Lecture 10

BCS – Trial wavefunction and the Bogoliubov method

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1 Cooper's problem

Cooper contributed a key insight for the understanding of the nature of superconductivity – pairing of electrons. Today we call these pairs Cooper pairs. The point is the formation of bound states, hence, the nature of superconductivity is non-pertubative if we start from the normal state. Later we will see the superconducting gap function $\Delta \propto \hbar\omega_D e^{-\frac{1}{N_0 g}}$ where ω_D is the Debye frequency, N_0 is the density of state at the Fermi surface, g is the effective attractive interaction strength. Since the interaction strength appears in the denominator of the exponent, it is an intrinsic singularity and cannot be expanded as a power series. This is the difficulty of superconductivity – it cannot be reached by performing perturbative solutions from the normal state.

As a starting point, Cooper considered an idealized problem of just two electrons. Idealization plays an important role in the study of physics, which can put the complicated but secondary factors aside for a moment so that we can concentrate on the most crucial points. Assume that there is a fully-filled Fermi surface with the Fermi wavevector k_f. On top of it, add two electrons with momenta and spins as $(\mathbf{k}, \uparrow)$ and $(-\mathbf{k}, \downarrow)$. We neglect that effect that electrons inside the Fermi surface actually can be scattered outside, i.e., the Fermi surface is rigid and simply plays the role of blocking the phase space. We assume an attractive interaction between these two electrons with the following Hamiltonian as

$$\begin{aligned} H &= H_0 + U \\ H_0 &= \sum_k (\epsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} \quad U = -\frac{g}{V} \sum_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{-k,\downarrow} c_{-k,\downarrow} c_{k,\uparrow}. \end{aligned} \tag{1}$$

The origin of the negative g is due to the electron-phonon interaction we learned before. For simplicity, we neglect its retarded nature, and assume it is instanious. Furthemore, we assume it is momentum independent, which corresponds to the isotropic s-wave superconductivity.

The interaction part causes the scattering $(\mathbf{k}, \uparrow; -\mathbf{k}, \downarrow) \rightarrow (\mathbf{k}' \uparrow; -\mathbf{k}, \downarrow)$ maintaining the total momentum zero. The the eigenstate states of the pair will a superposition of these pairs

$$|\Psi\rangle = \sum_k \alpha(k) c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} |F\rangle, \tag{2}$$

where $|F\rangle$ is the reference state of fully filled Fermi sphere. It is easy to check that

$$\begin{aligned} &H_0 c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} |F\rangle = (2\epsilon_k + E_0) c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} |F\rangle, \\ &U c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} |F\rangle = \frac{u}{V} \sum_{k'} c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} |F\rangle. \end{aligned} \tag{3}$$

Then we write down the Schrödinger equation $H\Psi\rangle = E|\Psi\rangle$ as

$$\begin{aligned} H\Psi &= \sum_k \alpha(k)(2\epsilon_k - 2\mu + E_0) c^\dagger_{k\uparrow} c^\dagger_{k,\downarrow} - \frac{u}{V} \sum_{k,k'} \alpha(k) c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} |F\rangle \\ &= \sum_k \Big((2\epsilon_k - 2\mu + E_0)\alpha(k) - \frac{u}{V} \sum_{k'} \alpha(k') \Big) c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} |F\rangle = E \sum_k \alpha(k) c^\dagger_{k',\uparrow} c^\dagger_{-k',\downarrow} |F\rangle, \end{aligned}$$

then,

$$\begin{aligned} \alpha(k) &= \frac{u/V}{2(\epsilon_k - \mu) - \Delta E} \sum_{k'} \alpha(k') \\ \frac{1}{u} &= \frac{1}{V} \sum_k \frac{1}{-\Delta E + 2(\epsilon_k - \mu)}, \end{aligned} \tag{4}$$

where $\Delta E = E - E_0$.

