Lecture 3: BCS theory of superconductivity - part 1

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I. GROUND STATE OF A NORMAL METAL

As we will see below, the superconducting state at temperature $T = 0$ can be understood as a consequence of the electrons in a metal forming a ground state which is qualitatively different of the regular ground state of the electrons in a metal. Therefore we start by discussing the structure of the ground state of the electrons in a metal; more precisely we discuss Sommerfeld's model, or the non-interacting free electron gas [1].

The allowed single electron states are $|\mathbf{k}\alpha\rangle$[1]. The two labels are the wavevector $\mathbf{k}$ and the spin value $\alpha = \pm 1$. This state has the position (or orbital) component $f_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} \exp i\mathbf{k}\mathbf{r}$ with $\mathbf{r}$ the position and V the total volume occupied by the electron; the factor $\frac{1}{\sqrt{V}}$ leads to proper normalization. The spin component is $|\alpha\rangle$, with $|1\rangle = |\uparrow\rangle$ and $|-1\rangle = |\downarrow\rangle$ the two possibilities for spin states. The allowed values of $\mathbf{k}$ are given by the so-called periodic boundary conditions: we assume that electrons occupy a parallelepiped of edges L_1, L_2, and L_3 and that the electron wavefunction has the same values for corresponding values on the two faces, ie $f_{\mathbf{k}}(\mathbf{r} + L_i\mathbf{e}_i) = f_{\mathbf{k}}(\mathbf{r})$, $i = \overline{1,3}$, with $\mathbf{e}_i$ the unit vectors along the three directions. Using periodic boundary conditions, we determine the allowed values of

$$\mathbf{k} = (\frac{2\pi}{L_1}n_1, \frac{2\pi}{L_2}n_2, \frac{2\pi}{L_3}n_3), \tag{1}$$

with n_i integers.

Electrons are fermions and therefore each single particle level can be occupied by at most one electron. The ground state of the free electron gas is obtained by placing electrons successively in states with increasingly larger values of $|\mathbf{k}|$. The largest energy level is characterized by the wavevector k_F and energy $E_F = \hbar^2 k_F^2/2m$, called respectively the Fermi vector and energy. Another useful quantity is the Fermi temperature defined by $k_B T_F = E_F$. For typical metals the Fermi temperature is a few 10^4 K [1]. Based on this, the energy density of states can be introduced. In $\mathbf{k}$ *space*, the volume occupied by a single state is $((2\pi)^3/(L_1 L_2 L_3)) = (2\pi)^3/V$ (see Fig. 1). The total number of electrons is

$$N_{el}(k_F, V) = 2\frac{\frac{4\pi}{3}k_F^3}{\frac{(2\pi)^3}{V}}, \tag{2}$$

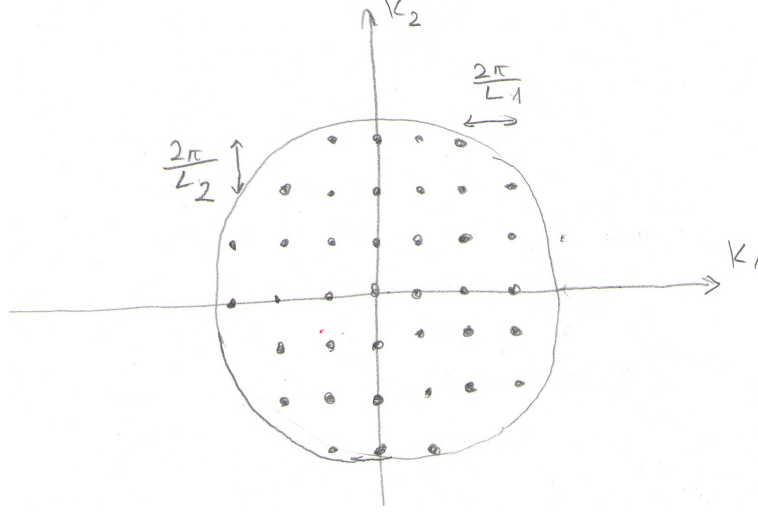[1] We use here the Dirac "bra/ket" notation for quantum states.

