Chap 4 The theory of superconductor

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I. SCREENING OF ELECTRON INTERACTION

In Chap 3, we have derived the static dielectric function at long wave length,

$$\epsilon_e(q) = 1 + \frac{k_0^2}{q^2}, \tag{1}$$

where $k_0^2 = 4\pi e^2 D(\varepsilon_F)$ is the Thomas-Fermi wave vector, $D(\varepsilon_F)$ is the density of states at the Fermi energy. As a result, the Coulomb interaction between electrons is modified as

$$V_0(q) = \frac{4\pi e^2}{q^2} \to V(q) = \frac{4\pi e^2}{\epsilon_e(q) q^2} = \frac{4\pi e^2}{q^2 + k_0^2}. \tag{2}$$

By Fourier transforming back to the real space, we have the modified interaction,

$$V(r) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} V(q) = \frac{e^2}{r} e^{-k_0 r}. \tag{3}$$

This is a screened Coulomb interaction with a screening length $1/k_0$.

The electrons in a solid is also under the influence of positive ions. When one brings a surplus electron to a location, it would not only repel the other electrons, but also attract surrounding (mobile) ions. The screening of ions also contributes to the dielectric function. If we approximate the ions as an ion gas, instead of a vibrating lattice, then the analysis in Chap 3 can be applied directly. However, since the ions have a much larger mass M than electron's, they respond to the surplus electron slowly. It is therefore more appropriate to employ the dielectric function at high frequency,

$$\epsilon_i(\omega) = 1 - \frac{\Omega_p^2}{\omega^2}, \tag{4}$$

where $\Omega_p^2 = 4\pi n e^2/M$ is the plasma frequency for the ion gas.

The total dielectric function felt by electrons is given as

$$\epsilon(q,\omega) = 1 + \frac{k_0^2}{q^2} - \frac{\Omega_p^2}{\omega^2}. \tag{5}$$

A rigorous argument that leads to this result can be found in, e.g., Chap 26 of Ashcroft and Mermin's. We will not repeat the analysis here. This dielectric function can be written in an alternative form,

$$\frac{1}{\epsilon(q,\omega)} = \frac{1}{1 + k_0^2/q^2} \cdot \frac{\omega^2}{\omega^2 - \omega(q)^2}, \tag{6}$$

where $\omega(q)^2 = \Omega_p^2/\varepsilon_e(q)$ is the screened ionic plasma frequency, which is of the order of the Debye frequency ω_D.

After including the contribution from mobile ions (or, phonons), the effective Coulomb interaction is

$$V_{eff}(q,\omega) = \frac{4\pi e^2}{\epsilon(q,\omega)q^2} = \frac{4\pi e^2}{q^2+k_0^2}\left[1+\frac{\omega^2(q)}{\omega^2-\omega^2(q)}\right]. \tag{7}$$

This can be regarded as an effective interaction between two electrons: $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ is the difference of their momenta, and $\hbar\omega = |\varepsilon_{k'} - \varepsilon_k|$ is the difference of their energies. Such a statement can be justified rigorously using the manybody formulation of electron-phonon interactions (see, e.g., Chap 17 of Bruus and Flensberg's).

Because of the frequency dependent correction within the square bracket in Eq. (7), the value of the interaction can be *negative*, when $\omega < \omega(q)$. This means that, instead of repulsion, the two electrons could attract each other, when their energy difference is less than $\omega(q)$. This is called **over screening**, and is crucial to the formation of Cooper pairs.

II. COOPER PAIR

For two electrons residing deep inside a Fermi sphere, the over screening cannot take effect, since the two electrons have nowhere to go. Only electrons near the Fermi surface can stretch their legs and attract each other. Cooper showed that such an attraction leads to a bound state, no matter how weak the attraction is. His argument is as follows.

Consider two electrons with the following wave function,

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \psi(\boldsymbol{\rho})e^{i\mathbf{q}\cdot\mathbf{R}}, \tag{8}$$

in which $\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2$ is the relative coordinate, and $\mathbf{R}$ is the center-of-mass (c.m.) coordinate of two electrons. Since the electrons are close to the Fermi surface, according to the Fermi liquid theory, they are nearly free. Therefore, the c.m. state can be considered as a plane wave. Also, we consider only the state with $\mathbf{q} = 0$, which has the lowest c.m. energy.

The paired state satisfies the Schrodinger equation,

$$\left(\frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{V_0}\sum_k V(\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\right)\Psi(\mathbf{r}_1,\mathbf{r}_2) = E\Psi(\mathbf{r}_1,\mathbf{r}_2). \tag{9}$$

Expand the paired state as,

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \sum_k g_k e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}, \tag{10}$$

and substitute it to the Schrodinger equation, one can get

$$2\underbrace{\frac{\hbar^2 k^2}{2m}}_{\varepsilon_k^0} g_k + \frac{1}{V_0}\sum_{k'} V(\mathbf{k}-\mathbf{k}')g_{k'} = Eg_k. \tag{11}$$

The interaction between electrons is assumed to have the simplified form,

$$V(\mathbf{k}-\mathbf{k}') = \begin{cases} -V_e & \text{if } 0 < \varepsilon_k^0 - \varepsilon_F \text{ and } \varepsilon_{k'}^0 - \varepsilon_F < \hbar\omega_c \\ 0 & \text{otherwise,} \end{cases} \tag{12}$$

where $\hbar\omega_c$ is a cut-off energy of the order of the **Debye energy** $\hbar\omega_D$. As a result, Eq. (11) becomes

$$\left(E - 2\varepsilon_k^0\right) g_k = -\frac{V_e}{V_0}\sum_{k'\in \text{ shell}} g_{k'}. \tag{13}$$

One can divide both sides of the equation by $E - 2\varepsilon_k^0$, then sum over g_k to get

$$\begin{aligned} 1 &= -\frac{V_e}{V_0}\sum_{k\in \text{ shell}} \frac{1}{E-2\varepsilon_k^0} \\ &\simeq -V_e D(\varepsilon_F)\int_{\varepsilon_F}^{\varepsilon_F+\hbar\omega_c} d\varepsilon \frac{1}{E-2\varepsilon} \\ &= \frac{V_e}{2} D(\varepsilon_F)\ln\left(\frac{E-2\varepsilon_F-2\hbar\omega_c}{E-2\varepsilon_F}\right), \end{aligned} \tag{14}$$

in which $D(\varepsilon_F)$ is the density of states at Fermi energy, and we have chosen an energy shell with thickness $\hbar\omega_D$ near the surface.

In most conventional superconductors, $V_e D(\varepsilon_F) < 0.3$. One assumes $V_e D(\varepsilon_F) \ll 1$ (weak-coupling approximation) and gets

$$E \simeq 2\varepsilon_F - 2\hbar\omega_c e^{-2/V_e D(\varepsilon_F)}. \tag{15}$$

The second term is the binding energy of the two electrons near the Fermi surface. Notice that the binding energy is not analytic at $V_e = 0$. That is, one would fail to get this result with a theory that treats V_e as a perturbation parameter.