We can plot the left and right hand sides of Eq. 4. It is clear that it has a solution with negative energy, which corresponds to a bound state. By changing the summation to integral, we can analytically solve the bound state energy as

Figure 1: Pictorial representation of the bound state solution.

$$\begin{aligned} \frac{1}{u} &= N(0) \int_0^{\hbar\omega_D} d\epsilon \frac{1}{2\epsilon - \Delta E} = \frac{N(0)}{2} \ln \frac{2\hbar\Omega_D - \Delta E}{-\Delta E} \\ \frac{2}{N_0 u} &\approx \ln \frac{2\hbar\omega_D}{|\Delta E|} \Rightarrow \Delta E = -2\hbar\omega_D e^{\frac{2}{N(0)g}}. \end{aligned} \tag{5}$$

Later we will see the superconducting gap function Δ is roughly speaking the same order as $|\Delta E|$.

An important feature of Eq. 5 is that the bound state exists at infinitesimal value of g. This is in contrast in the free space that a finite strength of attraction is needed to form a bound state. This is the effect from the Fermi surface – the low energy density of states becomes a constant, rather than vanishing as in the free space. Effectively, Fermi surface renders the density of states to be two-dimensional like.

2 BCS trial wavefunction

We use the following BCS Hamiltonian

$$H = \sum_{k\sigma} \xi_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} - \frac{1}{V} \sum_{k_1, k_2, \sigma\sigma'} g(k_1, k_2) c^\dagger_{k_2,\uparrow} c^\dagger_{-k_2,\downarrow} c_{-k_1,\downarrow} c_{k_1,\uparrow}, \tag{6}$$

where $\xi_k = \epsilon_k - \mu$.

2.1 BCS Ansatz

BCS generalized a single Cooper pair to many pairs, and proposed the following wavefunction

$$\Psi_{BCS}(r_1, ..., r_N; \sigma_1, ...\sigma_N) = \mathcal{A}\Big\{\varphi(r_1, r_2; \sigma_1, \sigma_2)\varphi(r_3, r_4; \sigma_3, \sigma_4)....\varphi(r_{N-1}, r_N; \sigma_{N-1}, \sigma_N)\Big\}, \tag{7}$$

where $\mathcal{A}$ is the inter-pair antisymmetrization operation, and $\varphi(r_1, r_2; \sigma_1, \sigma_2)$ is antisymmetric for the intrapair exchange between two electrons. For the singlet superconductor, we have

$$\begin{aligned}
\varphi(r_1, r_2; \sigma_1, \sigma_2) &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)\varphi(|r_1 - r_2|) \\
&= \frac{1}{\sqrt{2}} \sum_k \chi(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{r_1}-\mathbf{r_2})}(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2) \\
&= \sum_k \chi(\mathbf{k}) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k},\downarrow} |vac\rangle
\end{aligned} \tag{8}$$

φ is an even function, hence, $\varphi(\mathbf{k}) = \varphi(-\mathbf{k})$.

Then the many-body state can be written as

$$\Psi_N = \mathcal{N}^{-\frac{1}{2}} \Big(\chi(\mathbf{k}) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k},\downarrow}\Big)^{\frac{N}{2}} |vac\rangle, \tag{9}$$

where $\mathcal{N}$ is a normalization factor. Such a wavefunction has a fixed particle number of N. Since it is not easy to work with the canonical ensemble, the BCS method releases the fixed particle number constraint by using the grand canonical ensemble. Then the wavefunction becomes

$$\begin{aligned}
|\Psi\rangle &= \exp\Big(\sum_k \chi(\mathbf{k}) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k},\downarrow}\Big)|vac\rangle = \Pi_k \exp\Big(\chi(\mathbf{k}) c^\dagger_\uparrow c^\dagger_\downarrow\Big)|vac\rangle \\
&= \Pi_k \Big(1 + \chi(\mathbf{k}) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\Big)|vac\rangle,
\end{aligned} \tag{10}$$

where all of the higher order terms vanish due to the $(c^\dagger_{k\uparrow})^2 = 0$. The particle number in the system is controlled by the choice of chemical potential.

