Lecture 4: BCS theory of superconductivity - part 2

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(Dated: 2013/09/20)

I. GROUND STATE WAVEFUNCTION AND ENERGY

The ground state wavefunction in the BCS theory is

$$\widetilde{\phi} = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{-\boldsymbol{k}\downarrow} \right) |vac\rangle. \tag{1}$$

Using the results from last section, the optimal BCS ground state is described by

$$\frac{v_{\boldsymbol{l}}^2}{|u_{\boldsymbol{l}}|^2 + |v_{\boldsymbol{l}}|^2} = \frac{1}{2} \left(1 - \frac{\xi_{\boldsymbol{l}}}{\sqrt{\xi_{\boldsymbol{l}}^2 + \Delta^2}} \right), \tag{2}$$

$$\frac{u_{\boldsymbol{l}}^2}{|u_{\boldsymbol{l}}|^2 + |v_{\boldsymbol{l}}|^2} = \frac{1}{2} \left(1 + \frac{\xi_{\boldsymbol{l}}}{\sqrt{\xi_{\boldsymbol{l}}^2 + \Delta^2}} \right). \tag{3}$$

Note that we neglected the fact that $\Delta_{\boldsymbol{k}}$ depends on $\boldsymbol{k}$ (for the particular model chosen for the interaction), which is justified as long as $\Delta \ll \hbar\omega_D$ (valid as long as $N(0)\overline{V} \ll 1$). The occupation probability $f_{\boldsymbol{k}\alpha}$ for a state $\boldsymbol{k}\alpha$ is given by the expectation value of $c^{\dagger}_{\boldsymbol{k}\alpha} c_{\boldsymbol{k}\alpha}$. Using a result from the previous section, $f_{\boldsymbol{k}\alpha} = \frac{v_{\boldsymbol{l}}^2}{|u_{\boldsymbol{l}}|^2 + |v_{\boldsymbol{l}}|^2}$, and using 2 we find

$$f_{\boldsymbol{k}\alpha} = \frac{1}{2} \left(1 - \frac{\xi_{\boldsymbol{l}}}{\sqrt{\xi_{\boldsymbol{l}}^2 + \xi_{\boldsymbol{l}}^2}} \right). \tag{4}$$

This is plotted in Fig. 1. The occupation probability is similar to that of a normal metal, except for a narrow region of extent Δ around the chemical potential μ.

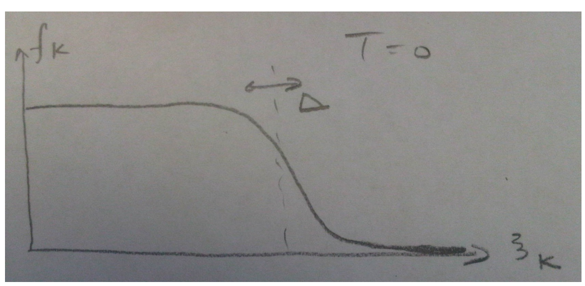

FIG. 1. Representation of the probability for a state $\boldsymbol{k}$ to be occupied in the ground state.

We next evaluate the expression for the total energy of the superconductor in the BCS ground state. We compare $\langle \phi_{BCS} | H - \mu N | \phi_{BCS} \rangle$, with $|\phi_{BCS}\rangle$ the optimized BCS wavefunction expressed in terms of the parameters in 3 and 2, and $\langle \phi_N | H - \mu N | \phi_N \rangle$ with $\phi_N = \left(\prod_{\frac{\hbar^2 \boldsymbol{k}^2}{2m} < \mu, \sigma} c^{\dagger}_{\boldsymbol{k}\sigma} \right) |vac\rangle$. We omit the details of the calculation here (see *eg* [1] or [2]). The result is

$$\delta E_{BCS} = -\frac{1}{2} N(0) V \Delta^2. \tag{5}$$

This is the main result of the BCS theory. It shows that for one particular model of weak attractive electron-electron interactions there exists one quantum state lower in energy that the free electron gas ground state. The lowering in energy corresponds qualitatively to a number $N(0)V\Delta$ of electrons lowering their energy by an amount Δ. Given the fact that the total number of electrons in a normal metal is $3/2N(0)V\mu$, the fraction of electrons who have their energies significantly modified is $\approx \Delta/\mu$, a very small number when considering typical values $\Delta = k_B \times$ 1 K and $\mu = k_B \times 10^4$ K.