The eigen-states depend on g_k, which is

$$g_k = \frac{C}{E-2\varepsilon_k^0}, \quad \text{where } C = -\frac{V_e}{V_0}\sum_{k'} g_{k'}. \tag{16}$$

Since this function depends on $|\mathbf{k}|$, it is isotropic in k-space. Therefore, the corresponding wave function in r-space (see Eq. (8) with $q = 0$) is also isotropic. In order for the Fermion

wave function to change sign under an exchange of particles, the spin part needs to be a singlet (antisymmetric).

Two remarks are in order: First, the size of the Cooper pair can be calculated via

$$\rho_C^2 = \int d^3\rho |\psi(\rho)|^2 \rho^2. \tag{17}$$

This gives $\rho_C = \frac{2}{\sqrt{3}} \frac{\hbar v_F}{E}$, where E is of the order of $k_B T_c$ (see Ref. 1). Here we give an estimate based on the uncertainty relation,

$$\Delta x \sim \frac{\hbar}{\Delta p} \sim \frac{\hbar}{\Delta E / v_F}, \tag{18}$$

where $\Delta E \sim k_B T_c$. Therefore,

$$\Delta x \sim \frac{\hbar v_F}{k_B T_c} \sim 1 \ \mu m. \tag{19}$$

This is the **coherence length** of the superconductor.

The fraction of electrons condensed by the superconducting (SC) transition is about $T_c/T_F \sim 10^{-4}$. Therefore, the average spacing between condensed electrons is about 10^{-2} μm. Within a Cooper pair radius (1 μm), there are about $1/(10^{-2})^3 \sim 10^6$ Cooper pairs. So the Cooper pairs are very loosely bounded and mix with each other to form a complex (but ordered) web.

Second, if $V(\mathbf{k} - \mathbf{k}')$ varies strongly with the angle $\angle(\mathbf{k}, \mathbf{k}')$, then there may be several bound states. They are anisotropic states with more complicated spin dependence (Ref. 1, p.96).

III. BCS WAVE FUNCTION

BCS theory is different from most of the theoretical investigations in condensed matter physics. It does not solve the wave function from a manybody Hamiltonian, which is an extremely difficult task. Instead, one writes down the wave function directly, then check to see if it fits with the superconductivity in reality.

Let's consider a partially filled energy band with N electrons and M k-states ($2M > N$). A superconductor ground state of these N electrons is likely to be

$$|\Psi_N\rangle = \sum_{\{k\}} g(k_1, k_2, \cdots, k_{N/2}) c^\dagger_{k_1\uparrow} c^\dagger_{-k_1\downarrow} \cdots c^\dagger_{k_{N/2}\uparrow} c^\dagger_{-k_{N/2}\downarrow} |\mathbf{0}\rangle. \tag{20}$$

We have written the operators in a Cooper-pair ready form: if the state $(\mathbf{k}, \uparrow)$ is filled, then the state $(-\mathbf{k}, \downarrow)$ is filled also.

With an insight that later proves to be valid, Schrieffer proposed the following form for the superconductor ground state (see App. A),

$$|\Psi_G\rangle = \prod_{k=k_1,k_2,\cdots,k_M} \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right) |\mathbf{0}\rangle, \tag{21}$$

where u_k and v_k are complex numbers and

$$|u_k|^2 + |v_k|^2 = 1, \quad \text{for each } k. \tag{22}$$

Obviously, $|v_k|^2$ is the probability of the $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$-state to be occupied (not necessarily bounded), while $|u_k|^2$ is the probability of this state to be un-occupied.

What's special about this BCS state is that it is a direct product of Cooper pair states, and every Cooper pair state has the same form. Also, the particle number in this state is *not* fixed, but ranges from 0 to $2M$. This is in sharp contrast to the state in Eq. (20), which has N electrons. This feature turns out to be essential for the superconducting order parameter Δ_k to be non-zero.

The average number of electrons in the BCS can be calculated from

$$\begin{aligned} \bar{N} &= \langle\Psi_G| \sum_{ks} c^\dagger_{ks} c_{ks} |\Psi_G\rangle \\ &= 2\sum_k \langle\Psi_G| c^\dagger_{k\uparrow} c_{k\uparrow} |\Psi_G\rangle. \end{aligned} \tag{23}$$

Out of the many products in the BCS state, only the one with momentum k has non-trivial expectation value,

$$\langle 0| \left(u^*_k + v^*_k c_{-k\downarrow} c_{k\uparrow}\right) c^\dagger_{k\uparrow} c_{k\uparrow} \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right) |0\rangle = |v_k|^2. \tag{24}$$

Therefore,

$$\bar{N} = 2\sum_k |v_k|^2, \tag{25}$$

which is of the order of 10^{23}.

The fluctuation of the particle number δN^2 is

$$\begin{aligned} & \langle \hat{N}^2 \rangle - \bar{N}^2 \\ = & \ 2 \sum_{k_1 k_2} \langle \Psi_G | c^\dagger_{k_1\uparrow} c_{k_1\uparrow} c^\dagger_{k_2\uparrow} c_{k_2\uparrow} | \Psi_G \rangle \\ + & \ 2 \sum_{k_1 k_2} \langle \Psi_G | c^\dagger_{k_1\uparrow} c_{k_1\uparrow} c^\dagger_{k_2\downarrow} c_{k_2\downarrow} | \Psi_G \rangle - 4 \sum_{k_1 k_2} |v_{k_1}|^2 |v_{k_2}|^2 \\ = & \ 4 \sum_{k_1} |v_{k_1}|^2 + 4 \sum_{k_1 \neq k_2} |v_{k_1}|^2 |v_{k_2}|^2 - 4 \sum_{k_1 k_2} |v_{k_1}|^2 |v_{k_2}|^2 \\ = & \ 4 \sum_{k} |u_k|^2 |v_k|^2. \end{aligned} \tag{26}$$

In next section, we will see that $|v_k|^2$ drops from 1 to 0 near the Fermi energy, with a transition width of the order of $k_B T_c$. On the other hand, $|u_k|^2 = 1 - |v_k|^2$ increases from 0 to 1 near the Fermi energy (see Fig. 1). So their product $|u_k|^2 |v_k|^2$ is nonzero around the Fermi energy within a range $k_B T_c$. Therefore,

$$\delta N^2 \sim \frac{T_c}{T_F} \bar{N}, \tag{27}$$

and

$$\frac{\delta N}{N} \sim \left(\frac{T_c}{T_F} \right)^{1/2} \frac{1}{\sqrt{\bar{N}}} \sim 10^{-13}. \tag{28}$$

The fluctuation is quite small for a macroscopic system, but could be significant in a mesoscopic system.

The number of electrons that can bind with each other are those near the Fermi surface. Their number is of the order of $N_C/\bar{N} \sim T_c/T_F \sim 10^{-4}$. These Cooper pairs lower the energy of the whole system by an amount $\sim N_C k_B T_c$. This is a tiny fraction of the total energy,

$$\frac{N_C T_c}{\bar{N} T_F} \sim 10^{-8}. \tag{29}$$

It's impossible for a theorist to account for all of the dynamical details up to such a fine scale (In Chap 2, we have seen how far off one can get in calculating the energy of an electronic system). Therefore, a successful theory must pick up a mechanism that is most crucial for this slight change of energy, while ignoring those that are irrelevant (but could involve much larger energy scales).

