

## **Many-body Theory, especially in Superconductivity**

BCS Theory by John R. Schrieffer

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## 1. Introduction of superconductivity and many-body theory

Many remarkable efforts were devoted after the discovery of superconductivity by Heike Kamerlingh Onnes in 1911, however, none of them had successful interpretation on electron-phonon interactions and microscopic origin of superconductivity. In 1957, a remarkable milestone was announced as Bardeen–Cooper–Schrieffer (BCS) theory, which describes superconductivity as a microscopic effect caused by a condensation of Cooper pairs into a bosonic state. <sup>[1]</sup>

Inspired by Prof. Tomonaga's approach to pion nucleon interactions, <sup>[2,3]</sup> Prof. Schrieffer made essential contribution to BCS wave functions, energy gap calculations and other extensions on free fermi gas and perturbation, which was achieved by solving many-body problems with Hartree–Fock Approximation, many-body perturbation theory, Green's function, etc. The many-body problem is to study properties of microscopic systems consisted of a large number of interacting particles, where the repeated interactions between particles create quantum correlations, or entanglement. <sup>[4]</sup>

BCS theory efficiently provided the approximation of many-body states of particles interaction. Fundamental fact is that the attractive interaction between electrons caused by virtual exchange of phonons appears when the energy difference between the electron states occupied is less than the phonon energy,  $\hbar\omega$ . <sup>[5]</sup>

## 2. Many-body problem applied to superconductivity

### 2.1. Mathematical Fundament

Being essential in wave function, the matrix element for electron-phonon interaction is given by,

$$|M_k|^2 = |v_k|^2 \left( \frac{\hbar}{2\omega_k} \right). \quad (2.1)$$

In which the  $v_k$  is the effective matrix element for electron-phonon interaction,  $\omega_k$  is the longitudinal sound wave frequency. <sup>[6]</sup> From the view of BCS theory, the attractive phonon interaction dominates the Coulomb interaction while the interaction is negative and less than phonon energy. <sup>[5]</sup> For simplicity it is assumed that a constant matrix element,  $-V$ , for transitions within an average phonon energy  $\hbar\omega$  of the Fermi surface, and the repulsive interaction outside this region is negligible, <sup>[7]</sup>

$$-V = \left\langle -\frac{2|M_k|^2}{\hbar\omega_k} + \frac{4\pi e^2}{k^2} \right\rangle < 0. \quad (2.2)$$

It will be extremely difficult when representing more than two electrons in a system. Conveniently, Slater determinant was applied to specify N-electron antisymmetrized product functions, which can be expressed by using creation operator,  $c^*$ , and annihilation operator,  $c$ , <sup>[8]</sup>

$$b_k = c_{-k\downarrow} c_{k\uparrow} \quad (2.3)$$

$$b_k^* = c_{-k\downarrow}^* c_{k\uparrow}^*. \quad (2.4)$$

Which are satisfied in Fermi commutation relations for bosonic system,

$$[b_k, b_{k'}^*]_- = (1 - n_{k\downarrow} - n_{k\uparrow})\delta_{kk'} \quad (2.5)$$

$$[b_k, b_{k'}]_- = 0 \quad (2.6)$$

$$[b_k, b_{k'}]_- = 2b_k b_{k'}(1 - \delta_{kk'}). \quad (2.7)$$

Where  $n$  is the single-particle number operator denoted by the multiple of creation operator,  $c^*$  and annihilation operator,  $c$ .  $\delta_{ij}$  is the Kronecker delta, which is a mathematical expression of  $i$  and  $j$  variables. When  $i$  is equal to  $j$ ,  $\delta$  is one, otherwise,  $\delta$  turns to be zero.