The BCS trial wavefunction $|\Psi\rangle$ is no longer a Slater determinant state which is a product of single particle state. In contrast, we decompose the many-body Hilbert space into the product of sectors of pairs. The question is how the different pairs communicate with each other – how do they share phase information? Let us just consider the sector spanned by the modes of $\mathbf{k}\uparrow$ and $-\mathbf{k}\downarrow$. They span four states marked as

$$|0\rangle, \quad c^\dagger_{-k,\downarrow}|0\rangle, \quad c^\dagger_{k,\uparrow}|0\rangle, \quad c^\dagger_{k,\uparrow}c^\dagger_{-k,\downarrow}|0\rangle. \tag{11}$$

Then

$$|\Psi\rangle = \Pi_k\Big(|0\rangle + \chi(k)c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}|0\rangle\Big) \Rightarrow \Pi_k\Big(u_k + v_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\Big)|0\rangle, \tag{12}$$

where we set $|u_k|^2 + |v_k|^2 = 1$. We can set u_k to be real and positive, and then v_k can be determined up to a phase $v_k e^{i\phi}$. For the conventional superconductors, ϕ is independent of $\mathbf{k}$. This means that different pairs share the same phase, and this is the global phase coherence. Then we have

$$|\Psi(\phi)\rangle = \Pi_k\Big(|u_k| + |v_k|e^{i\phi}c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\Big)|0\rangle, \tag{13}$$

which is called the phase eigenstate. We can project out the fixed particle state via Fourier transform as

$$|\Psi_N\rangle = \int_0^{2\pi} \Psi(\varphi)e^{-i\frac{N\varphi}{2}}d\varphi. \tag{14}$$

In this sense, the number of Cooper pairs $N/2$ and the condensation phase ϕ are a pair of conjugate variables.

2.2 Optimization of the BCS wavefunction

Let us calculate the ground state energy expectation value of the BCS wavefunction

$$E = \langle K\rangle + \langle H_{int}\rangle, \tag{15}$$

where

$$\begin{aligned}
\langle K\rangle &= \langle\sum_{k\sigma}\xi_i c^\dagger_{k\sigma}c_{k\sigma}\rangle = 2\sum_k \xi_k|v_k|^2 \\
\langle H_{int}\rangle &= -\frac{1}{2V}\sum_{k_1,k_2} g(k_1,k_2)\langle c^\dagger_{k\sigma}c^\dagger_{-k,\sigma'}c_{-k\sigma'}c_{k,\sigma}\rangle \approx -\frac{1}{V}\sum_{k_1,k_2} g(k_1,k_2)\langle c^\dagger_{k_2,\uparrow}c^\dagger_{-k_2,\downarrow}\rangle\langle c_{-k_1,\downarrow}c_{k_1,\uparrow}\rangle.
\end{aligned}$$

We define

$$F_k = u^*_k v_k = \langle 0_{k\uparrow}0_{-k\downarrow}|c_{-k,\downarrow}c_{k,\uparrow}|1_{k\uparrow}1_{-k\downarrow}\rangle, \tag{16}$$

then

$$\langle H_{int} \rangle = -\frac{1}{V} \sum_{k_1,k_2} g(k_1,k_2) F_{k1} F^*_{k_2}. \tag{17}$$

and the total energy

$$E = 2\sum_k \xi_k |v_k|^2 - \frac{1}{V} \sum_{k_1,k_2} g(k_1,k_2) u^*_{k1} v_{k_1} u_{k2} v^*_{k2}. \tag{18}$$

Using the commonly used parameterization scheme

$$u_k = \cos\theta_k, \quad v_k = \sin\theta_k, \tag{19}$$

we have

$$\begin{aligned} E &= 2\sum_k \xi_k \sin^2\theta_k - \frac{1}{4V} \sum_{k_1,k_2} g(k_1,k_2) \sin 2\theta_{k1} \sin 2\theta_{k_2} \\ &= \sum_k \xi_k (-\cos 2\theta_k + 1) - \frac{1}{4} \sum_{k_1} \sin 2\theta_{k1} \sum_{k2} \frac{g(k_1,k_2)}{V} \sin 2\theta_{k2}. \end{aligned} \tag{20}$$