IV. BCS PAIRING HAMILTONIAN

The general Hamiltonian for interacting electrons is

$$\begin{aligned} H &= \sum_{k,s} \varepsilon_k^0 c_{k,s}^\dagger c_{k,s} \\ &+ \frac{1}{2V_0} \sum_{ks,k's',q} V_q^{eff} c_{k+q,s}^\dagger c_{k'-q,s'}^\dagger c_{k's'} c_{ks}. \end{aligned} \tag{30}$$

We have included the phonon effect in the effective interaction (see. Eq. (7)) The interaction term describes two electrons in states $(\mathbf{k}, \mathbf{k}')$ being scattered to $(\mathbf{k}+\mathbf{q}, \mathbf{k}'-\mathbf{q})$. We now relabel the momenta and consider two electrons in states $(\mathbf{k}, -\mathbf{k}+\mathbf{q})$ being scattered to $(\mathbf{k}', -\mathbf{k}'+\mathbf{q})$. The interaction term can be decomposed as

$$\begin{aligned} &\frac{1}{2V_0} \sum_{ks,k's',q} V_{kk'}^{eff} c_{k's}^\dagger c_{-k'+q,s'}^\dagger c_{-k+q,s'} c_{ks} \\ &= \frac{1}{V_0} \sum_{kk'} V_{kk'}^{eff} c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger c_{-k\downarrow} c_{k\uparrow} \quad \leftarrow \text{ singlet pairs} \\ &+ \frac{1}{V_0} \sum_{kk'} V_{kk'}^{eff} c_{k'\uparrow}^\dagger c_{-k'\uparrow}^\dagger c_{-k\uparrow} c_{k\uparrow} \quad \leftarrow \text{ triplet pairs} \\ &+ \frac{1}{2V_0} \sum_{ks,k's',q\neq 0} V_{kk'}^{eff} c_{k's}^\dagger c_{-k'+q,s'}^\dagger c_{-k+q,s'} c_{ks}. \end{aligned} \tag{31}$$

If each of the momenta $\mathbf{k}, \mathbf{k}'$ has N possible values, then there are N^2 singlet-pair terms (the same for the triplet-pair terms). For the summation with $q \neq 0$, there are about $N^3 - N^2$ terms. Even though much larger in number, they are random in signs when sandwiched between the BCS state and would cancel with each other. On the contrary, each of the singlet-pair term is negative, so they make coherent contributions: $-\frac{V_e}{V_0} N^2$ (Ref. 2, p.313). The triplet-pair terms are crucial in the p-wave superconductors, but not in the s-wave superconductors. Therefore, we would only keep the singlet-pair terms, and ignore the rest of the terms:

$$H_{BCS} = \sum_{k,s} \varepsilon_k^0 c_{k,s}^\dagger c_{k,s} + \frac{1}{V_0} \sum_{kk'} V_{kk'} c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger c_{-k\downarrow} c_{k\uparrow}, \tag{32}$$

where $V_{kk'} = -V_e$ if the magnitude of both $\varepsilon_k \equiv \varepsilon_k^0 - \varepsilon_F$ and $\varepsilon_{k'} \equiv \varepsilon_{k'}^0 - \varepsilon_F$ are smaller than a cutoff energy $\hbar\omega_c$.

Even though we only keep the singlet-pair terms, the neglected interactions are required for things like collective plasma mode, excitation states within SC energy gap, and damping effect (Ref. 3, p.27).

A. Determination of u_k and v_k

The BCS wave function is essentially a variational wave function, and u_k and v_k are its parameters. They can be determined by the method of variation,

$$\delta\langle\Psi_G|H_{BCS}-\mu\hat{N}|\Psi_G\rangle=0. \tag{33}$$

A Lagrange multiplier (the chemical potential) has been added to fix the total number of particles. First we need to evaluate the expectation values, which involve terms like (see Eq. (24))

$$\langle\Psi_G|c^\dagger_{k\uparrow}c_{k\uparrow}|\Psi_G\rangle=|v_k|^2. \tag{34}$$

It is left as an exercise to show that

$$\langle\Psi_G|c^\dagger_{k'\uparrow}c^\dagger_{-k'\downarrow}c_{-k\downarrow}c_{k\uparrow}|\Psi_G\rangle=u_{k'}v^*_{k'}u^*_kv_k. \tag{35}$$

This is the probability amplitude for electrons scattering from states $(\mathbf{k},-\mathbf{k})$ to states $(\mathbf{k}',-\mathbf{k}')$.

Later we will show that if u_k are taken as real numbers, then v_k would be a real number multiplied by a *k-independent* phase shift $e^{i\phi}$ (ϕ is the phase of the macroscopic condensate). Therefore,

$$\langle\Psi_G|H_{BCS}-\mu\hat{N}|\Psi_G\rangle=2\sum_k\varepsilon_k|v_k|^2+\frac{1}{V_0}\sum_{kk'}V_{kk'}u_{k'}|v_{k'}|u_k|v_k|, \tag{36}$$

where $\varepsilon_k\equiv\varepsilon^0_k-\mu$.

Since $|u_k|^2+|v_k|^2=1$, they can be parameterized as

$$u_k=\cos\theta_k,\quad v_k=\sin\theta_ke^{i\phi}. \tag{37}$$

Then,

$$\langle\cdots\rangle=\sum_k\varepsilon_k(1-\cos2\theta_k)+\frac{1}{4V_0}\sum_{kk'}V_{kk'}\sin2\theta_{k'}\sin2\theta_k. \tag{38}$$

Minimize the expectation value with respect to the parameters, $\partial\langle\cdots\rangle/\partial\theta_k=0$, one will get

$$\tan2\theta_k=-\frac{\frac{1}{V_0}\sum_{k'}V_{kk'}\sin2\theta_{k'}}{2\varepsilon_k}. \tag{39}$$

Before solving this equation, let's introduce the superconductor **gap function**,

$$\begin{aligned}\Delta_k&\equiv-\frac{1}{V_0}\sum_{k'}V_{kk'}\langle c_{-k'\downarrow}c_{k'\uparrow}\rangle \\ &=-\frac{1}{V_0}\sum_{k'}V_{kk'}u_{k'}v_{k'}=-\frac{1}{2V_0}\sum_{k'}V_{kk'}\sin2\theta_{k'}e^{i\phi}.\end{aligned} \tag{40}$$

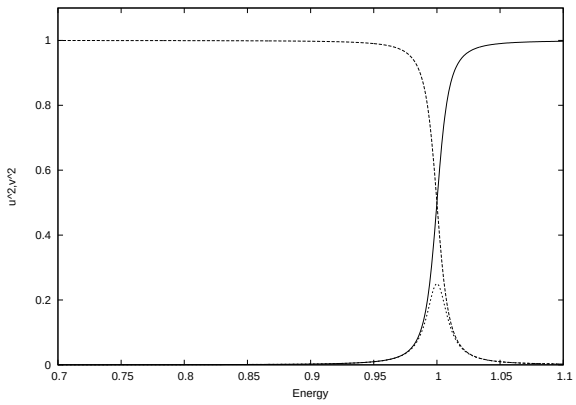

FIG. 1: The functions $|u_k|^2$ (solid line), $|v_k|^2$ (dotted line), and $|u_k|^2|v_k|^2$. The energy is in units of the Fermi energy, and $\Delta/\varepsilon_F = 0.01$.

