum_{\mathbf{k}} c_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_1} e^{-i\mathbf{k}\mathbf{r}_2} \quad (2)$$

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[*]until further notice, consider clean samples and neglect crystal-lattice effects (corresponds to Sommerfeld model for normal state).

If $V_{\mathbf{kk'}}$ ($\equiv V_{\mathbf{k-k'}}$) is matrix element for scattering $(\mathbf{k}, -\mathbf{k}) \to (\mathbf{k'}, -\mathbf{k'})$, the time independent Schrödinger equation has the form:

$$(2\xi_{\mathbf{k}} - \tilde{\epsilon}_0)c_{\mathbf{k}} = -\sum_{\mathbf{k'}} V_{\mathbf{kk'}}c_{\mathbf{k'}} \tag{3}$$

($\mathbf{k'}$ sums over all wave vectors, $\tilde{\epsilon}_0$ = energy eigenvalue).

For sufficiently weak (negative) $V_{\mathbf{kk'}}$ in 3D this has no negative energy solutions (also, of course, not for positive V).

Now modify the problem by occupying states up to Fermi surface k_{F} with other electrons, thus excluding the scattering pair from the states $k < k_{\mathrm{F}}$. The only difference, now, is that the sum over $\mathbf{k'}$ on the r.h.s. of (3) now only runs over $k' > k_{\mathrm{F}}$. Now the interesting question is: Does there exist a state with energy less than $2\epsilon_{\mathrm{F}} \equiv 2\mu$? Rewrite (3) in terms of $\epsilon_{\mathbf{k}}$ and $\epsilon_0 = \tilde{\epsilon}_0 - 2\mu$:

$$(2\epsilon_{\mathbf{k}} - \epsilon_0)c_{\mathbf{k}} = -\sum_{k'>k_{\mathrm{F}}} V_{\mathbf{kk'}}c_{\mathbf{k'}} \tag{4}$$

If $V_{\mathbf{kk'}} > 0$, in general still no bound state solution. But if $V_{\mathbf{kk'}} < 0$ and approaches finite limit as $k, k' \to k_{\mathrm{F}}$, always exist a solution with $\epsilon_0 < 0$, i.e. 'bound' relative to state of two free particles!

Example: Cooper's original problem, $V_{\mathbf{kk'}} = -V_0$ for $|\epsilon_{\mathbf{k}}|$, $|\epsilon_{\mathbf{k}}|$ both $< \epsilon_c$, otherwise 0.

$$c_{\mathbf{k}} = \frac{V_0}{2\epsilon_{\mathbf{k}} - \epsilon_0}\sum_{\mathbf{k'}} c_{\mathbf{k'}} \Rightarrow \left[\sum_{\mathbf{k}} c_{\mathbf{k}}\right] = \sum_{\mathbf{k}} \frac{V_0}{2\epsilon_{\mathbf{k}} - \epsilon_0}\left[\sum_{\mathbf{k'}} c_{\mathbf{k'}}\right] \Rightarrow$$

$$1 = \sum_{\mathbf{k}} \frac{V_0}{2\epsilon_{\mathbf{k}} - \epsilon_0}, \text{ or putting } \sum_{\mathbf{k}} = N(0)\int d\epsilon_k, 1 = N(0)V_0\int_0^{\epsilon_c} d\epsilon\, \frac{1}{2\epsilon - \epsilon_0} = \frac{N(0)V_0}{2}\ln(1 + 2\epsilon_c/|\epsilon_0|)$$

$$\Rightarrow \epsilon_0 = \frac{-2\epsilon_c}{e^{2/N(0)V_0} - 1} \approx -2\epsilon_c\, e^{-2/N(0)V_0} \quad \text{if } N(0)V_0 \ll 1$$

Note nonanalyticity in $V_0 \Rightarrow$ cannot be obtained by perturbation theory. In 3D free space argument fails because $\sum_{\mathbf{k}} \to \int \epsilon^{1/2}\, d\epsilon \neq \text{const} \int d\epsilon$.