If we do variation,

$$0 = \frac{\partial}{\partial \theta_k} E = 2\xi_k \sin 2\theta_k - \cos 2\theta_k \frac{1}{V} \sum_{k'} g(k,k') \sin 2\theta_{k'}. \tag{21}$$

Define the gap function

$$\Delta_k = \frac{1}{2V} \sum_{k'} g(k,k') \sin 2\theta_{k'}, \tag{22}$$

then

$$\tan 2\theta_k = \frac{\Delta_k}{\xi_k}, \Rightarrow \cos 2\theta_k = \frac{\xi_k}{E_k}, \quad \sin 2\theta_k = \frac{\Delta_k}{E_k}, \tag{23}$$

where $E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$. Then the self-consistent condition is

$$\Delta_k = \frac{1}{V} \sum_{k'} g(k,k') \frac{\Delta'_k}{2E'_k}, = \int \frac{dk'}{(2\pi)^3} g(k,k') \frac{\Delta'_k/2}{\sqrt{\xi^2_{k'} + \Delta^2_{k'}}}. \tag{24}$$

which is the celebrated BCS gap equation (at $T = 0$).

3 The self-consistent Bogoliubov method

The above variational method is physically intuitive. Nevertheless, it is not so easy to generalize to spatial inhomogeneous systems. It is equivalent to the Bogoliubov mean-field theory, and later was generalized to inhomogenous systems such as vortex and impurity problems – called the Bogoliubov-de Gennes (B-deG) formalism.

3.1 Bogoliubov transformation

The technical part of the mean-field theory is to decompose the 4-fermion interaction into fermion bilinears based on

$$O_1O_2 = O_1\langle O_2\rangle + \langle O_1\rangle O_2 - \langle O_1\rangle\langle O_2\rangle + \delta O_1\delta O_2 \approx O_1\langle O_2\rangle + \langle O_1\rangle O_2 - \langle O_1\rangle\langle O_2\rangle \quad (25)$$

where $O_{1,2}$ are fermion bilinear operators, and $\delta O_i = O_i - \langle O_i\rangle$. $\delta O_1\delta O_2$ is viewed as a high order fluctuation term, and is neglected at the mean-field level. Following this, we decompose the 4-fermion interaction term in Eq. 6 into

$$\sum_k c^\dagger_{k\uparrow}c^\dagger_{-k,\downarrow}\Delta_k + c_{-k\downarrow}c_{k\uparrow}\Delta^*_k + \sum_{k_1,k_2} g(k_1,k_2)\langle c^\dagger_{k\uparrow}c^\dagger_{-k,\downarrow}\rangle\langle c_{-k\downarrow}c_{k\downarrow}\rangle, \quad (26)$$

where

$$\Delta_k = -\frac{1}{V}\sum_{k'} g(k,k')\langle c_{-k'\downarrow}c_{k'\uparrow}\rangle. \quad (27)$$

Then we arrive at the following decoupled mean-field Hamiltonian as

$$H = \sum_k \Big\{H_k + \xi_k\Big\} + \sum_{k_1,k_2} g(k_1,k_2)\langle c^\dagger_{k\uparrow}c^\dagger_{-k,\downarrow}\rangle\langle c_{-k\downarrow}c_{k\downarrow}\rangle. \quad (28)$$

with

$$H_k = (c^\dagger_{k\uparrow}, c_{-k\downarrow})\begin{pmatrix} \xi_k & \Delta_k \\ \Delta^*_k & -\xi_k \end{pmatrix}\begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k,\downarrow} \end{pmatrix}. \quad (29)$$