Notice that Δ_k has the same phase $e^{i\phi}$ as v_k's. From Eq. (39), one has

$$\tan 2\theta_k = \frac{|\Delta_k|}{\varepsilon_k}, \tag{41}$$

which leads to

$$\begin{aligned} \sin 2\theta_k (= 2u_k|v_k|) &= \frac{|\Delta_k|}{E_k}, \\ \cos 2\theta_k (= u_k^2 - |v_k|^2) &= +\frac{\varepsilon_k}{E_k}, \\ \text{where} \quad E_k &\equiv \sqrt{\varepsilon_k^2 + |\Delta_k|^2}. \end{aligned} \tag{42}$$

The positive sign of $\cos 2\theta_k$ is chosen so that $|v_k|^2 \to +1$ as $\varepsilon_k \ll 0$.

From Eq. (40), we then have the self-consistent **gap equation**,

$$\Delta_k = -\frac{1}{2V_0} \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{E_{k'}}. \tag{43}$$

Since the interaction potential $V_{kk'}$ is a constant $-V_e$ when both electrons are near the Fermi surface, the gap function would be k-independent, $|\Delta_k| = \Delta$. Then from Eq. (43), we have

$$1 = \frac{V_e}{2V_0} \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + \Delta^2}} = V_e D(\varepsilon_F) \underbrace{\frac{1}{2} \int_{-\hbar\omega_c}^{\hbar\omega_c} \frac{d\varepsilon}{\varepsilon^2 + \Delta^2}}_{\log\left(\varepsilon + \sqrt{\varepsilon^2+\Delta^2}\right)\Big|_0^{\hbar\omega_c}}. \tag{44}$$

It is not difficult to show that

$$\Delta = \frac{\hbar\omega_c}{\sinh\left(\frac{1}{D(\varepsilon_F)V_e}\right)} \overset{D(\varepsilon_F)V_e \ll 1}{\sim} 2\hbar\omega_c e^{-1/D(\varepsilon_F)V_e}. \tag{45}$$

In realistic cases, we have $D(\varepsilon_F)V_e \leq 0.3$, and the approximation is accurate to within 1% (compare with Eq. (15)).

Finally, the values of u_k and $|v_k|$ are given by

$$\begin{aligned} u_k^2 &= \frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right) \\ |v_k|^2 &= \frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right). \end{aligned} \tag{46}$$

The distribution of $|v_k|^2$ is plotted in Fig. 1. It is the probability of the states $(\mathbf{k}, -\mathbf{k})$ being occupied.

V. EXCITATIONS IN SUPERCONDUCTOR

A. Mean-field theory of superconductor

We now rely on the BCS Hamiltonian to study various properties of a superconductor. Cooper pairs are the main players of superconductivity, and the interactions between them is less crucial. Therefore, we will use the following mean-field approximation (with hindsight, such an approximation proves to be very successful),

$$\begin{aligned} & c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow} c_{-k\downarrow} c_{k\uparrow} \\ \simeq\ & c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow} \langle c_{-k\downarrow} c_{k\uparrow}\rangle + \langle c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\rangle c_{-k\downarrow} c_{k\uparrow} \\ -\ & \langle c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\rangle \langle c_{-k\downarrow} c_{k\uparrow}\rangle. \end{aligned} \tag{47}$$

Notice that this is not the usual MFA introduced in Chap 2, since two creation (or annihilation) operators are grouped together here.

The BCS mean-field Hamiltonian can then be written as,

$$\begin{aligned} H_{BCS} &= \sum_{ks} \varepsilon_k c^\dagger_{ks} c_{ks} - \sum_k \Delta_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - \sum_k \Delta^*_k c_{-k\downarrow} c_{k\uparrow} \\ &- \sum_{kk'} V_{kk'} \langle c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\rangle \langle c_{-k\downarrow} c_{k\uparrow}\rangle. \end{aligned} \tag{48}$$

B. Bogoliubov-Valatin transformation

The quadratic Hamiltonian in Eq. (48) can be diagonalized as follows. First, rewrite the first term of H_{BCS} as,

$$\sum_k \varepsilon_k \left(c^\dagger_{k\uparrow} c_{k\uparrow} - c^\dagger_{k\downarrow} c_{k\downarrow} \right) + \sum_k \varepsilon_k, \tag{49}$$

then the Hamiltonian can be written in a matrix form,

$$H_{BCS} = \sum_k (c^\dagger_{k\uparrow} c_{-k\downarrow}) \begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta^*_k & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} + A, \tag{50}$$

where

$$A = \sum_k \varepsilon_k - \sum_{kk'} V_{kk'} \langle c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow} \rangle \langle c_{-k\downarrow} c_{k\uparrow} \rangle. \tag{51}$$

The 2×2 matrix can be diagonalized with a similarity transformation (the **Bogoliubov-Valatin transformation**),

$$\begin{aligned} \begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta^*_k & -\varepsilon_k \end{pmatrix} &= U \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} U^\dagger, \\ U &= \begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix}, \end{aligned} \tag{52}$$

where $\pm E_k = \pm\sqrt{\varepsilon_k^2 + |\Delta_k|^2}$ are the eigenvalues, and $(\alpha_{1/2}, \beta_{1/2})^T$ are the eigen-vectors of the first/second eigenvalues.

It can be shown that

$$\begin{aligned} |\alpha_1|^2 &= \underbrace{\frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right)}_{|u_k|^2} = |\beta_2|^2, \\ |\beta_1|^2 &= \underbrace{\frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)}_{|v_k|^2} = |\alpha_2|^2. \end{aligned} \tag{53}$$

There is some freedom in choosing the phases of $\alpha_{1/2}$ and $\beta_{1/2}$. Again we assume that u_k are all real, then choose

$$U = \begin{pmatrix} u_k & v_k \\ -v^*_k & u_k \end{pmatrix}. \tag{54}$$

As a result,

$$\begin{aligned} H_{BCS} &= \sum_k (\gamma^\dagger_{k\uparrow}\gamma_{-k\downarrow}) \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix} + A \\ &= \sum_k E_k \left(\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + \gamma^\dagger_{-k\downarrow}\gamma_{-k\downarrow} \right) \underbrace{- \sum_k E_k + A}_{\equiv E_G^S} . \end{aligned} \tag{55}$$

The rotated operators are defined as

$$\begin{aligned} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix} &= \begin{pmatrix} u_k & -v_k \\ v_k^* & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} , \\ \text{or} \quad \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} &= \begin{pmatrix} u_k & v_k \\ -v_k^* & u_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix} . \end{aligned} \tag{56}$$

Two remarks are in order:

First, the quasi-particles created by $\gamma^\dagger_{ks}$ in Eq. (55) do not interact with each other. So H_{BCS} is a Hamiltonian of free (quasi-)particles. The terms in the parenthesis of Eq. (55) are the number operators of the quasi-particles. Therefore, the lowest energy of the BCS Hamiltonian is E_G^S (when there is no quasi-particle). The first excited state has 1 quasi-particle, with an excitation energy E_k. We will call the quasi-particle as a **bogolon**. Notice that it has a definite energy, momentum, and spin, but does not have a definite charge.