FIG. 1. Allowed values of the wavevector (represented in two dimensions), with the occupied states inside the region $k < k_F$.

with a factor of 2 introduced to take spin degeneracy into account. In terms of the energy E,

$$N_{el}(E, V) = 2\frac{\frac{4\pi}{3}(2mE/\hbar^2)^{3/2}}{\frac{(2\pi)^3}{V}}, \tag{3}$$

which allows finding the density of states

$$\frac{dN}{dE}. \tag{4}$$

The ground state of the electron gas is

$$\Psi_G(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, .., \boldsymbol{r}_N\sigma_N) = \mathcal{A}g_{\boldsymbol{k}_1\alpha_1}(\boldsymbol{r}_1, \sigma_1)g_{\boldsymbol{k}_2\alpha_2}(\boldsymbol{r}_2, \sigma_2)..g_{\boldsymbol{k}_N\alpha_N}(\boldsymbol{r}_N, \sigma_N), \tag{5}$$

with the single particle wavefunctions

$$g_{\boldsymbol{k}\alpha}(\boldsymbol{r}, \sigma) = \frac{1}{\sqrt{V}}\exp i\boldsymbol{k}\boldsymbol{r}\delta_{\alpha,\sigma} \tag{6}$$

and the values $\boldsymbol{k}_i$ chosen to fill each level with wavevector lower than k_F (see Fig. 1); two values of α, ± 1, are available for each value of $\boldsymbol{k}$. The operator $\mathcal{A}$ is the antisymmetrization operator which guarantees that on interchange of two sets of coordinates the wavefunction changes sign, as needed for a fermion wavefunction. When applied to a N-particle wavefunction $u(p_1, p_2, .., p_N) = f_1(p_1)f_2(p_2)...f_N(p_N)$ (here p_i is a label for the combination $r_i\sigma_i$), the transformation is

$$(\mathcal{A}u)(p_1, p_2, .., p_N) = \frac{1}{\sqrt{N!}}\sum_P \text{sgn}(P)f_1(p_{P(1)})f_2(p_{P(2)})...f_N(p_{P(N)}) \tag{7}$$

with P all the permutations of order N. The $\frac{1}{\sqrt{N!}}$ has the role of enforcing normalization (if the single particle states form an orthonormal basis). Expression 7 is called a Slater determinant.

It is convenient to introduce the second quantization notation for many-particle states. This is done with reference to one particular complete and orthonormal set of single particle states, $g_{\boldsymbol{k}\alpha}(\boldsymbol{r},\sigma)$. A quantum state of N electrons occupying levels $\boldsymbol{k}_1\alpha_1$, $\boldsymbol{k}_2\alpha_2$, ..., $\boldsymbol{k}_N\alpha_N$ is the properly symmetrized state defined in 5, and is denoted by

$$c^\dagger_{\boldsymbol{k}_1\alpha_1} c^\dagger_{\boldsymbol{k}_2\alpha_2}..c^\dagger_{\boldsymbol{k}_N\alpha_N}|vac\rangle. \tag{8}$$

We introduced the creation operators $c^\dagger_{\boldsymbol{k}\alpha}$ which create an electron in state $\boldsymbol{k}\alpha$. The $|vac\rangle$ state is a state with no particles present. The action of these operators is simple when defined on states of the type $|n_{\boldsymbol{l}_1,-1} n_{\boldsymbol{l}_1 1} n_{\boldsymbol{l}_2,-1} n_{\boldsymbol{l}_2 1}..n_{\boldsymbol{l}_i,-1} n_{\boldsymbol{l}_i 1}..\rangle$. The different indices $\boldsymbol{l}_i$ represent the *infinite* set of single particle states in Eq. 1 (where some order is assumed). The different occupation numbers are $n_{\boldsymbol{k}\alpha} \in \{0,1\}$. The action of the creation operators is

$$c^\dagger_{\boldsymbol{k}\alpha}|..n_{\boldsymbol{k}\alpha}..\rangle = \begin{cases} (-1)^{\sum_{\boldsymbol{l}\beta < \boldsymbol{k}\alpha} n_{\boldsymbol{l}\beta}}|..n_{\boldsymbol{k}\alpha}+1..\rangle & \text{if } n_{\boldsymbol{k}\alpha} = 0 \\ 0 & \text{if } n_{\boldsymbol{k}\alpha} = 1 \end{cases}. \tag{9}$$