II. EXCITATIONS IN A SUPERCONDUCTOR

Different methods exist to deal with energy excitations in superconductors. We follow here closely the treatment in Tinkham [2] based on Bogoliubov transformations.

The interaction Hamiltonian of the BCS theory has the form

$$H_{int} = \sum_{\boldsymbol{k},\boldsymbol{l}} V_{\boldsymbol{k},\boldsymbol{l}} b^\dagger_{\boldsymbol{k}} b_{\boldsymbol{l}} \tag{6}$$

where we introduced the pair creation and annihilation operators

$$b_{\boldsymbol{k}} = c_{-\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\uparrow} \tag{7}$$

and

$$b^\dagger_{\boldsymbol{k}} = c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}. \tag{8}$$

The BCS ground state is such that the expectation value of $b_{\boldsymbol{k}}$ has a relatively well defined value and small quantum fluctuations. . . For this reason we can write

$$b_{\boldsymbol{k}} = \overline{b_{\boldsymbol{k}}} + \delta_{\boldsymbol{k}}, \tag{9}$$

where $\overline{b_{\boldsymbol{k}}}$ is the expectation value of $b_{\boldsymbol{k}}$ and $\delta_{\boldsymbol{k}}$ accounts for the small quantum fluctuations around the average. We rewrite the Hamiltonian 6 up to terms which are second order in the fluctuations $\delta_{\boldsymbol{k}}$:

$$H_{int,M} = \sum_{\boldsymbol{k},\boldsymbol{l}} V_{\boldsymbol{k},\boldsymbol{l}} (b^\dagger_{\boldsymbol{k}} \overline{b_{\boldsymbol{l}}} + \overline{b_{\boldsymbol{k}}}^* b_{\boldsymbol{l}} - \overline{b_{\boldsymbol{k}}}^* \overline{b_{\boldsymbol{l}}}). \tag{10}$$

We write next the total model Hamiltonian, formed by the sum of the single particle Hamiltonian and the approximate interaction Hamiltonian in 10 and the single particle Hamiltonian:

$$H_M = \sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k},\boldsymbol{l}} V_{\boldsymbol{k},\boldsymbol{l}} (\overline{b_{\boldsymbol{l}}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} + \overline{b_{\boldsymbol{k}}}^* c_{-\boldsymbol{l}\downarrow} c_{\boldsymbol{l}\uparrow} - \overline{b_{\boldsymbol{k}}}^* \overline{b_{\boldsymbol{l}}}). \tag{11}$$

As done earlier when dealing with the ground state of the BCS superconductor, we define

$$\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k},\boldsymbol{l}} V_{\boldsymbol{k},\boldsymbol{l}} \overline{b_{\boldsymbol{l}}}. \tag{12}$$

With the new notation 11 becomes:

$$H_M = \sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}} (\Delta_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow} + \Delta^*_{\boldsymbol{k}} c_{-\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\uparrow} - \Delta_{\boldsymbol{k}} \overline{b_{\boldsymbol{k}}}^*). \tag{13}$$

This Hamiltonian is quadratic and therefore it can be diagonalized by a linear transformation. We take suitable combinations of creation/annihilation operators for states $\pm\boldsymbol{k}\uparrow$ and $\pm\boldsymbol{k}\downarrow$:

$$c_{\boldsymbol{k}\uparrow} = u^*_{\boldsymbol{k}} \gamma_{\boldsymbol{k}0} + v_{\boldsymbol{k}} \gamma^\dagger_{\boldsymbol{k}1}, \tag{14}$$

$$c^\dagger_{-\boldsymbol{k}\downarrow} = -v^*_{\boldsymbol{k}} \gamma_{\boldsymbol{k}0} + u_{\boldsymbol{k}} \gamma^\dagger_{\boldsymbol{k}1}. \tag{15}$$