Second, it can be shown that

$$\{\gamma_{ks}, \gamma^\dagger_{k's'}\} = \delta_{kk'}\delta_{ss'}. \tag{57}$$

That is, the bogolons are fermions.

C. Condensation energy

Before the superconducting transition, the normal state has energy

$$E_G^N = 2 \sum_{k<k_F} \varepsilon_k. \tag{58}$$

After the transition, the superconduting state has energy (see Eqs. (51) and (55))

$$E_G^S = \sum_k \left(\varepsilon_k - E_k + \Delta_k \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle \right) . \tag{59}$$

Their difference, $\delta E_G = E_G^S - E_G^N$, is called the **condensation energy**. You can check that the normal state energy E_G^N can be obtained from the SC state energy E_G^S with $\Delta_k = 0$.

Recall that the Cooper pair amplitude is

$$\langle c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \rangle = \frac{1}{2} \sin 2\theta_k e^{-i\phi} = \frac{1}{2} \frac{\Delta_k^*}{E_k}. \tag{60}$$

It is nonzero only within a thin shell near the Fermi surface. Let $|\Delta_k| = \Delta$ within that shell, then

$$E_G^S = \sum_k \left(\varepsilon_k - \frac{\varepsilon_k^2}{E_k} \right) - \frac{\Delta^2}{V_e} V_0, \tag{61}$$

where we have used $\frac{V_e}{2V_0} \sum_k \frac{1}{E_k} = 1$ (see Eq. (43) and below).

After some more calculations, one can show that (Ref. 4, p.57)

$$\delta E_G = -\frac{1}{2} D(\varepsilon_F) \Delta^2 V_0. \tag{62}$$

According to an independent thermodynamic analysis, this energy should be equal to $H_c^2/8\pi$, where H_c is the critical magnetic field (at $T = 0$).

D. Density of states

Since the electron operator c_{ks} is connected with the bogolon operator γ_{ks} with an unitary transformation, one expects

$$D_N(\varepsilon) d\varepsilon = D_S(E) dE. \tag{63}$$

This leads to the following density of states near the Fermi energy,

$$\begin{aligned} D_S(E) &= D_N(\varepsilon) \frac{d\varepsilon}{dE} \\ &= \begin{cases} D_N(\varepsilon_F) \frac{E}{\sqrt{E^2 - \Delta^2}} & \text{if } E > \Delta \\ 0 \qquad\qquad \text{if} \quad E < \Delta. \end{cases} \end{aligned} \tag{64}$$

In Fig. 2, one can see that the SC transition opens a gap with a magnitude Δ around the Fermi energy. This is the result of the Cooper instability mentioned earlier in Sec. II.

E. Excited states of the BCS mean-field Hamiltonian

The SC ground state can be defined as the vacuum of bogolons,

$$\gamma_{k\uparrow} |\Psi_G\rangle = \gamma_{-k\downarrow} |\Psi_G\rangle = 0. \tag{65}$$

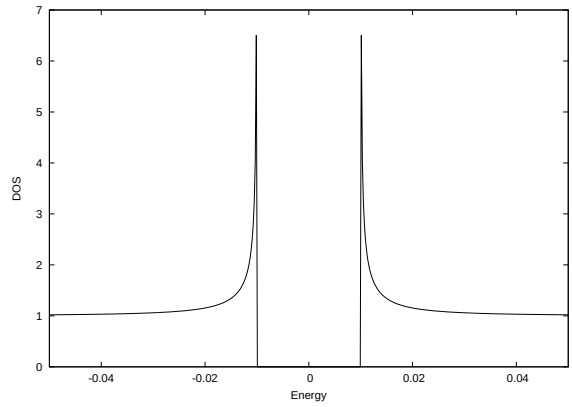

FIG. 2: The density of states (in units of $D_N(\varepsilon_F)$) near the Fermi energy. The energy is in units of ε_F and $\Delta = 0.01$.

This definition is consistent with the BCS ground state $|\Psi_G\rangle$ in Eq. (21). For example, one can check that,

$$\begin{aligned} \gamma_{k\uparrow}|\Psi_G\rangle &= \left(u_k c_{k\uparrow} - v_k c^\dagger_{-k\downarrow}\right) \prod_{k'} \left(u_{k'} + v_{k'} c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\right) |\mathbf{0}\rangle \\ &= 0. \end{aligned} \tag{66}$$

This explains why we write the eigen-vectors in Eq. (54) with those specific forms.

The excited states with one bogolon are

$$\begin{aligned} \gamma^\dagger_{k\uparrow}|\Psi_G\rangle &= c^\dagger_{k\uparrow} \prod_{k'\neq k} \left(u_{k'} + v_{k'} c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\right) |\mathbf{0}\rangle, \\ \gamma^\dagger_{-k\downarrow}|\Psi_G\rangle &= c^\dagger_{-k\downarrow} \prod_{k'\neq k} \left(u_{k'} + v_{k'} c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow}\right) |\mathbf{0}\rangle. \end{aligned} \tag{67}$$

As we have shown earlier (see Eq. (34)), the number of electrons in state-k of the BCS ground state is

$$\begin{aligned} \langle\Psi_G| \sum_s c^\dagger_{ks} c_{ks} |\Psi_G\rangle &= 2|v_k|^2 \\ &= 2 \;\to\; 0 \text{ as energy increases.} \end{aligned} \tag{68}$$

On the other hand, the number of electrons in state-k of the 1-bogolon state is

$$\langle\Psi_G|\gamma_{k\uparrow} \sum_{s'} c^\dagger_{ks'} c_{ks'} \gamma^\dagger_{k\uparrow} |\Psi_G\rangle = 1. \tag{69}$$

Compared to the ground state, the 1-bogolon state has one less electron below the Fermi energy, but one more electron above the Fermi energy. Therefore, the excited state moves one electron from below the Fermi energy to above.

Finally, if one fills the vacuum with bogolons, then it can be shown that

$$\prod_k \gamma_{-k\downarrow}\gamma_{k\uparrow}|\mathbf{0}\rangle = \prod_k (-v_k)\left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|\mathbf{0}\rangle, \tag{70}$$

which is nothing but $|\Psi_G\rangle$ after suitable normalization.

F. Thermal excitations

Once the BCS states are described in terms of the non-interacting bogolons, the quasi-particle excitations can be studied easily. For example, we can study the temperature effect on the gap function,

$$\Delta_k = -\sum_{k'} V_{kk'}\langle c_{-k'\downarrow} c_{k'\uparrow}\rangle.$$

First, write the electron operators in terms of bogolon operators (see Eq. (56)),

$$\begin{aligned} c_{k\uparrow} &= u_k\gamma_{k\uparrow} + v_k\gamma^\dagger_{-k\downarrow} \\ c_{-k\downarrow} &= -v_k\gamma^\dagger_{k\uparrow} + u_k\gamma_{-k\downarrow}. \end{aligned} \tag{72}$$

Then,

$$\langle c_{-k\downarrow} c_{k\uparrow}\rangle = -u_k v_k\langle\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + \gamma^\dagger_{-k\downarrow}\gamma_{-k\downarrow} - 1\rangle. \tag{73}$$

Terms like $\langle\Psi_G|\gamma^\dagger_{k\uparrow}\gamma^\dagger_{-k\downarrow}|\Psi_G\rangle$ are zero. This is true also for n-bogolon excited states as well, where n is any positive integer. Therefore, the thermal average $\langle\gamma^\dagger_{k\uparrow}\gamma^\dagger_{-k\downarrow}\rangle = 0$.