The notation $\boldsymbol{l}\beta < \boldsymbol{k}\alpha$ indicates that according to the chosen order the state $\boldsymbol{l}\beta$ comes before $\boldsymbol{k}\alpha$. The role of the sign is to maintain the proper sign of a Slater determinant. In addition to the creation operators, we define annihilation operators

$$c_{\boldsymbol{k}\alpha} = \left(c^\dagger_{\boldsymbol{k}\alpha}\right)^\dagger. \tag{10}$$

Their action on number states is

$$c_{\boldsymbol{k}\alpha}|..n_{\boldsymbol{k}\alpha}..\rangle = \begin{cases} 0 & \text{if } n_{\boldsymbol{k}\alpha} = 0 \\ (-1)^{\sum_{\boldsymbol{l}\beta < \boldsymbol{k}\alpha} n_{\boldsymbol{l}\beta}}|..n_{\boldsymbol{k}\alpha}-1..\rangle & \text{if } n_{\boldsymbol{k}\alpha} = 1 \end{cases}. \tag{11}$$

The annihilation and creation operators satisfy the following anticommutation relations:

$$\{c_{\boldsymbol{k}_1\alpha_1}, c_{\boldsymbol{k}_2\alpha_2}\} = 0 \tag{12}$$

$$\{c^\dagger_{\boldsymbol{k}_1\alpha_1}, c^\dagger_{\boldsymbol{k}_2\alpha_2}\} = 0 \tag{13}$$

$$\{c_{\boldsymbol{k}_1\alpha_1}, c^\dagger_{\boldsymbol{k}_2\alpha_2}\} = \delta_{\boldsymbol{k}_1\boldsymbol{k}_2}\delta_{\alpha_1\alpha_2}. \tag{14}$$

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The second quantization notation does not bring anything new to the description of physical systems. The creation and annihilation operators allow for changing the number of particles, however the representation of "regular" Hamiltonians always involves pairs of annihilation and creation operators so that the number of particles is conserved. The usefulness of the second quantization formalism is in the compact representation of many particle states and in the implicit taking into account of the symmetry of many particle states. Later in the lecture we will deal with second quantization representation of bosonic modes. We will use the second quantization representation when discussing the Bardeen-Cooper-Schrieffer (BCS) theory below.

II. EFFECTIVE INTERACTION DUE TO PHONONS

The essential ingredient of superconductivity is an effective *attractive* electron-electron interaction. The regular electron-electron interaction, due to Coulomb force, is repulsive. In a solid, an attractive interaction arises due to phonons. Quantitatively, this can be understood as follows: an electron polarizes the lattice creating therefore an excess of positive charge; this positive charge attracts a second electron. Formally, the interaction potential between two electrons can be represented as a process which involves two electrons initially in states $|\boldsymbol{k_1}\alpha_1\rangle$ and $|\boldsymbol{k_2}\alpha_2\rangle$ and which emerge in final states $|\boldsymbol{k_1}+\boldsymbol{q}\alpha_1\rangle$ and $|\boldsymbol{k_2}-\boldsymbol{q}\alpha_2\rangle$. The process conserves the total momentum and the spin of each particle. Using second quantization notation, the effective interaction can be written as

$$V_{eff} = \frac{1}{2} \sum_{\boldsymbol{k_1},\alpha_1,\boldsymbol{k_2},\alpha_2,\boldsymbol{q}} \widetilde{V}(\boldsymbol{k_1}+\boldsymbol{q}, \boldsymbol{k_2}-\boldsymbol{q}|\boldsymbol{k_1},\boldsymbol{k_2}) c^{\dagger}_{\boldsymbol{k_1}+\boldsymbol{q}\alpha_1} c^{\dagger}_{\boldsymbol{k_2}-\boldsymbol{q}\alpha_2} c_{\boldsymbol{k_2}\alpha_2} c_{\boldsymbol{k_1}\alpha_1}. \tag{15}$$

The calculation of 15 is a complicated solid state problem. An excellent discussion of this is given in [2]. As we will see, the exact form of the effective interaction is not essential for explaining superconductivity.