If we require that

$$|u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1, \tag{16}$$

these transformation preserve the Fermi anticommutation relations: if the operators c are fermionic, then so are the γ operators, and viceversa. . When we use 14 and 15 in 13 we find a sum which contains products of the form $\gamma\gamma$, $\gamma^\dagger\gamma^\dagger$, and $\gamma^\dagger\gamma$, and $\gamma\gamma^\dagger$. We require that the coefficients of the terms $\gamma\gamma$ and $\gamma^\dagger\gamma^\dagger$ vanish, as suitable for proper single particle operators. We skip here the actual details of the calculation (straightforward algebra). The result is:

$$2\xi_{\boldsymbol{k}} u_{\boldsymbol{k}} v_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}} v^2_{\boldsymbol{k}} - \Delta_{\boldsymbol{k}} u^2_{\boldsymbol{k}} = 0. \tag{17}$$

We multiply the above by $\Delta^*_{\boldsymbol{k}}/u^2_{\boldsymbol{k}}$ and solve for $\Delta^*_{\boldsymbol{k}} v_{\boldsymbol{k}}/u_{\boldsymbol{k}}$. We find

$$\frac{v_{\boldsymbol{k}}}{u_{\boldsymbol{k}}} = \frac{\epsilon_{\boldsymbol{k}} - \xi_{\boldsymbol{k}}}{\Delta^*_{\boldsymbol{k}}}, \tag{18}$$

where $\epsilon_{\boldsymbol{k}} = \sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2}$. Together with normalization condition 16 this leads to

$$|v_{\boldsymbol{k}}|^2 = 1 - |u_{\boldsymbol{k}}|^2 = \frac{1}{2}\left(1 - \frac{\xi_{\boldsymbol{k}}}{\epsilon_{\boldsymbol{k}}}\right). \tag{19}$$

This is exactly the same as the expression obtained previously using the minimization of energy for the BCS wavefunction. However, the gain is that the treatment here results in an effective Hamiltonian which describes elementary excitations of the superconductor

$$H_m = \text{constant} + \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} (\gamma^\dagger_{\boldsymbol{k}1} \gamma_{\boldsymbol{k}1} + \gamma^\dagger_{\boldsymbol{k}0} \gamma_{\boldsymbol{k}0}). \tag{20}$$

The operators $\gamma_{\boldsymbol{k}1}^{\dagger}$ and $\gamma_{\boldsymbol{k}0}^{\dagger}$ create elementary excitations in the superconductor of energy $\epsilon_{\boldsymbol{k}}$. Excitations corresponding to different operators are independent as long as their number is not too large. The proper criterion to use is the self-consistency conditions. That is, we require that

$$\overline{b_{\boldsymbol{k}}} = \langle\widetilde{\phi}_{exc}|c_{-\boldsymbol{k}\downarrow}c_{\boldsymbol{k}\uparrow}|\widetilde{\phi}_{exc}\rangle \tag{21}$$

where $|\widetilde{\phi}_{exc}\rangle$ is an excited state obtained by application of a number of Bogoliubov operators

$$|\widetilde{\phi}_{exc}\rangle = \left(\prod_{\text{finite set of } \boldsymbol{k}\beta \text{ values}} \gamma_{\boldsymbol{k}\beta}^{\dagger}\right)|\widetilde{\phi}\rangle \tag{22}$$

or more generally a statistical mixture of states as above. This will be in fact the key for the theory of a superconductor at finite temperatures. Using 21, 14 and 15 we find

$$\overline{b_{\boldsymbol{k}}} = \langle\widetilde{\phi}_{exc}|u_{\boldsymbol{k}}^{*}v_{\boldsymbol{k}}\left(1-\gamma_{\boldsymbol{k}1}^{\dagger}\gamma_{\boldsymbol{k}1}-\gamma_{\boldsymbol{k}0}^{\dagger}\gamma_{\boldsymbol{k}0}\right)|\widetilde{\phi}_{exc}\rangle, \tag{23}$$

where we used the anticommutation relation for the Bogoliubov operators, as well assumed that the expectation value is over a mixture of excited states so that expectation values for products $\gamma\gamma$ and $\gamma^{\dagger}\gamma^{\dagger}$ are vanishing. Using 23 in the definition 12 we find

$$\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k},\boldsymbol{l}} V_{\boldsymbol{k},\boldsymbol{l}}u_{\boldsymbol{l}}^{*}v_{\boldsymbol{l}}\left\langle 1-\gamma_{\boldsymbol{l}1}^{\dagger}\gamma_{\boldsymbol{l}1}-\gamma_{\boldsymbol{l}0}^{\dagger}\gamma_{\boldsymbol{l}0}\right\rangle \tag{24}$$