As mentioned earlier, the bogolons are free fermions. Therefore (same for the $(-\mathbf{k}\downarrow)$ bogolon),

$$\langle\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow}\rangle = f(E_k) = \frac{1}{e^{E_k/k_BT}+1}. \tag{74}$$

This is a Fermi distribution with zero chemical potential. The average bogolon number reduces to zero as $T \to 0$.

The gap function now becomes

$$\Delta_k = -\frac{1}{V_0}\sum_{k'} V_{kk'}u_{k'}v_{k'}\left[1 - 2f(E_{k'})\right]. \tag{75}$$

Use Eq. (60), and let $\Delta_k = \Delta e^{i\phi}, V_{kk'} = -V_e$ as before, then we have the gap equation at finite temperature,

$$1 = \frac{V_e}{2V_0} \sum_{k\in\text{shell}} \frac{1}{E_k} \tanh \frac{E_k}{2k_BT}. \tag{76}$$

This is a generalization of Eq. (44).

G. Determine the critical temperature T_c

At critical temperature $T = T_c$, $E_k = \varepsilon_k$, so

$$\begin{aligned} 1 &= V_e D(\varepsilon_F) \int_0^{\hbar\omega_c} d\varepsilon \frac{1}{\varepsilon} \tanh \frac{\varepsilon}{2k_BT_c} \\ &\simeq V_e D(\varepsilon_F) \ln \left(\frac{2e^\gamma}{\pi} \frac{\hbar\omega_c}{k_BT_c} \right), \end{aligned} \tag{77}$$

where $\gamma \simeq 0.557$ is the Euler constant. This leads to (see Eq. (45))

$$k_BT_c = \underbrace{\frac{2e^\gamma}{\pi}}_{\simeq 1.13} \hbar\omega_c e^{-1/D(\varepsilon_F)V_e} = \frac{1.13}{2}\Delta(0). \tag{78}$$

That is,

$$\frac{2\Delta(0)}{k_BT_c} \simeq 3.53. \tag{79}$$

This is the famous result predicted by the BCS theory. Most of the conventional superconductors have this ratio within the range of $3.0 \sim 4.5$. For example, the value of tin is 3.46; the value of lead is 4.29. Superconductors with this ratio larger than 4.5 are called *strong-coupling superconductors*. Their explanation requires a modified BCS theory (Eliashberg's theory).

H. Temperature dependence of the superconducting gap $\Delta(T)$

Let's go back to the gap function at $T < T_c$,

$$\begin{aligned} 1 &= V_e D(\varepsilon_F) \int_0^{\hbar\omega_c} d\varepsilon \frac{(\tanh \sqrt{\varepsilon^2 + \Delta^2}/2k_BT)}{\sqrt{\varepsilon^2 + \Delta^2}} \\ &= V_e D(\varepsilon_F) \int_0^{\frac{\hbar\omega_c}{k_BT}} dx \frac{\tanh \frac{1}{2}\left[x^2 + (\Delta/k_BT)^2\right]^{1/2}}{\left[x^2 + (\Delta/k_BT)^2\right]^{1/2}}. \end{aligned} \tag{80}$$

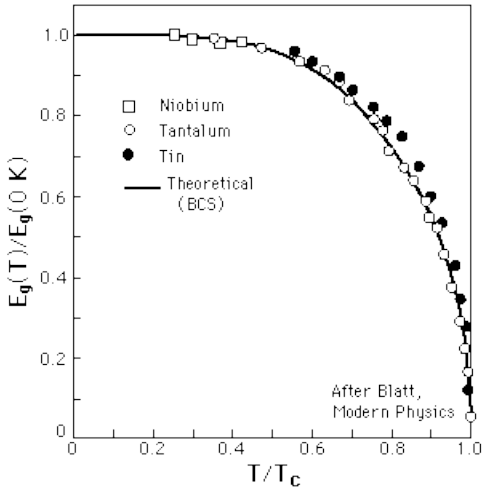

FIG. 3: Superconducting energy gap reduces to zero as the temperature approached the critical temperature [the figure is adopted from hyperphysics website].

At low temperature with $\hbar\omega_c/k_BT_c \gg 1$, the upper limit of the integral can be extended to infinity. The integral is then only a function of $\Delta(T)/k_BT$. Therefore,

$$\frac{\Delta(T)}{\Delta(0)} = f\left(\frac{T}{T_c}\right). \tag{81}$$

The functional form of f is the same for different materials. Fig. 3 shows the temperature dependence of $\Delta(T)$ calculated from the gap equation above. When T is near T_c, it can be shown that

$$\frac{\Delta(T)}{\Delta(0)} \simeq 1.74\left(1-\frac{T}{T_c}\right)^{1/2}. \tag{82}$$

VI. MEISSNER EFFECT

A. London theory of the Meissner effect

London showed that, if the electric current density is proportional to the vector potential (CGS),

$$\mathbf{J}^e(\mathbf{r}) = -\frac{c}{4\pi\lambda_L^2}\mathbf{A}(\mathbf{r}), \tag{83}$$

then from the Ampere equation $\nabla\times\mathbf{B} = \frac{4\pi}{c}\mathbf{J}^e$, we should get

$$\nabla^2\mathbf{B} - \frac{1}{\lambda_L^2}\mathbf{B} = 0. \tag{84}$$

This implies the repulsion of magnetic field from a superconductor.

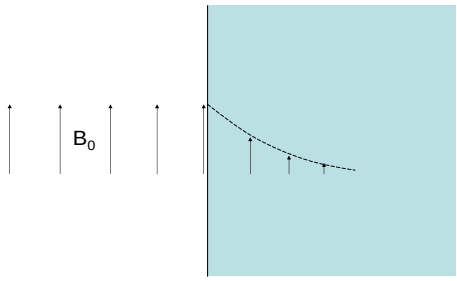

FIG. 4: A uniform magnetic field cannot penetrate deep inside a superconductor.

For example, in Fig. 4 there is a semi-infinite SC in the region $x > 0$. Assume there is a uniform magnetic field $B_0\hat{z}$ outside the SC and is parallel to the surface of the SC, then from Eq. (84) and the boundary condition at $x = 0$, we get (for $x > 0$)

$$B(x) = B_0 e^{-x/\lambda_L}. \tag{85}$$

That is, the static magnetic field cannot penetrate deep into the bulk of the SC. The parameter λ_L is called the **London penetration depth**, which is of the order of 0.1 μm for type-I superconductor.