III. THE COOPER PROBLEM

Cooper's discovery is one of the most important insights preceding the development of the theory of superconductivity by BCS [3]. He considered the following problem: two electrons are interacting with each other, through a weak attractive potential. The two electrons

are added "on top" of an already occupied Fermi sphere. In other words, the electrons are allowed to occupy any state $|\boldsymbol{k}\sigma\rangle$ as long as $|\boldsymbol{k}| > k_F$.

We do not adopt at this stage second quantization notation for the wavefunction. Cooper assumed a two electron wavefunction which is obtained by pairing states $|\boldsymbol{k}\uparrow\rangle$ and $|-\boldsymbol{k}\downarrow\rangle$. This can be justified if we require anisotropy (hence the choice of opposite values of $\boldsymbol{k}$) and lack of magnetic ordering (zero total spin), both of which are consistent with observed properties of the superconducting state. The wavefunction is obtained by summing over all the possible values of $\boldsymbol{k}$. . The wavefunction with these characteristics is given by

$$\Psi_{CP}(\boldsymbol{r}_1, \sigma_1, \boldsymbol{r}_2, \sigma_2) = \sum_{|\boldsymbol{k}|>k_F} h_{\boldsymbol{k}} \mathcal{A}\left(f_{\boldsymbol{k}}(\boldsymbol{r}_1)\delta_{\sigma_1,+1} f_{-\boldsymbol{k}}(\boldsymbol{r}_2)\delta_{\sigma_2,-1}\right), \tag{16}$$

with $f_{\boldsymbol{k}}(\boldsymbol{r})$ the single electron eigenstates (plane waves) and $h_{\boldsymbol{k}}$ constants to be optimized later. We can assume $h_{\boldsymbol{k}} = h_{-\boldsymbol{k}}$, which leads to writing 16 as

$$\Psi_{CP}(\boldsymbol{r}_1, \sigma_1, \boldsymbol{r}_2, \sigma_2) = \psi_{CP}(\boldsymbol{r}_1 - \boldsymbol{r}_2)\chi_s(\sigma_1, \sigma_2) \tag{17}$$

with

$$\psi_{CP}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{|\boldsymbol{k}|>k_F} h_{\boldsymbol{k}} f_{\boldsymbol{k}}(\boldsymbol{r}_1) f_{-\boldsymbol{k}}(\boldsymbol{r}_2) \tag{18}$$

and

$$\chi_s(\sigma_1, \sigma_2) = \frac{1}{\sqrt{2}}\left(\delta_{\sigma_1,+1}\delta_{\sigma_2,-1} - \delta_{\sigma_1,-1}\delta_{\sigma_2,+1}\right) \tag{19}$$

the singlet spin state. Note that the orbital part 18 is fully symmetric and the spin part 19 is antisymmetric. The Hamiltonian for this two-electron problem is

$$H_{2e} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V(\boldsymbol{r}_1, \boldsymbol{r}_2). \tag{20}$$

The Schrodinger equation can be written as

$$H_{2e}\psi_{CP}(\boldsymbol{r}_1, \boldsymbol{r}_2) = (E + 2E_F)\psi_{CP}(\boldsymbol{r}_1, \boldsymbol{r}_2), \tag{21}$$

as the Hamiltonian is independent of spin. E is the energy with respect to $2E_F$, the minimum value when the interactions are absent. Multiplying 21 with $\frac{1}{\sqrt{V}}e^{-i\boldsymbol{k}(\boldsymbol{r}_1-\boldsymbol{r}_2)}$ and integrating over the volume V, we obtain

$$\frac{\hbar^2}{m}\boldsymbol{k}^2 h_{\boldsymbol{k}} + \sum_{|\boldsymbol{k}'|>k_F} V_{\boldsymbol{k},\boldsymbol{k}'} h_{\boldsymbol{k}'} = (E + 2E_F)h_{\boldsymbol{k}}, \tag{22}$$

where

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \frac{1}{V} \int d\boldsymbol{r} e^{-i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{r}} V(\boldsymbol{r}). \tag{23}$$

We consider the following form for the interaction Hamiltonian:

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \begin{cases} -\frac{\overline{V}}{V} & \text{if } \frac{\hbar^2 k^2}{2m} < E_F + \hbar\omega_D \text{ and } \frac{\hbar^2 k'^2}{2m} < E_F + \hbar\omega_D \\ 0 & \text{in other cases} \end{cases}. \tag{24}$$