When the expectation value of the ground state is considered in 24 (that is we take $\left\langle\gamma_{\boldsymbol{k}1}^{\dagger}\gamma_{\boldsymbol{k}1}\right\rangle = 0$ and $\left\langle\gamma_{\boldsymbol{k}0}^{\dagger}\gamma_{\boldsymbol{k}0}\right\rangle = 0$), we obtain

$$\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{l}} V_{\boldsymbol{k},\boldsymbol{l}}u_{\boldsymbol{l}}^{*}v_{\boldsymbol{l}}. \tag{25}$$

This result is the same as obtained in the BCS treatment. When we insert the values of $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ from 18 we obtain the same equation for the gap as in the BCS approach considered earlier (which was based on variational calculus as opposed to the mean field approach taken here).

III. SUPERCONDUCTORS AT FINITE TEMPERATURE

We only outline here the finite temperature theory, without detailed calculations. A very concise treatment of finite temperature effects is given in [2]. The treatment builds on the mean field theory of the previous section. The main ingredients are as follows:

- the mean field Hamiltonian 13 is valid

- at finite temperature, the expectation values

$$\left\langle \gamma^{\dagger}_{\boldsymbol{k}1}\gamma_{\boldsymbol{k}1}\right\rangle = \left\langle \gamma^{\dagger}_{\boldsymbol{k}0}\gamma_{\boldsymbol{k}0}\right\rangle = f_{FD}(\epsilon_{\boldsymbol{k}}) \tag{26}$$

  with

$$f_{FD}(\epsilon_{\boldsymbol{k}}) = (1 + e^{\beta\epsilon_{\boldsymbol{k}}})^{-1} \tag{27}$$

  the Fermi-Dirac distribution ($\beta = 1/k_B T$). Note that $\epsilon_{\boldsymbol{k}}$ is a function of the $\Delta_{\boldsymbol{k}}$ parameter through $\epsilon_{\boldsymbol{k}} = \sqrt{\xi^2_{\boldsymbol{k}} + |\Delta_{\boldsymbol{k}}|^2}$.

- the self-consistency equation 24 is used in the following form

$$\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k},\boldsymbol{l}} V_{\boldsymbol{k},\boldsymbol{l}} u^*_{\boldsymbol{l}} v_{\boldsymbol{l}} (1 - 2 f_{FD}(\epsilon_{\boldsymbol{l}})). \tag{28}$$

  The $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ parameters depend again on $\Delta_{\boldsymbol{k}}$ through relations 18 and 19.

Equation 28 can be solved to find the value of Δ as a function of temperature. We take the same simplified model for the potential as considered in the previous lecture, that is

$$V_{\boldsymbol{l},\boldsymbol{m}} = \begin{cases} -\overline{V} & \text{if } |\xi_{\boldsymbol{l}}|,|\xi_{\boldsymbol{m}}| < \hbar\omega_D \\ 0 & \text{in other cases} \end{cases}. \tag{29}$$

The selfconsistency condition becomes

$$\frac{1}{\overline{\overline{V}}} = \frac{1}{2} \sum_{\boldsymbol{k}} \frac{\tanh \beta\epsilon_{\boldsymbol{k}}/2}{\epsilon_{\boldsymbol{k}}} \tag{30}$$

The gap decreases as a function of temperature and it eventually reaches zero, the point at which the structure of the excitations is the same as in the normal state. This is the critical temperature T_c. We replace $\epsilon_{\boldsymbol{k}}$ with $\xi_{\boldsymbol{k}}$ in equation 30. The integral can be done by first noting the symmetry around $\xi = 0$ and using the variable $x = \beta\xi$. The result is

$$\frac{1}{N(0)\overline{\overline{V}}} = \int_0^{\beta_c \hbar\omega_D} dx \frac{\tanh x}{x}. \tag{31}$$

where $\beta_c = 1/(k_B T_c)$. The result is

$$k_B T_c = 1.13 \hbar\omega_D e^{-\frac{1}{N(0)\overline{V}}}. \tag{32}$$

One can express this in terms of the result we obtained earlier which connects the $T = 0$ energy gap $\Delta(0)$ with the cutoff frequency ω_D and the strength of the potential V. We obtain

$$\frac{\Delta(0)}{k_B T_c} = 1.764. \tag{33}$$

This is a central result of the theory of superconductivity. It provides an experimentally verifiable prediction for the ratio of $\Delta(0)$ to $k_B T_c$ which is independent of the strength of the phonon mediated electron-electron coupling[1].