B. Microscopic theory of the London equation

To study the connection between external potential $\mathbf{A}$ and electric current, one uses the Kubo formula in Chap 3:

$$\langle J^e_\alpha(\mathbf{q},\omega)\rangle = \chi^e_{\alpha\beta}(\mathbf{q},\omega)A_\beta(\mathbf{q},\omega), \tag{86}$$

where

$$\chi^e_{\alpha\beta}(\mathbf{q},\omega) = -e^2\left[\delta_{\alpha\beta}\frac{\rho(\mathbf{q},\omega)}{m} + \chi^p_{\alpha\beta}(\mathbf{q},\omega)\right]. \tag{87}$$

The paramagnetic response function is

$$\chi^p_{\alpha\beta}(\mathbf{q},\omega) = -\frac{i}{V_0}\int_0^\infty dt e^{i\omega t}\langle[J_\alpha(\mathbf{q},t), J_\beta(-\mathbf{q},0)]\rangle. \tag{88}$$

In the following discussion, we will show that, at zero temperature, a static $\mathbf{A}(\mathbf{r}) = \mathbf{A}_q e^{i\mathbf{q}\cdot\mathbf{r}}$ at long wave length ($q \to 0$) would not generate a paramagnetic current. Therefore, in this case the electric current in a SC is entirely the diamagnetic current.

In Eq. (88), we have terms of the form ($T = 0$),

$$\begin{aligned} & \langle J_\alpha(\mathbf{q},t)J_\beta(-\mathbf{q},0) - J_\beta(-\mathbf{q},0)J_\alpha(\mathbf{q},t)\rangle_G \\ = & \sum_l \langle\Psi_G|J_\alpha(\mathbf{q})e^{-iE_l t}|\Psi_l\rangle\langle\Psi_l|J_\beta(-\mathbf{q})|\Psi_G\rangle \\ - & \sum_l \langle\Psi_G|J_\beta(-\mathbf{q})|\Psi_l\rangle\langle\Psi_l|e^{iE_l t}J_\alpha(\mathbf{q})|\Psi_G\rangle, \end{aligned} \tag{89}$$

where $\{|\Psi_l\rangle\}$ form a complete set, and E_l is the eigenenergy of state $|\Psi_l\rangle$ (the ground state energy is set to zero). Recall that the current operator is

$$\mathbf{J}(\mathbf{q}) = \frac{\hbar}{m}\sum_{ks}\left(\mathbf{k}+\frac{\mathbf{q}}{2}\right)c^\dagger_{ks}c_{k+q,s}. \tag{90}$$

It's always easier to let the operators act on the ground state, so we will use the dual relation,

$$\langle\Psi_G|J_\alpha(\mathbf{q}) = \left[J_\alpha(-\mathbf{q})|\Psi_G\rangle\right]^\dagger, \tag{91}$$

At the core of the calculation is

$$\begin{aligned} & c^\dagger_{ks}c_{k-q,s}|\Psi_G\rangle \\ = & \left(u_k\gamma^\dagger_{ks} + v^*_k\gamma_{-k-s}\right)\left(u_{k-q}\gamma_{k-q,s} + v_{k-q}\gamma^\dagger_{-k+q,-s}\right)|\Psi_G\rangle \\ = & u_k v_{k-q}\underbrace{\gamma^\dagger_{ks}\gamma^\dagger_{-k+q,-s}|\Psi_G\rangle}_{\text{an excited state } |\Psi_l\rangle} + |v_k|^2\delta_{q,0}|\Psi_G\rangle. \end{aligned} \tag{92}$$

After some straightforward calculations, we have

$$\begin{aligned} & \langle\Psi_G|J_\alpha(\mathbf{q},t)J_\beta(-\mathbf{q},0)|\Psi_G\rangle \\ = & \frac{2\hbar^2}{m^2}\sum_{ks}\left(k_\alpha - \frac{q_\alpha}{2}\right)\left(k_\beta - \frac{q_\beta}{2}\right) \\ \times & \left(u_k^2|v_{k-q}|^2 - u_k u_{k-q}v_k v^*_{k-q}\right)e^{-i(E_k+E_{k-q})t}, \end{aligned} \tag{93}$$

where $E_q + E_{k-q}$ is the eigenenergy of the 2-bogolon state in Eq. (92). For the other term in the commutator, one just use the result in Eq. (93), but exchange α with β, and $\mathbf{q}$ with $-\mathbf{q}$,

$$\begin{aligned} & \langle\Psi_G|J_\beta(-\mathbf{q},0)J_\alpha(\mathbf{q},t)|\Psi_G\rangle \\ = & \frac{2\hbar^2}{m^2}\sum_{ks}\left(k_\alpha + \frac{q_\alpha}{2}\right)\left(k_\beta + \frac{q_\beta}{2}\right) \\ \times & \left(u_k^2|v_{k+q}|^2 - u_k u_{k+q}v_k v^*_{k+q}\right)e^{i(E_k+E_{k+q})t}. \end{aligned} \tag{94}$$

Shift $\mathbf{k}$ to $\mathbf{k}-\mathbf{q}$, and combine with Eqs. (93), and carry out the integration over time to get ($\omega = 0$)

$$\begin{aligned} \chi^p_{\alpha\beta}(\mathbf{q}) &= -\frac{\hbar^2}{m^2}\frac{2}{V_0}\sum_k \left(k_\alpha - \frac{q_\alpha}{2}\right)\left(k_\beta - \frac{q_\beta}{2}\right) \\ &\times \frac{|u_{k-q}v_k - u_k v_{k-q}|^2}{E_k + E_{k-q}}. \end{aligned} \tag{95}$$

The numerator (sometimes called the **coherence factor**) is (see Eq. (46))

$$\begin{aligned} & |u'v \pm uv'|^2 \\ &= \frac{1}{4}\left(\sqrt{1+\frac{\varepsilon'}{E'}}\sqrt{1-\frac{\varepsilon}{E}} \pm \sqrt{1+\frac{\varepsilon}{E}}\sqrt{1-\frac{\varepsilon'}{E'}}\right)^2 \\ &= \frac{1}{2}\left(1 - \frac{\varepsilon\varepsilon'}{EE'} \pm \frac{\Delta^2}{EE'}\right). \end{aligned} \tag{96}$$

It is zero when $q \to 0$. Therefore, the paramagnetic response function $\chi^p_{\alpha\beta}(0)$ in Eq. (95) vanishes as a result.

Finally, we have

$$\langle \mathbf{J}^e \rangle = -\frac{e^2\rho}{mc}\mathbf{A}. \tag{97}$$

This is the London equation. Compare with Eq. (83), one gets

$$\lambda_L = \left(\frac{mc^2}{4\pi\rho e^2}\right)^{1/2} = \frac{c}{\omega_p}, \quad \omega_p = \sqrt{\frac{4\pi\rho e^2}{m}}. \tag{98}$$

VII. FLUX QUANTIZATION THROUGH A SUPERCONDUCTING RING

The magnetic flux Φ inside a SC ring must be quantized. Such a quantization was first suggested by Onsager. Here we follow the discussion in Byers and Yang's paper (Ref. 5). For electrons in a metal ring, the Schrodinger equation is

$$\sum_i \frac{1}{2m}\left[\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right]^2 \Psi + V\Psi = E\Psi, \tag{99}$$

where $\mathbf{A}$ is the vector potential due to the magnetic flux, and V could include electron-phonon and electron-electron interactions.