One can rewrite 22 as

$$\left(-\frac{\hbar^2 k^2}{m} + E + 2E_F\right) h_{\boldsymbol{k}} = \sum_{|\boldsymbol{k}'|>k_F} V_{\boldsymbol{k},\boldsymbol{k}'} h_{\boldsymbol{k}'}. \tag{25}$$

In view of 24 the RHS of 25 is independent of the index $\boldsymbol{k}$ as long as $\frac{\hbar^2 k^2}{2m} < E_F + \hbar\omega_D$ and vanishes otherwise. Therefore

$$h_{\boldsymbol{k}} = \frac{C}{\left(-\frac{\hbar^2 k^2}{m} + E + 2E_F\right)} \text{ for } \frac{\hbar^2 k^2}{2m} < E_F + \hbar\omega_D. \tag{26}$$

Noting that constant C in 26 is the RHS of 25 we find

$$1 = \frac{\overline{V}}{V} \sum_{E_F < \frac{\hbar^2 k^2}{2m} < E_F + \hbar\omega_D} \frac{1}{\left(-\frac{\hbar^2 k^2}{m} + E + 2E_F\right)}. \tag{27}$$

For a large volume system, one can replace the sum by an integral. The density of electronic states appears as a factor under the integral. Assuming that $\hbar\omega_D \ll E_F$ we take this density of states to be a constant, $N(0)V$.. Eq. 27 becomes

$$1 = N(0)\overline{V} \int_0^{\hbar\omega_D} d\xi \frac{1}{2\xi - E}. \tag{28}$$

Assuming in addition that $N(0)V \ll 1$ (an assumption in agreement with results derived from BCS theory) we find

$$E = -\hbar\omega_D e^{-\frac{2}{N(0)\overline{V}}}. \tag{29}$$

We find that two electrons experiencing an attractive interaction and constrained to occupy states outside an occupied Fermi sphere have a bound state of negative energy[2]. This would not be the case if the two electrons were allowed to occupy single particle states of any wavevector (see [2]). This result provided one of the main ingredients used in formulating the BCS theory of superconductivity.

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[2] Showing that the state is bound requires in fact showing that the probability for the relative position is concentrated on a finite region in space. It can be shown that this region has a size of approximately $\hbar v_F/|E|$, with v_F the Fermi energy and E the energy of the bound state.

IV. BCS ANSATZ

Bardeen, Cooper, and Schrieffer formulated the theory of superconductivity in 1957 [4]. Their discovery is one of the most important discoveries in physics. BCS assumed a ground state of the following form:

$$\widetilde{\phi} = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger} \right) |vac\rangle, \tag{30}$$

where the product is over *all* values of $\boldsymbol{k}$ consistent with periodic boundary conditions and the $u_{\boldsymbol{k}}$ and $u_{\boldsymbol{k}}$ are for the moment arbitrary constants. The wavefunction 30 has the disturbing feature of being a superposition of states with different (even) numbers of electrons, *ie*

$$\widetilde{\phi} = \sum_{N\text{even}} \lambda_N \phi_N. \tag{31}$$

It can be shown (see [2]) that the distribution of the λ_Ns in 31 is peaked around its average value $< N >$ with fluctuations of order $1/\sqrt{< N >}$. In addition, the expectation values of "simple" operators is the same when calculated on the state 30 and on a state which is the projection $\phi_{<N>}$ of $\widetilde{\phi}$ on the $< N >$-particle subspace (for a discussion of this point see [5]). Using the "unphysical" state in 30 has the advantage of simplifying calculations. The state 30 preserves one of the features which was essential in the Cooper problem, namely pairing of electrons in states $\boldsymbol{k}\uparrow$ and $-\boldsymbol{k}\downarrow$. .