Structure of the relative wave function: for $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$ and $c_{\mathbf{k}} \sim 1/(2\epsilon_{\mathbf{k}} - \epsilon_0)$ we have

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}}e^{i\mathbf{kr}} = \sum_{k>k_{\mathrm{F}}} \frac{e^{i\mathbf{kr}}}{2\epsilon_{\mathbf{k}} - \epsilon_0} \approx \frac{1}{r}\int_{k_{\mathrm{F}}}^{k_c} dk\, \frac{k\sin kr}{2\epsilon_k + |\epsilon_0|}$$

$$\approx -\frac{1}{r}\frac{d}{dr}\left\{\cos k_{\mathrm{F}}r \underbrace{\int_0^{\epsilon_c} \frac{\cos \epsilon r/\hbar v_{\mathrm{F}}}{\epsilon + |\epsilon_0|/2}\, d\epsilon}_{\equiv J(r)}\right\}$$

where $k - k_{\mathrm{F}} \approx \epsilon_k/\hbar v_{\mathrm{F}}$ was used.

The wave function is thus essentially that of two freely scattering particles, $r^{-1}\sin k_{\mathrm{F}}r$, times the integral $J(r)$. It is clear that the latter is roughly constant for $r < \hbar v_{\mathrm{F}}/|\epsilon_0|$

and thereafter falls off as different components start to interfere. It can be shown that $J(r)$ falls off as $1/r$, thus $\Psi(r) \sim 1/r^2$ and now state is bound in space of the relative coordinate.[†] The 'radius' of the bound state is about $\hbar v_{\mathrm{F}}/|\epsilon_0|$, hence exponentially large as $V_0 \to 0$.
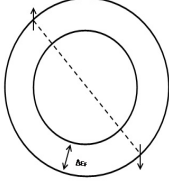
Depairing: Note that the existence of a bound state solution to Cooper problem rests essentially on the fact that the DOS of available states goes to a constant as $\epsilon \to 0$. Suppose we split the Fermi surface, e.g. by a Zeeman field, so that $\epsilon_{\mathrm{F}\uparrow} \neq \epsilon_{\mathrm{F}\downarrow}$. Then for a pair with $K = 0$ minimum excitation energy relative to 'zero' (two free particles) is $\Delta\epsilon_{\mathrm{F}} = \epsilon_{\mathrm{F}\uparrow} - \epsilon_{\mathrm{F}\downarrow}$. Then

$$1 = N(0)V_0 \int_0^{\epsilon_c} \frac{d\epsilon}{2\epsilon + \Delta\epsilon_{\mathrm{F}} - \epsilon_0} \tag{5}$$

and now $|\epsilon_0| = |\epsilon_0^{(0)}| - \Delta\epsilon_{\mathrm{F}}$. So, when $\Delta\epsilon_{\mathrm{F}}$ is $\geq$ the binding energy of the state for $\Delta\epsilon_{\mathrm{F}} = 0$, no bound state solution possible.

Another example of depairing: Suppose $\Delta\epsilon_{\mathrm{F}} = 0$ but we require pair to have finite center of mass momentum K relative to Fermi sea. Then it is fairly clear that minimum value of ϵ_k is of order $\hbar v_{\mathrm{F}} K$, so, again, solution disappears when $K \gtrsim |\epsilon_0|/\hbar v_{\mathrm{F}}$. (Could we 'cancel' these two effects against one another?).

Cooper calculation unsatisfactory, in that it treats two electrons as 'special', rest only as blocking states in Fermi sea. Obviously, would like to treat all electrons on equal footing.

3 BCS wave function

To emphasize generality of BCS concepts, initially make no particular assumption about potential, etc. Fundamental assumption, as above, is that ground state wave function (GSWF) is in class:

$$\Psi(\mathbf{r}_1\sigma_1 \dots \mathbf{r}_N\sigma_N) = \mathcal{A}\left[\phi(\mathbf{r}_1\sigma_1; \mathbf{r}_2\sigma_2)\phi(\mathbf{r}_3\sigma_3; \mathbf{r}_4\sigma_4) \dots \phi(\mathbf{r}_{N-1}\sigma_{N-1}; \mathbf{r}_N\sigma_N)\right] \tag{6}$$

and $\mathcal{A}$ is antisymmetrizer. ϕ must be antisymmetric under exchange $\mathbf{r}_1\sigma_1 \rightleftharpoons \mathbf{r}_2\sigma_2$. Note all pairs have same ϕ.

Specialize to

(a) spin singlet pairing;

[†]As it stands this argument is not convincing, since $\langle r^2 \rangle$ diverges. (However, Cooper used this argument!). But see de Gennes problem on p. 96 (who cheats: $\partial g/\partial \xi$ has singularity at ϵ_c!)