We would like to diagonalize H_k. For simplicity, we assume that Δ_k is real, such that the diagonalization can be performed by a 2D rotation as,

$$\begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u^*_k & -v_k \\ v^*_k & u_k \end{pmatrix}\begin{pmatrix} \alpha_{k\uparrow} \\ \alpha^\dagger_{-k\downarrow} \end{pmatrix} \Rightarrow \begin{pmatrix} \alpha_{k\uparrow} \\ \alpha^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v^*_k & u^*_k \end{pmatrix}\begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} \quad (30)$$

then

$$(c^\dagger_{k\uparrow}, c_{-k\downarrow}) = (\alpha^\dagger_{k\uparrow}, \alpha_{-k\downarrow})\begin{pmatrix} u_k & v_k \\ -v^*_k & u^*_k \end{pmatrix} \Rightarrow (\alpha^\dagger_{k\uparrow}, \alpha_{-k\downarrow}) = (c^\dagger_{k\uparrow}, c_{-k\downarrow})\begin{pmatrix} u^*_k & -v_k \\ v^*_k & u_k \end{pmatrix} \quad (31)$$

Then

$$\begin{aligned} H_k &= (\alpha^\dagger_{k\uparrow}, \beta_{-k\downarrow})\begin{pmatrix} u_k & v_k \\ -v^*_k & u^*_k \end{pmatrix}\begin{pmatrix} \xi_k & \Delta_k \\ \Delta^*_k & -\xi_k \end{pmatrix}\begin{pmatrix} u^*_k & -v_k \\ v^*_k & u_k \end{pmatrix}\begin{pmatrix} \alpha_{k\uparrow} \\ \beta^\dagger_{-k,\downarrow} \end{pmatrix} \\ &= (\alpha^\dagger_{k\uparrow}, \beta_{-k\downarrow})M_k\begin{pmatrix} \alpha_{k\uparrow} \\ \beta^\dagger_{-k,\downarrow} \end{pmatrix}. \end{aligned}$$

where

$$M_k = \begin{pmatrix} \xi_k(|u_k|^2 - |v_k|^2) + \Delta_k u^*_k v_k + \Delta^*_k u_k v^*_k & \Delta_k u^2_k - \Delta^*_k v^2_k - 2\xi_k u_k v_k \\ \Delta^*_k u^{*2}_k - \Delta_k v^{*2}_k - 2\xi_k u^*_k v^*_k & \xi_k(|u_k|^2 - |v_k|^2) + \Delta_k u^*_k v_k + \Delta^*_k u_k v^*_k \end{pmatrix} \quad (32)$$

Consider the case that Δ_k is real, so that we can $u_k = \cos\theta_k$ and $v_k = \sin\theta_k$, we have

$$M_k = \begin{pmatrix} \xi_k \cos 2\theta_k + \Delta_k \sin 2\theta_k & -\xi_k \sin 2\theta_k + \Delta_k \cos 2\theta_k \\ -\xi_k \sin 2\theta_k + \Delta_k \cos 2\theta_k & -\xi_k \cos 2\theta_k - \Delta_k \sin 2\theta_k \end{pmatrix} \quad (33)$$

Then we can diagonalize M_k by setting

$$\begin{aligned} \tan 2\theta_k &= \frac{\Delta_k}{\xi_k}, \Rightarrow \cos 2\theta_k = \frac{\xi_k}{E_k}, \quad \sin 2\theta_k = \frac{\Delta_k}{E_k}, \\ u_k^2 &= \cos^2\theta_k = \frac{1}{2}\Big(1 + \frac{\xi_k}{E_k}\Big) \\ v_k^2 &= \sin^2\theta_k = \frac{1}{2}\Big(1 - \frac{\xi_k}{E_k}\Big). \end{aligned} \quad (34)$$

where $E_k = \sqrt{\xi_k^2 + |\Delta_k|^2}$.