The equation 30 also allows finding the temperature dependence of the superconducting gap.

IV. DENSITY OF STATES, TUNNELING EXPERIMENTS

Equations 14 and 15 show that each excitation in a normal superconductor, which is normally associated with a vector $\boldsymbol{k}$ and of either of the two possible values of spin, is mapped onto an excitation which is also uniquely related to a vector $\boldsymbol{k}$ and the two different types of Bogoliubov operators, 14 and 15. There is thus a one-to-one mapping between excitations in the normal and in the superconducting state; the energy is however connected through the relation $\epsilon = \sqrt{\xi^2 + \Delta^2}$, where ϵ and ξ are the excitation energies in the superconductor and the normal state respectively. As a result one can define a density of states of excitations by the following relation:

$$N_s(E) = \begin{cases} 0 & \text{if } E < \Delta \\ N(E_F)\frac{E}{\sqrt{E^2-\Delta^2}} & \text{if } E > \Delta \end{cases}. \tag{34}$$

This density of states can be probed directly in experiments on tunneling between a superconductor and a normal metal.

V. CONNECTION BETWEEN MICROSCOPIC THEORY AND GINZBURG LANDAU THEORY

The Ginzburg Landau theory can be derived rigourously from the microscopic theory[4]. The details of this derivation are very involved and we only discuss here very briefly the

[1] See Table 34.3 in [3]

result. It is found that the order parameter in the GL theory is related in the following way to the microscopic theory:

$$\Psi_{GL}(\boldsymbol{R}) = const \times F(\boldsymbol{R}, \boldsymbol{\rho}) \tag{35}$$

with

$$F(\boldsymbol{R}, \boldsymbol{\rho}) = \langle \psi_\uparrow \left(\boldsymbol{R} + \frac{\boldsymbol{\rho}}{2} \right) \psi_\downarrow \left(\boldsymbol{R} - \frac{\boldsymbol{\rho}}{2} \right) \rangle. \tag{36}$$

We used the operators

$$\psi_\sigma \left(\boldsymbol{r} \right) = \sum_{\boldsymbol{k}} g_{\boldsymbol{k}}(\boldsymbol{r}) c^\dagger_{\boldsymbol{k}\sigma} \tag{37}$$

with $g_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\boldsymbol{r}}$ the single particle states introduced in previous lectures. The operator $\psi_\sigma \left(\boldsymbol{r} \right)$ annihilates a particle of spin σ at position $\boldsymbol{r}$.

Leggett [4] gives a detailed account of the derivation of the Ginzburg-Landau equations from the microscopic equations. The key point is that the free energy of the system, which is given by microscopic theory as formulated in previous sections, is minimized with the constraint that the expectation value $\langle \psi_\uparrow \left(\boldsymbol{R} \right) \psi_\downarrow \left(\boldsymbol{R} \right) \rangle$ is the given function $\Psi_{GL}(\boldsymbol{R})$. A (again) self consistent procedure results in expressing the free energy of the system as a *functional* of Ψ_{GL}. The Ginzburg Landau equation is a good model for temperatures close to T_c.

VI. FURTHER READING

Tinkham [2], de Gennes [1], and Leggett [4] give an excellent account of the microscopic theory.

The chapter by Rickayzen in [5] is a very good discussion of the mean field theory for superconductors.

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[1] P. de Gennes, *Superconductivity of metals and alloys* (WA Benjamin, 1966).

[2] M. Tinkham, *Introduction to superconductivity*, 2nd ed., edited by J. Shira and E. Castellano, Physics and Astronomy (McGraw-Hill, 1996).

[3] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Harcourt College Publishing, 1976).

[4] A. Leggett, *Quantum Liquids, Bose condensation and Cooper pairing in condensed-matter systems* (Oxford University Press, 2006).

[5] R. Parks, ed., *Superconductivity, vol 1*, Vol. 1 (Marcel Dekker Inc., 1969).