(b) orbital s-wave state;

(c) center of mass at rest.

Then we can assume

$$\phi(\mathbf{r}_1\sigma_1;\mathbf{r}_2\sigma_2) = 2^{-1/2}\,(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2) \times \phi(\mathbf{r}_1 - \mathbf{r}_2) \tag{7}$$

and ϕ is even in $\mathbf{r}_1 - \mathbf{r}_2$. Make Fourier expansion of ϕ

$$\phi(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} \chi(\mathbf{k})e^{i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)}, \quad \chi(\mathbf{k}) = \chi(|\mathbf{k}|),\ \text{ so that } \chi(-\mathbf{k}) = \chi(\mathbf{k}) \tag{8}$$

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

$$\Psi_N = (\Omega^{\dagger})^{N/2}|\text{vac}\rangle \tag{9}$$

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

$$\Psi_N^{\text{norm}} = \prod_{k<k_{\mathrm{F}}} a^{\dagger}_{\mathbf{k}\uparrow}a^{\dagger}_{-\mathbf{k}\downarrow}|\text{vac}\rangle \overset{\text{Fermi statistics}}{\equiv} \left(\sum_{k<k_{\mathrm{F}}} a^{\dagger}_{\mathbf{k}\uparrow}a^{\dagger}_{-\mathbf{k}\downarrow}\right)^{N/2}|\text{vac}\rangle \tag{10}$$

which is special case with $\chi(\mathbf{k}) = \theta(k_{\mathrm{F}} - |\mathbf{k}|)$. However, in this case

$$\phi(\mathbf{r}_1 - \mathbf{r}_2) \equiv \phi(\mathbf{r}) = \text{const}\int_{\text{FS}} d\mathbf{k}\,\exp i\mathbf{k}\mathbf{r} = \text{const}\frac{1}{r^3}\,(\sin k_{\mathrm{F}}r - k_{\mathrm{F}}r\cos k_{\mathrm{F}}r) \tag{11}$$

Thus $P(r) \sim r^{-4}$ as $r \to \infty$, and the mean square radius $4\pi\int r^2 P(r)\,d^3\mathbf{r}$
$\equiv \text{const.} \int_0^\infty r^4 P(r)\mathrm{d}r$ diverges.

4 BCS method[§]

Relax particle number conservation and minimize not $\hat{H}$ but $\hat{H} - \mu\hat{N}$ (Bogoliubov, 1948). One obvious way of doing this is to replace $\left(\Omega^\dagger\right)^{N/2}$ by (assuming N even)

$$\exp\Omega^\dagger \equiv \sum_{N/2}^{\infty} \left(\Omega^\dagger\right)^{N/2}/(N/2)! \tag{12}$$

Thus neglecting for the moment normalization,

$$\Psi = \exp\left\{\sum_{\mathbf{k}} \chi(\mathbf{k})a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow}\right\}|\text{vac}\rangle \equiv \prod_{\mathbf{k}}\exp\left\{\chi(\mathbf{k})a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow}\right\}|\text{vac}\rangle \tag{13}$$

But since $(a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow})^2 = 0$, this is just equivalent to

$$\Psi = \prod_{\mathbf{k}}\left(1 + \chi(\mathbf{k})a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow}\right)|\text{vac}\rangle \tag{14}$$

Go over to representation in terms of occupation spaces of $\mathbf{k}\uparrow, -\mathbf{k}\downarrow$: $|00\rangle_{\mathbf{k}}$, $|10\rangle_{\mathbf{k}}$, $|01\rangle_{\mathbf{k}}$, $|11\rangle_{\mathbf{k}}$. Then

$$\Psi = \prod_{\mathbf{k}}\Phi_{\mathbf{k}}, \quad \Phi_{\mathbf{k}} \equiv |00\rangle_{\mathbf{k}} + \chi_{\mathbf{k}}|11\rangle_{\mathbf{k}} \tag{15}$$

Above is not normalized, so multiply by $(1 + |\chi_{\mathbf{k}}|^2)^{-1/2}$ and write

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

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

$$\Psi_{\text{BCS}} = \prod_{k}\left(u_{\mathbf{k}}|00\rangle_{\mathbf{k}} + v_{\mathbf{k}}|11\rangle_{\mathbf{k}}\right) = \boxed{\prod_{\mathbf{k}}\left(u_{\mathbf{k}} + v_{\mathbf{k}}a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow}\right)|\text{vac}\rangle} \tag{16}$$