Then set θ_k as before according to Eq. 34, we have the diagonalized form

$$H_k = E_k\Big(\alpha^\dagger_{k\uparrow}\alpha_{k\uparrow} + \alpha^\dagger_{-k\downarrow}\alpha_{-k\downarrow} - 1\Big). \quad (35)$$

Now we can drive the gap equation as the self-consistent condition

$$\begin{aligned} \Delta_k &= -\frac{1}{V}\sum_{k'} g(k,k')\langle c_{-k\downarrow}c_{k\uparrow}\rangle \\ &= \frac{1}{V}\sum_{k'} g(k,k')\sin\theta_k\cos\theta_k\Big\{\frac{1}{2} - \langle\alpha^\dagger_{k\uparrow}\alpha_{k\uparrow}\rangle + \frac{1}{2} - \langle\beta^\dagger_{-k\downarrow}\beta_{-k\downarrow}\rangle\Big\} \\ &= \frac{1}{2V}\sum_{k'} g(k,k')\sin 2\theta_k \tanh\frac{\beta E_k}{2}, \end{aligned} \quad (36)$$

then we arrive the gap equation at finite temperatures

$$\Delta_k = \int \frac{dk'}{(2\pi)^3} g(k,k')\frac{\Delta'_k/2}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}} \tanh\frac{\beta\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}}{2}. \quad (37)$$

3.2 The BCS vacuum

The BCS vacuum should be annihilated by $\alpha_{k\uparrow}$ and $\alpha_{-k\downarrow}$, i.e.,

$$\alpha_{k\uparrow}|\Psi_{GP}\rangle = \alpha_{-k\downarrow}|\Psi_{GP}\rangle = 0, \quad (38)$$

We can define to meet the above requirements:

$$|\Phi_{GP}\rangle = \Big(u_k - v_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\Big)|0\rangle. \quad (39)$$

(It seems a sign difference from the variational construction – need check.) In other words, the BCS vacuum can be viewed as a squeezed state of the particle number vacuum. Then the single Bogoliubov excitations above the superconducting vacuum are just the ordinary spin up and down fermions referring to the particle vacuum

$$\alpha^\dagger_{k\uparrow}|\Phi_{GP}\rangle = c^\dagger_{k\uparrow}|0\rangle, \quad \alpha^\dagger_{-k\downarrow}|\Phi_{GP}\rangle = c^\dagger_{-k\downarrow}|0\rangle. \quad (40)$$

And then the double excitation becomes

$$|\Phi_{EP}\rangle = \alpha^\dagger_{k\uparrow}\alpha^\dagger_{-k\downarrow}|\Phi_{GP}\rangle = \Big(v_k^* + u_k^* c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\Big)|\Phi_{GP}\rangle \quad (41)$$

4 Solution to the gap equation

Let us consider the simplest case that $|g(k, k')| = g$, i.e., Δ_k is independent on k, then Eq. 37 is simplified to

$$\Delta = gN_0 \int_{-\hbar\omega_D}^{\hbar\omega_D} d\epsilon \frac{\Delta}{2E_k} \tanh \frac{\beta E_k}{2} \Rightarrow \frac{1}{gN_0} = \int_0^{\hbar\omega_D} d\epsilon \frac{1}{E_k} \tanh \frac{\beta E_k}{2}. \tag{42}$$

4.1 Gap function at zero temperature

First, consider the zero temperature, then by setting $\beta \to +\infty$ we have

$$\begin{aligned} \frac{1}{gN_0} &= \int_0^{\hbar\omega_D} d\epsilon \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} = \int_0^{\frac{\hbar\omega_D}{\Delta}} \frac{dx}{\sqrt{1+x^2}} = \sinh^{-1} \frac{\hbar\omega_D}{\Delta} \\ \Delta &= \frac{\hbar\omega_D}{\sinh \frac{1}{N_0 g}} \Rightarrow \Delta \approx 2\hbar\omega_D e^{-\frac{1}{N_0 g}} \quad \text{at} \quad gN_0 \ll 1. \end{aligned} \tag{43}$$