We minimize the energy of the system, $\langle\widetilde{\phi}|H|\widetilde{\phi}\rangle$ (where H is the Hamiltonian of the interacting electron system) with respect to variations of the $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ parameters in 30. To work with a constant number of particles, we minimize the quantity

$$\langle\widetilde{\phi}|H|\widetilde{\phi}\rangle - \mu\langle\widetilde{\phi}|N|\widetilde{\phi}\rangle. \tag{32}$$

The expression $-\mu\langle\widetilde{\phi}|N|\widetilde{\phi}\rangle$ is a Lagrange multiplier. The operator in 33 has the following terms

$$H - \mu N = H_0 + H_{int}, \tag{33}$$

with

$$H_0 = H_{kinetic} - \mu N, \tag{34}$$

where $H_{kinetic}$ is the kinetic energy operator for the Hamiltonian. We have

$$H_0 = \sum_{\boldsymbol{k}\alpha} \xi_{\boldsymbol{k}} c_{\boldsymbol{k}\alpha}^{\dagger} c_{\boldsymbol{k}\alpha}, \tag{35}$$

with

$$\xi_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m} - \mu. \tag{36}$$

The interaction Hamiltonian was defined in 15. We proceed with the calculation of these contributions to the energy. Before doing this we need one additional result, which is the calculation of two wavefunctions of the form 30. We take

$$\widetilde{\phi}^a = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}}^a + v_{\boldsymbol{k}}^a c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger} \right) |vac\rangle \tag{37}$$

and

$$\widetilde{\phi}^b = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}}^b + v_{\boldsymbol{k}}^b c_{\boldsymbol{k}\uparrow}^{\dagger} c_{-\boldsymbol{k}\downarrow}^{\dagger} \right) |vac\rangle. \tag{38}$$

Their scalar product is

$$\langle \widetilde{\phi}^a | \widetilde{\phi}^b \rangle = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}}^{a*} u_{\boldsymbol{k}}^b + v_{\boldsymbol{k}}^{a*} v_{\boldsymbol{k}}^b \right), \tag{39}$$

as one can show by using the commutation/anticommutation relations for the creation/annihilation operators in 12, 13, and 14.. Applying this relation to 30 results in

$$\langle \widetilde{\phi} | \widetilde{\phi} \rangle = \prod_{\boldsymbol{k}} \left(|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 \right) = 1. \tag{40}$$

The contribution of $\langle \widetilde{\phi} | H_0 | \widetilde{\phi} \rangle$ can be calculated as follows. Consider first the operator H_0. Applying $c_{\boldsymbol{k}\uparrow}^{\dagger} c_{\boldsymbol{k}\uparrow}$ to $|\widetilde{\phi}\rangle$ results in $(u_{\boldsymbol{k}}, v_{\boldsymbol{k}}) \to (0, v_{\boldsymbol{k}})$, whereas applying $c_{\boldsymbol{k}\downarrow}^{\dagger} c_{\boldsymbol{k}\downarrow}$ results in $(u_{-\boldsymbol{k}}, v_{-\boldsymbol{k}}) \to (0, v_{-\boldsymbol{k}})$ (all the other sets of $(u_{\boldsymbol{k}}, v_{\boldsymbol{k}})$ being left unaffected). Using the result 40 we find that

$$\langle \widetilde{\phi} | H_0 | \widetilde{\phi} \rangle = 2 \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} \frac{|v_{\boldsymbol{k}}|^2}{|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2}. \tag{41}$$

The calculation of the expectation value of the interaction Hamiltonian is more complicated. One first point to consider is the fact that the Hamiltonian 15 applied to a state as in the BCS ansatz (30) leads to a state which may be in general not of the same general form. To eliminate this possibility, we need to restrict the values of $\{\boldsymbol{k}_1 + \boldsymbol{q}\alpha_1, \boldsymbol{k}_2 - \boldsymbol{q}\alpha_2 \boldsymbol{k}_2\alpha_2, \boldsymbol{k}_1\alpha_1\}$ to correspond to the particle states represented by two pairs, that is $\{\boldsymbol{l}\uparrow, -\boldsymbol{l}\downarrow, \boldsymbol{m}\uparrow, -\boldsymbol{m}\downarrow\}$. After elimination of interaction terms which are of the same form as in the normal state, we find

$$\langle \widetilde{\phi} | V_{eff} | \widetilde{\phi} \rangle = \sum_{l,m} V_{l,m} \frac{u_l^* v_l v_m^* u_m}{(|u_l|^2 + |v_l|^2)(|u_m|^2 + |v_m|^2)}. \tag{42}$$