## 2.2. Ground State Wave Function

In physical interpretation of ground state, energy levels are completely occupied below Fermi energy, levels above are vacant without excited electrons. In the pictures of BCS theory, linearly combined low-lying normal states form ground state wave function where the Bloch states, describing the conduction of electrons in crystalline solids, are occupied by opposite spin pairs. [5]

Before delving into details, several prime conditions and assumptions are set: exchange interaction of phonons and Coulomb interactions between electrons provide the energy difference between normal and superconducting state. Other interactions are assumed to cancel the energy difference. Attractive interaction is the fundamental condition for wave functions. This was proved by Leon N. Cooper, after computing a wave function of a single pair of electrons that excited above the Fermi surface, it turned out that a bound state was formed for negative interaction no matter how weak the interaction was. [10]

Hereby, the ground state wave function is based on two-body interaction potentials in dense system of fermions, which is also applied for excitation state. In an easily approached way, net momentum,  $q$ , is considered zero with only opposite spin pair. The general ground state wave function of opposite spin is,

$$\Psi_{\text{grd}} = \sum_{k_1 \dots k_n} [h(k_1 \dots k_n)]^{\frac{1}{2}} f[\dots 1(k_1) \dots 1(k_n) \dots]. \quad (2.8)$$

Being represented by specific wave factor  $k'$ ,

$$\Psi_{\text{grd}} = h_{k'}^{\frac{1}{2}} \varphi_1 + (1 - h_{k'})^{\frac{1}{2}} \varphi_0. \quad (2.9)$$

Where,  $\varphi$  are normalized functions,  $\varphi_0$  is empty state,  $\varphi_1$  is the pair state,  $h_k$  is the probability that state  $k$  is occupied. BCS held the view that it would be a good approximation to apply Hartree self-consistent field to describe large number of involved particles, where the occupancy of each state  $k$  is dependent on the average occupancy of other states. [8] By using Hartree-like methods, and being represented by product integral operator,

$$\varphi_1 = b_k^* \prod_{k \neq k'} [(1 - h_k)^{\frac{1}{2}} + h_k^{\frac{1}{2}} b_k^*] \Phi_0. \quad (2.10)$$

In quantum field theory,  $\Phi_0$  is vacuum state with no particles present. Although it is not truly empty, it has the lowest possible energy compared to other states.

### 2.3. Ground State Energy and Energy Gap Function

When it comes to ground state energy, it is dependent on two terms,

$$W_0 = W_{KE} + W_I. \quad (2.11)$$

Where  $W_{KE}$  is for kinetic energy, and  $W_I$  is interaction energy.

$$W_{KE} = 2 \sum_{k>k_F} h_k \epsilon_k + 2 \sum_{k<k_F} (1 - h_k) |\epsilon_k| \quad (2.12)$$

$$W_I = - \sum_{k,k'} V_{kk'} [h_k (1 - h_k) h_{k'} (1 - h_{k'})]^{\frac{1}{2}}. \quad (2.13)$$

For  $k < k_F$ , it refers to electron occupation, and  $k > k_F$  represents hold occupation. Where  $\epsilon_k$  is the Bloch energy which is designed for particles in periodically-repeated system. By minimizing the  $W_0$  with  $h_k$ , distribution function is achieved,

$$\frac{[h_k(1-h_k)]^{\frac{1}{2}}}{1-2h_k} = \frac{\sum_{k'} V_{kk'} [h_{k'}(1-h_{k'})]^{\frac{1}{2}}}{2\epsilon_k}. \quad (2.14)$$

As mentioned in Sec.2.1, simplified matrix element  $V$  was introduced as approximation for all  $V_{kk'}$  for  $k$  states out to a cutoff energy  $\hbar\omega$  away from Fermi energy, and  $V_{kk'}$  is equal to zero above Fermi energy. [8] While the band and crystal structure was neglected and replacing the periodic ion potential by  $V$ , [9]

$$V = \langle V_{kk'} \rangle_{ave} \quad (2.15)$$

$$[h_k = \frac{1}{2} [1 - \frac{\epsilon_k}{2(\epsilon_k^2 + \epsilon_0^2)^{\frac{1}{2}}}] \quad (2.16)$$

$$[h_k(1 - h_k)]^{\frac{1}{2}} = \frac{\epsilon_0}{2(\epsilon_k^2 + \epsilon_0^2)^{\frac{1}{2}}}. \quad (2.17)$$