4.2 Gap function around T_c

Around T_c, $\Delta \to 0$, we have

$$\frac{1}{gN_0} = \int_0^{\hbar\omega_D} d\epsilon \frac{\tanh \frac{\beta_c \epsilon}{2}}{\epsilon} = \int_0^{\frac{1}{2}\beta_c\hbar\omega_D} dx \frac{\tanh x}{x}. \tag{44}$$

Since $\tanh x/x \to 1$ at small values of x, and $\to 1/x$ at large values of x, we can approximate $\int_0^a dx \frac{\tanh x}{x} \approx \int_0^1 dx + \int_1^a dx/x = \ln a + 1$ at $a \gg 1$. A more accurate estimate shows that

$$\int_0^a dx \frac{\tanh x}{x} \approx \ln 2.28x. \tag{45}$$

Hence, we have

$$\frac{1}{gN_0} = \ln 1.14\beta_c\hbar\omega_D \Rightarrow k_B T_c = 1.14\hbar\omega_D e^{-\frac{1}{gN_0}} \tag{46}$$

A more careful analysis shows that the gap function $\Delta(T)$ at $T \to T_c$ behaves

$$\frac{\Delta}{k_B T_c} \sim 3.2\Big(1 - \frac{T}{T_c}\Big)^{\frac{1}{2}} \tag{47}$$

The sketch of the temperature dependence of the gap function $\Delta(T)$ based on the BCS theory is presented in Fig 2.

4.3 Universal relation between Δ and T_c

Compare Eq. 43 and Eq. 46, we have the universal relation for the weak coupling BCS superconductors that

Figure 2: The temperature dependence of the gap function $\Delta(T)$.

$$\frac{\Delta(T=0)}{k_B T_c} \approx 1.76. \tag{48}$$

This is a famous result of BCS theory, and widely used in literature for judge weak or strong coupling superconductivity. For strong coupling superconductors, it has significant deviations: $\frac{\Delta(T=0)}{k_B T_c} \approx 2.3$ and 2.6 for Hg and Pb, respectively. Certainly for high T_c superconductors, it can reach much larger values at the order of 10.

5 The isotope effect

The superconducting transition temperature $T_c = 1.14\hbar\omega_D e^{-\frac{1}{N_0 g}}$. ω_D inversely depends on $M_{ion}^{-\frac{1}{2}}$ due to Newton's equation, hence, $T_c \propto M^{-\frac{1}{2}}$. Historically, this isotope effect has been seen in a variety of superconductors such as Hg, Pb, Mg, Sn, Tl, etc. It was the motivation of electron-phonon mechanism for superconductivity.

6 The McMillan formula

So far, we have neglected the retarded nature of the phonon renormalized effective electron-electron interaction. In fact, such an interaction contains two parts: a screened Coulomb interaction, and a phonon-intermediated interaction. The overall effect is that the interaction is repulsive at $\omega > \omega_D$ and attractive at $\omega < \omega_D$. Let us neglect the angular dependence of $g_{k,k'}$ on $\mathbf{k} \cdot \mathbf{k}'$, but only keep their dependence on the radial part of momentum, which is equivalent to the energy dependence

$$-g(k, k') = V_c - V_{ph}(\frac{\xi_k - \xi_{k'}}{\hbar}). \tag{49}$$

This not a fully treatment to the retarded nature of the frequency dependent phonon-renormalized interaction. Rather, we approximate the interaction by its value at the on-shell frequency, but it is still constant of frequency. Then the gap equation close to T_c is reformatted as

$$\Delta(\xi) = -N_0 \int_{-\Lambda}^{\Lambda} d\xi' \Big(V_c - V_{ph}(\frac{\xi - \xi'}{\hbar})\Big) \Delta(\xi') \frac{\tanh \frac{\beta_c \xi'}{2}}{2\xi'}, \tag{50}$$

where $\Lambda \gg \hbar\omega_D$ is a high energy cut off. Basically, $\Delta(\xi)$ represents the gap function from those electrons with energy ξ to the Fermi surface.