Note this is very general, e.g. we need not even assume (as we did above) that $\chi_{\mathbf{k}}$, hence $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, are functions only of $|\mathbf{k}|$. (But to introduce triplet pairing needs some modification). It is clear that multiplying the $u_{\mathbf{k}}$ and the $v_{\mathbf{k}}$ simultaneously by $\exp i\phi_{\mathbf{k}}$ ($\phi_{\mathbf{k}}$ real but arbitrary) only multiplies the total Ψ by a phase factor and has no physical effect: thus, we can take all the $u_{\mathbf{k}}$ real (and will do so). Then it turns out (cf. below) that physical quantities depend only on the magnitudes $|u_{\mathbf{k}}|$, $|v_{\mathbf{k}}|$ and the *relative* phases of the $v_{\mathbf{k}}$: thus, multiplying all $v_{\mathbf{k}}$ by same factor $\exp i\phi$ ($\phi \neq f(\mathbf{k})$) affects nothing physical. A very important observation for the conceptual formulation is that an N-conserving many body wave functions can be obtained by the trick

$$\Psi_N = \frac{1}{2\pi}\int_0^{2\pi} d\phi\, \Psi_{\text{BCS}}(\phi)\exp{-iN\phi} \tag{17}$$

[§]For a particle-conserving method of deriving the same results, see AJL, Quantum Liquids, section 5.4.

where

$$\Psi_{\mathrm{BCS}}(\phi) \equiv \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + (v_{\mathbf{k}} \exp i\phi) a_{\mathbf{k}\uparrow}^{\dagger} a_{-\mathbf{k}\downarrow}^{\dagger} \right) |\mathrm{vac}\rangle \tag{18}$$

This approach effectively justifies the BCS trick of relaxing particle number conservation. (Note $\Delta N^2 \sim N$).

5 The 'pair wave function'

A very important quantity, which turns out effectively to play the role of the relative wave function of a Cooper pair, is (at $T = 0$)

$$F_{\mathbf{k}} \equiv u_{\mathbf{k}} v_{\mathbf{k}} \tag{19}$$

or its Fourier transform $F(\mathbf{r}) = \sum_{\mathbf{k}} F_{\mathbf{k}} \exp i\mathbf{kr}$. To see why, let us consider the evaluation on the many body wave function (16) of a spin-independent 2-particle quantity such as the potential energy $\langle V \rangle$ (we take this for definiteness, but could replace it by any 2-particle operator). Quite generally we have

$$\langle V \rangle = \frac{1}{2} \sum_{\substack{\mathbf{pp'q} \\ \sigma\sigma'}} V_{\mathbf{pp'q}} \langle a_{\mathbf{p}+\mathbf{q}/2,\sigma}^{\dagger} a_{\mathbf{p}'-\mathbf{q}/2,\sigma'}^{\dagger} a_{\mathbf{p}'+\mathbf{q}/2,\sigma'} a_{\mathbf{p}-\mathbf{q}/2,\sigma} \rangle \tag{20}$$

(where for a local potential, $V_{\mathbf{pp'q}} \equiv V(\mathbf{q})$, but for the moment we leave it general). It is fairly easy to see that if we apply the operator in $\langle \ \rangle$ to a Ψ of the form (16), most terms lead to wave fuctions which do not have the structure of Ψ and thus cannot contribute to $\langle \Psi | V | \Psi \rangle$. In fact, there are only 3 types of term which can contribute:

(1) Hartree terms: $(q = 0)$. These lead to

$$\langle V \rangle_{\mathrm{Hartree}} = \frac{1}{2} \sum_{\substack{\mathbf{pp'} \\ \sigma\sigma'}} V_{\mathbf{pp'}0} \ \langle n_{\mathbf{p}\sigma} n_{\mathbf{p}'\sigma'} \rangle \tag{21}$$

In case $V_{\mathbf{pp'}0} \equiv V_0$, these are just $\frac{1}{2} V_0 \langle N^2 \rangle \approx \frac{1}{2} V_0 \langle N \rangle^2$.