Where  $\epsilon_0$  is denoted as energy gap or the minimum excitation energy at Fermi surface,

$$\epsilon_0 = V \sum_{k'} [h_{k'}(1 - h_{k'})]^{\frac{1}{2}} = \frac{\hbar\omega}{\sinh[\frac{1}{N(0)V}]}. \quad (2.18)$$

Computing by (2.12), (2.13), (2.16), (2.17) and (2.18), the ground state energy is,

$$W_0 = 4N(0) \int_0^{\hbar\omega} [\epsilon - \frac{\epsilon^2}{(\epsilon^2 + \epsilon_0^2)^{\frac{1}{2}}}] d\epsilon - \frac{\epsilon_0^2}{V}. \quad (2.19)$$

Where  $N(0)$  denotes the density of states at the Fermi surface for electrons of one spin orientation [8]. And weak-coupling approximation can be applied when  $N(0)V \ll 1$ .

### 2.4. Energy Gap Relation at Absolute Zero

After minimizing the energy of wave function, energy gap can be achieved. The minimum energy needed from occupied ground state to excitation is as follows, which is the energy gap function at absolute zero represented by pair states.

$$W_{k',k''} - W_0 = \epsilon_{k'}(1 - 2h_{k'}) + \epsilon_{k''}(1 - 2h_{k''}) + 2V \sum_k [h_k(1 - h_k)]^{\frac{1}{2}} \{ [h_{k'}(1 - h_{k'})]^{\frac{1}{2}} + [h_{k''}(1 - h_{k''})]^{\frac{1}{2}} \}. \quad (2.20)$$

Where  $k'$  and  $k''$  were denoted as wave functions for different energy states, in this case,  $k'$  stands for spin-down states and  $k''$  hereby represents spin-up states. Use (2.16), (2.17), (2.18) and (2.20) for substituting variables,

$$W_{k',k''}-W_0 = \frac{\epsilon_{k'}^2}{E_{k'}} + \frac{\epsilon_{k''}^2}{E_{k''}} + \epsilon_0^2 \left( \frac{1}{E_{k'}} + \frac{1}{E_{k''}} \right). \quad (2.21)$$

Where  $E_k$  is the excitation energy,

$$E_k = (\epsilon_k^2 + \epsilon_0^2)^{\frac{1}{2}}. \quad (2.22)$$

While being at zero temperature state,  $\epsilon_k$  goes to zero,  $E_k$  goes to  $\epsilon_0$ . The minimum energy for excitation becomes  $2\epsilon_0$ . Moreover, as it goes to general form after being excited, the energy difference between two states are,

$$W_1 - W_2 = \sum_1 E_k - \sum_2 E_k. \quad (2.23)$$

Which is given by the sums of energy for each excitation state.

## 2.5. Excitation State Wave Function

As mentioned in Sec.2.1, the excited state shares the similar premise with ground state. Differently, the excited system is composed by the ground states,  $g$ , occupied by ground pairs, excited pairs state,  $p$ , and single particle state,  $s$ . Excited state wave function is described as follows.

$$\Psi_{\text{exc}} = \prod_{k(g)} [(1 - h_k)^{\frac{1}{2}} + h_k^{\frac{1}{2}} b_k^*] \prod_{k'(p)} [(1 - h_{k'})^{\frac{1}{2}} b_{k'}^* - h_{k'}^{\frac{1}{2}}] \prod_{k''(s)} c_{k''}^* \Phi_0. \quad (2.24)$$

According to solid state physics principle for different states with different energy, the excited state wave function is orthogonal to ground state wave function (2.8).