We denote

$$A = -N_0 \int_{-\Lambda}^{\Lambda} d\xi' V_c \Delta(\xi') \frac{\tanh \frac{\beta_c \xi'}{2}}{2\xi'}, \tag{51}$$

then $\Delta(\xi) \approx A$ at $|\xi| \geq \hbar\omega_D$, where $V_{ph}(\omega)$ is already suppressed, and $\Delta(\xi)$ is nearly ξ-independent. Further, we define the average value of Δ over the region of $|\xi| \leq \hbar\omega_D$ is B. Then we have

$$B = N_0 \bar{V}_{ph} \int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi' B \frac{\tanh \frac{\beta_c \xi'}{2}}{2\xi'} + A \approx B N_0 \bar{V}_{ph} \ln \frac{\hbar\omega_D}{k_B T_c} + A, \tag{52}$$

where $\bar{V}_{ph}$ is the average of $V_{ph}(\xi - \xi')$ in the low frequency region.

On the other hand,

$$\begin{aligned} A &= -N_0 \int_{-\Lambda}^{\Lambda} d\xi' V_c \Delta(\xi') \frac{\tanh \frac{\beta_c \xi'}{2}}{2\xi'} \\ &= -N_0 V_c \Big(B \int_{-\hbar\omega_D}^{\hbar\omega_D} + A \int_{\hbar\omega_D}^{\Lambda} + A \int_{-\Lambda}^{-\hbar\omega_D} \Big) d\xi' \frac{\tanh \frac{\beta_c \xi'}{2}}{2\xi'} \\ &= -N_0 V_c \Big(B \ln \frac{\hbar\omega_D}{k_B T_c} + A \ln \frac{\Lambda}{\omega_D} \Big). \end{aligned} \tag{53}$$

Combine the above two equations, we have the following relation

$$\begin{aligned} B\Big(1 - N_0 \bar{V}_{ph} \ln \frac{\hbar\omega_D}{k_B T_c}\Big) &= A \\ A(1 + N_0 V_c \ln \frac{\hbar\omega_c}{\Lambda}) &= -N_0 V_c \ln \frac{\hbar\omega_D}{k_B T_c} B, \end{aligned} \tag{54}$$

hence,

$$\begin{aligned} 1 - N_0 \bar{V}_{ph} \ln \frac{\hbar\omega_D}{k_B T_c} &= -\frac{N_0 V_c \ln \frac{\hbar\omega_D}{k_B T_c}}{1 + N_0 V_c \ln \frac{\hbar\omega_c}{\Lambda}} \\ 1 = N_0 \ln \frac{\hbar\omega_D}{k_B T_c} &\Big(\bar{V}_{ph} - \frac{V_c}{1 + N_0 V_c \ln \frac{\hbar\omega_c}{\Lambda}} \Big). \end{aligned} \tag{55}$$

Hence, we arrive at the famous McMillan formula for T_c

$$T_c = \hbar\omega_D \exp\Big\{ -\frac{1}{N_0 \bar{V}_{ph} - \mu^*} \Big\} \tag{56}$$

where μ^* reads

$$\mu^* = \frac{N_0 V_c}{1 + N_0 V_c \ln \frac{\Lambda}{\omega_D}}. \tag{57}$$

μ^* reflect the renormalized Coulomb interaction to the superconductivity. It weakens the electron-phonon interaction strength from $N_0 \bar{V}_p h \to N_0 \bar{V}_p h - \mu^*$. A few remarks

1. Hence, Coulomb interaction is not sufficient to suppress superconductivity, due to the renormalized effect in the denominator.

2. The isotope effect is weakened due to the dependence of μ^* on ω_D. Enhancing ion mass lowers the Debye frequency ω_D, which certainly lowers T_c. On the other hand, the two energy scales of ω_D and Λ of phonons and Coulomb interaction are more separated, then the Coulomb interaction is more strongly renormalized. Hence μ^* is weakened which compensates partly the effect of lowering ω_D.