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

$$\langle V \rangle_{\mathrm{Fock}} = -\frac{1}{2} \sum_{\mathbf{pq}\sigma} V_{\mathbf{ppq}} \ \langle n_{\mathbf{p}+\mathbf{q}/2\sigma} n_{\mathbf{p}-\mathbf{q}/2\sigma} \rangle \tag{22}$$

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

$$-\frac{1}{2} \sum_{\mathbf{pq}\sigma} V_{\mathbf{ppq}} \ \langle n_{\mathbf{p}+\mathbf{q}/2\sigma} n_{\mathbf{p}-\mathbf{q}/2\sigma} \rangle = -\frac{1}{2} \sum_{\mathbf{pq}\sigma} V_{\mathbf{ppq}} \ |v_{\mathbf{p}+\mathbf{q}/2}|^2 |v_{\mathbf{p}-\mathbf{q}/2}|^2 \tag{23}$$

(cf. below on KE). In general we should keep these terms, but in the usual limit considered by BCS, there is a standard argument that they are essentially the same in the normal and superconducting phases and thus can be neglected in analyzing the transition; see next lecture.

(3) The pairing terms (the interesting term!). These correspond to $\mathbf{p} + \mathbf{q}/2 = -(\mathbf{p}' - \mathbf{q}/2)$, $\sigma' = -\sigma$. Writing for convenience: $\mathbf{p} + \mathbf{q}/2 = \mathbf{k}'$, $\mathbf{p} - \mathbf{q}/2 = \mathbf{k}$, we have

$$\langle V \rangle = \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\sigma} V_{\mathbf{k}\mathbf{k}'} \, \langle a^\dagger_{\mathbf{k}'\sigma} a^\dagger_{-\mathbf{k}'-\sigma} a_{\mathbf{k}\sigma} a_{-\mathbf{k}-\sigma} \rangle \tag{24}$$

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 that expression (24) 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

$$\langle V \rangle_{\text{pair}} = \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\sigma} V_{\mathbf{k}\mathbf{k}'} \, \langle a^\dagger_{\mathbf{k}'\sigma} a^\dagger_{-\mathbf{k}'-\sigma} \rangle \langle a_{-\mathbf{k}-\sigma} a_{\mathbf{k}\sigma} \rangle \tag{25}$$

or using the spin singlet nature of the wave function

$$\langle V \rangle_{\text{pair}} = \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'\sigma} V_{\mathbf{k}\mathbf{k}'} \, \langle a^\dagger_{\mathbf{k}'\uparrow} a^\dagger_{-\mathbf{k}'\downarrow} \rangle \langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \rangle \tag{26}$$

It remains to evaluate the quantity

$$
\begin{aligned}
\langle a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} \rangle &\equiv \langle \Psi_{\text{BCS}} | a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} | \Psi_{\text{BCS}} \rangle \\
&= \langle \phi_{\mathbf{k}} | a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} | \phi_{\mathbf{k}} \rangle = u^*_{\mathbf{k}} v_{\mathbf{k}} \langle 00 | a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} | 11 \rangle = u^*_{\mathbf{k}} v_{\mathbf{k}} = u_{\mathbf{k}} v_{\mathbf{k}}
\end{aligned}
\tag{27}
$$

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

$$\langle V \rangle_{\text{pair}} = \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} F_{\mathbf{k}} F^*_{\mathbf{k}'}, \quad F_{\mathbf{k}} \equiv u_{\mathbf{k}} v_{\mathbf{k}} \tag{28}$$

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

$$\langle V \rangle_{\text{pair}} = \int d\mathbf{r} \, V(\mathbf{r}) |F(\mathbf{r})|^2 \tag{29}$$

Compare for 2 particles in free space: $V(\mathbf{r}) = \int d\mathbf{r} \, V(\mathbf{r}) |\psi(\mathbf{r})|^2$. Thus, for the paired degenerate Fermi system, $F(\mathbf{r})$ essentially plays the role of the relative wave function $\psi(\mathbf{r})$. (at least for the purpose of calculating 2-particle quantities). It is a much simpler quantity to deal with than the quantity $\phi(\mathbf{r})$ which appears in the N-conserving formalism. [Note however, that $F(\mathbf{r})$ 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 $\int r^2 F^2 \, d\mathbf{r} / \int F^2 \, d\mathbf{r}$.

Emphasize: everything in sections 3–5 above very general and can be done independently of whether or not the state we are considering is actually the ground state.

(Anderson pseudospin representation)