## 2.6. Excited State Energy

Being similar to ground state energy,  $W$  is computed by the energy from ensemble average over the wave function of excitation state.  $W$  includes the kinetic energy and the ensemble average of interaction Hamiltonian, which are,

$$W_{KE} = \sum_k |\epsilon_k| [s_k + 2p_k + 2(1 - s_k - 2p_k)h_k(|\epsilon_k|)] \quad (2.25)$$

$$W_I = -\sum_{k,k'} V_{kk'} [h_k(1 - h_k)h_{k'}(1 - h_{k'})]^{\frac{1}{2}} \times \{(1 - s_k - 2p_k)(1 - s_{k'} - 2p_{k'})\} \quad (2.26)$$

$$s_k = 2f_k(1 - f_k) \quad (2.27)$$

$$p_k = f_k^2. \quad (2.28)$$

Where,  $s_k$  is the probability that either spin-up state is occupied or spin-down state is occupied,  $p_k$  is the probability that both spin-up state and spin-down state are occupied. The energy is finite to excite an electron from ground state, because the small excitation energy in total energy is proportional to the number of excited electrons. <sup>[5]</sup>

### 3. Important Theoretical Predictions

#### 3.1. Critical temperature

Once a specimen reaches superconducting state, it will have a striking decrease on resistance, where temperature is denoted as critical temperature,  $T_c$ . It is defined as the boundary of the region beyond which there is no real, positive  $\epsilon_0$  that satisfies (3.14). Above critical temperature, temperature dependence of the  $\epsilon_0$  becomes zero.

It can be deduced that the electron concentration plays important role in setting critical temperature. Below critical temperature, free energy minimization is achieved. The expressions of critical temperature and related energy gap are as follows. <sup>[5]</sup> From (3.3), it can be easily concluded that the energy gap turns to zero once reaching the critical temperature.

$$kT_c = 1.13\hbar\omega_c e^{-1/N(0)V} \quad (3.1)$$

$$\frac{\epsilon_0}{kT_c} = 1.764. \quad (3.2)$$

$$\epsilon_0 = 3.2kT_c[1 - (T/T_c)]^{\frac{1}{2}}. \quad (3.3)$$

#### 3.12. Free energy

Thermodynamically, free energy is expressed as

$$F = W - TS. \quad (3.4)$$

Where,

$$W_0 = W_{KE} + W_I. \quad (3.5)$$

$$-TS = 2kT \sum_{k'} \{f_{k'} \ln f_{k'} + (1 - f_{k'}) \ln(1 - f_{k'})\}. \quad (3.6)$$

$$F_n = -4N(0)kT \int_0^\infty d\epsilon \log(1 + e^{-\beta\epsilon}) = -\frac{1}{3}\pi^2 N(0)(kT)^2. \quad (3.7)$$

$$F_s = -4N(0) \int_0^\infty d\epsilon E f(\beta E) + 2N(0) \int_0^{\hbar\omega} d\epsilon \left[ \epsilon - \frac{\epsilon^2}{E} \right] - \frac{\epsilon_0^2}{V}. \quad (3.8)$$

In which  $\beta$  is the reciprocal of  $kT$ .

#### 3.13. Minimization of the Free Energy

When minimizing the free energy with respect to  $h_k$ ,

$$\frac{[h_k(1-h_k)]^{\frac{1}{2}}}{1-2h_k} = \frac{\sum_{k'} V_{kk'} [h_{k'}(1-h_{k'})]^{\frac{1}{2}}}{2\epsilon_k} (1 - 2f_{k'}). \quad (3.9)$$

Which gives the minimum excitation  $\epsilon_0$ :

$$\epsilon_0 = V \sum_{k'} [h_{k'}(1 - h_{k'})]^{\frac{1}{2}} (1 - 2f_{k'}). \quad (3.10)$$