In the following we assume the $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ parameters in the BCS ansatz to be real[3]. We also define

$$\sin \theta_l = \frac{u_l}{\sqrt{|u_l|^2 + |v_l|^2}}, \tag{43}$$

$$\cos \theta_l = \frac{v_l}{\sqrt{|u_l|^2 + |v_l|^2}}. \tag{44}$$

With these definitions,

$$\langle \widetilde{\phi} | H - \mu N | \widetilde{\phi} \rangle = 2 \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} \cos^2 \theta_{\boldsymbol{k}} + \frac{1}{4} \sum_{l,m} V_{l,m} \sin 2\theta_l \sin 2\theta_m. \tag{45}$$

Minimization with respect to the angle θ_l results in

$$-2\xi_l \sin 2\theta_l + \sum_m V_{l,m} \cos 2\theta_l \sin 2\theta_m = 0, \tag{46}$$

which leads to

$$\xi_l \tan 2\theta_l = \frac{1}{2} \sum_m V_{l,m} \sin 2\theta_m \tag{47}$$

We define

$$\Delta_l = -\frac{1}{2} \sum_m V_{l,m} \sin 2\theta_m, \tag{48}$$

$$\epsilon_l = \sqrt{\Delta_l^2 + \xi_l^2} \tag{49}$$

So from 47 and 48 we find

$$\tan 2\theta_l = -\frac{\Delta_l}{\xi_l} \tag{50}$$

and

$$\sin 2\theta_l = \frac{\Delta_l}{\epsilon_l}. \tag{51}$$

The choice of sign in last equation is such that we have

$$\frac{|v_l|^2}{|u_l|^2 + |v_l|^2} = \frac{1 + \cos^2 \theta_l}{2} = \frac{1 - \frac{\xi_l}{\epsilon_l}}{2} \tag{52}$$

which in results in the probability of occupation of the a state $l\alpha$, given by v_l^2, being positive for negative values of ξ_l.

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[3] This point requires some more careful consideration. One can make all the $u_{\boldsymbol{k}}$ real, as this only leads to a global term in the wavefunction. Next take $v_{\boldsymbol{k}} = |v_{\boldsymbol{k}}| e^{i\phi_{\boldsymbol{k}}}$. The sum in 42 becomes $\frac{1}{2} \sum_{l,m} V_{l,m} \frac{|u_l||v_l||v_m||u_m| \cos(\phi_l - \phi_m)}{(|u_l|^2 + |v_l|^2)(|u_m|^2 + |v_m|^2)}$. The cosine factors contribute negatively to the lowering of the total energy due to the attractive interaction. Having all the phases equal leads to a minimum energy. With all the phases equal, only the absolute values of the $v_{\boldsymbol{k}}$ coefficients matter

Finally we can reexpress equation 48 as

$$\Delta_l = -\sum_m V_{l,m} \frac{\Delta_m}{2\sqrt{\Delta_l^2 + \xi_l^2}}. \tag{53}$$

We consider a simple model of the interaction potential (similar to the Cooper problem):

$$V_{l,m} = \begin{cases} -\frac{\overline{V}}{V} & \text{if } |\xi_l|,|\xi_m| < \hbar\omega_D \\ 0 & \text{in other cases} \end{cases}. \tag{54}$$

With this simple model Δ_l is a constant Δ if $|\xi_l|,|\xi_m| < \hbar\omega_D$ and vanishes otherwise. To find Δ we need to solve

$$\Delta = \sum_m \frac{\overline{V}}{V} \frac{\Delta}{2\sqrt{\Delta^2 + \xi_m^2}}. \tag{55}$$

Using an approach similar to the Cooper problem, we transform the sum into an integral:

$$\Delta = N(0)\overline{V} \int_{-\hbar\omega_D}^{\hbar\omega_D} \Delta \frac{d\xi}{2\sqrt{\Delta^2 + \xi}}. \tag{56}$$

with the solution

$$\Delta = \frac{\hbar\omega_D}{\sinh \frac{1}{N(0)V}}, \tag{57}$$

which reduces to

$$\Delta = 2\hbar\omega_D e^{-\frac{1}{N(0)\overline{V}}}. \tag{58}$$

Equation 58 is a very important result. Based on it, we can determine the values of the parameters $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ and hence find the expression of the BCS wavefunction which minimizes the energy as well as the optimized value of the energy.

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