It turned out that energy gap becomes  $2\epsilon_0$  for single-particle density of states. Hereby, the distribution of ground pairs is dependent on the magnitude of energy gap at that temperature. <sup>[5]</sup> When minimize the free energy with respect to  $f_k$ ,

$$2\epsilon_k(1 - 2h_k) + 4 \sum_{k'} V_{kk'} [h_k(1 - h_k)h_{k'}(1 - h_{k'})]^{\frac{1}{2}} \times (1 - 2f_{k'}) + 2kT \ln \left( \frac{f_k}{1-f_k} \right) = 0 \quad (3.11)$$

$$f_k = \frac{1}{e^{\beta E_k + 1}} = f(E_k). \quad (3.12)$$

The density of states is given by,

$$\frac{dN(E)}{dE} = \frac{dN(E)}{dE} = N(0) \frac{E}{(E^2 - \epsilon_0^2)^{\frac{1}{2}}}. \quad (3.13)$$

The energy gap determining condition is,

$$\frac{1}{N(0)V} = \int_0^{\hbar\omega} \frac{d\epsilon}{\epsilon} \tanh\left(\frac{1}{2}\beta_c \epsilon^2 + \epsilon_0^2\right). \quad (3.14)$$

### 3.14. Critical Field

Changes of magnetic field can also result in phase transition entering superconducting state. When applied magnetic field is high enough, specimen gain energy advantage to switch back to normal state. Superconductivity is destroyed via a first order phase transition. Therefore, the highest magnetic field before specimen return to normal state is described as critical field. In the picture of BCS theory, only Type I superconductors are considered, upper and lower critical field from Type II superconductors are not included. The critical field for a bulk specimen of unit volume is expressed as, [5]

$$\frac{H_S^2}{8\pi} = F_n - F_S. \quad (3.15)$$

According to (3.3), (3.8), and (3.15), critical field becomes,

$$\frac{H_S^2}{8\pi} = N(0)(\hbar\omega)^2 \left\{ \left[ 1 + \left( \frac{\epsilon_0}{\hbar\omega} \right)^2 \right]^{\frac{1}{2}} - 1 \right\} - \frac{\pi^2}{3} N(0)(kT)^2 \times \left\{ 1 - \beta^2 \int_0^\infty d\epsilon \left[ \frac{2\epsilon^2 + \epsilon_0^2}{E} \right] f(BE) \right\}. \quad (3.16)$$

### 3.15. Specific heat

The specific heat of superconducting state is given by,

$$C_{es} = T \frac{dS}{dT} = -\beta \frac{dS}{d\beta} = 4k\beta^2 \sum_{k>k_F} f_k (1 - f_k) \left[ E_k^2 + \frac{\beta d\epsilon_0^2}{2d\beta} \right]. \quad (3.17)$$

Owing to energy gap vanishing and the second phase transition at critical temperature, the specific heat of superconducting state will have a large jump compared with that of normal state. [5] The difference can be found as follows,

$$(C_{es} - C_{en})|_{T_c} = 2k\beta^2 \sum_{k>k_F} f_{kn} (1 - f_{kn}) \left[ \frac{d\epsilon_0^2}{d\beta} \right]_{T_c}. \quad (3.18)$$

Where

$$C_{en}|_{T_c} = \gamma_{T_c}. \quad (3.19)$$

Jump turns into

$$\frac{C_{es} - \gamma_{T_c}}{\gamma_{T_c}}|_{T_c} = 1.52. \quad (3.20)$$

Where  $\gamma$  is the specific heat at normal state.

## 4. Discussion

### 4.1. Significance

As the first microscopic superconducting theory, it provides essential guidance and accurate predictions to thermal, electrical transport and electromagnetic properties of superconductors. It leads to sufficient wave function and energy gap models for phase transition at superconducting state. <sup>[9]</sup>

### 4.2. Limits & Restrictions

Several limits exist in assumptions and premises, for example, as mentioned in Sec.2.2, the ground state stands for zero net momentum for spins. However, possibility may exist for the situation where no energy gap between states with nonzero net spin momentum. <sup>[5]</sup>

Electron-phonon interactions only prove critical temperature limits of 35 K, BCS theory hereby has inadequacy in high temperature superconductors whose mechanism is more complicated. With time going by, BCS theory is unable to predict increasing number of “unconventional” and compound superconductors. <sup>[9]</sup>

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