Due to the Meissner effect, $\nabla \times \mathbf{A} = 0$ inside the superconductor. This implies

$$\mathbf{A}(\mathbf{r}) = \nabla\chi \ \text{ inside the SC}, \tag{100}$$

the scalar function χ is not single-valued since

$$\oint \mathbf{A} \cdot d\boldsymbol{\ell} = \Delta\chi = \Phi. \tag{101}$$

As a pure gauge, χ can be eliminated from the Schrodinger equation by a gauge transformation,

$$\Psi \;\rightarrow\; \Psi' = \Psi e^{i\sum_i \frac{e}{\hbar c}\chi(\mathbf{r}_i)}. \tag{102}$$

Then,

$$\mathbf{p}_i\Psi' = e^{i\sum_i \frac{e}{\hbar c}\chi(\mathbf{r}_i)}\left(\mathbf{p}_i + \frac{e}{c}\nabla_i\chi\right)\Psi. \tag{103}$$

As a result, Eq. (99) becomes

$$\left(\sum_i \frac{p_i^2}{2m}\right)\Psi' + V\Psi' = E\Psi'. \tag{104}$$

Even though not in the Schrodinger equation, $\mathbf{A}$ changed the boundary condition of the wave function: Ψ' now is not single-valued. For example, after circling electron-p around the ring once (the other electrons remain fixed),

$$\Psi' \;\rightarrow\; e^{i\frac{e}{\hbar c}\Phi}\Psi'. \tag{105}$$

The extra factor is periodic in Φ with a period $\Phi_0 = \frac{hc}{e}$.

As a result, the eigenvalues E_n, and the partition function $Z = \sum_n e^{-\beta E_n}$, are all periodic in Φ. Also, one expects

$$E_n(-\Phi) = E_n(\Phi) \;\rightarrow\; Z(-\Phi) = Z(\Phi). \tag{106}$$

Therefore, $\partial Z/\partial\Phi = 0$ at $\Phi = 0$ and $\Phi_0/2$.

The Aharonov-Bohm phase results in the following shift of electron wavevector: $kL \rightarrow kL + 2\pi\Phi/\Phi_0$. Therefore,

$$\frac{1}{L}\frac{\partial E_n}{\hbar\partial k} = -\frac{c}{e}\frac{\partial E_n}{\partial\Phi}, \tag{107}$$

and the current circling the ring is

$$\begin{aligned} I \;&=\; -\frac{e}{L}\sum_k \frac{\partial E_n}{\hbar\partial k}\frac{e^{-\beta E_n}}{Z} \\ &=\; \frac{c}{\beta}\frac{\partial \ln Z}{\partial\Phi} = c\frac{\partial F}{\partial\Phi}, \end{aligned} \tag{108}$$

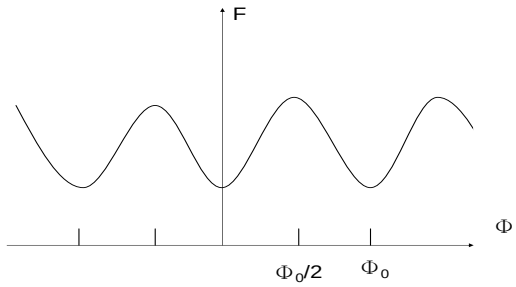

FIG. 5: The free energy of s SC ring is a periodic function of the threading magnetic flux.

where F is the free energy. It follows that $I = 0$ at $\Phi = 0$ and $\Phi_0/2$. A schematic plot of the free energy is shown in Fig. 5. One can see that the system is in stable equilibrium when $\Phi = \ell\Phi_0$ (ℓ is an integer), and the flux would be quantized at these values. If the applied flux does not satisfy this condition, then the current in Eq. (108) would flow. The current won't stop until the induced magnetic flux plus the external flux equals a quantized value.

However, experiments found that the flux inside a SC ring is quantized at $\Phi_0/2$, instead of Φ_0. This is of course due to the Cooper pair (which has charge $2e$), but what's wrong with the very general argument above?

Let's consider a thin ring with circumference L. The coordinate inside the ring is denoted as x. Since the two electrons of a Cooper pair are correlated, the condition

$$\Psi'(x_1, \cdots, x_p + L, \cdots) = \Psi'(x_1, \cdots, x_p, \cdots) \tag{109}$$

can be relaxed to (p, q are paired)

$$\Psi'(x_1, \cdots, x_p + L, \cdots, x_q + L, \cdots) = \Psi'(x_1, \cdots, x_p, \cdots, x_q, \cdots). \tag{110}$$

This allows the possibility of

$$\Psi'(x_1, \cdots, x_p + L, \cdots) = -\Psi'(x_1, \cdots, x_p, \cdots). \tag{111}$$

For example, consider the wave function of a Cooper pair in a ring (see Eqs. (8) and (10))

,

$$\psi = \left(\sum_l g_l e^{il(\phi_1 - \phi_2)} \right) e^{iM\frac{\phi_1+\phi_2}{2}}, \tag{112}$$

where l is the quantum number for the relative motion, and M is the angular momentum of the c.m. motion. If $M = 2m$ is an even integer, then

$$\psi = \sum_l g_l e^{i(m+l)\phi_1} e^{i(m-l)\phi_2}. \tag{113}$$

If $M = 2m + 1$, then

$$\psi = \sum_l g_l e^{i(m+\frac{1}{2}+l)\phi_1} e^{i(m+\frac{1}{2}-l)\phi_2}. \tag{114}$$

For the second case, a single-particle wave function changes sign when $\phi_{1,2} \to \phi_{1,2} + 2\pi$, but the wave function of the Cooper pair does not change sign. That is, a change of flux by $\Phi_0/2$ is enough to bring the system back to its initial state, so the free energy would be periodic in half of the flux quantum (see Ref. 3, p.242).

A. Persistent in a normal metal ring

Consider a clean metal ring at low temperature (but not superconducting), so that an electron would be able to maintain its phase coherence after circling the ring once. In reality the magnetic field can penetrate through the metal and the pure gauge condition (Eq. (100)) is not strictly valid. Nevertheless, the analysis above Eq. (108) still applies approximately, so that the free energy is periodic in Φ_0.

Since there is no Meissner effect to screen out the magnetic flux, the flux threading through the ring does not have to be quantized. Therefore, in general $\partial F/\partial\Phi \neq 0$, and according to Eq. (108) there is a current inside the ring. This is called a **persistent current** since it persists as long as the external flux is there. Such a non-dissipative current has been verified by experiments in 1989.

APPENDIX A: CONNECTION WITH COHERENT STATE

1. Boson coherent state

Firstly, a short review of boson coherent state:

$$\begin{aligned} |\lambda\rangle &= e^{-|\lambda|^2/2} e^{\lambda a^\dagger} |0\rangle \\ &= e^{-|\lambda|^2/2} \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle. \end{aligned} \tag{A1}$$

It is an eigenstate of the annihilation operator,

$$a|\lambda\rangle = \lambda|\lambda\rangle, \quad \text{and} \quad \bar{n} = \langle\lambda|\hat{n}|\lambda\rangle = |\lambda|^2. \tag{A2}$$

In general,

$$\lambda = |\lambda|e^{i\theta} = \sqrt{\bar{n}}e^{i\theta}. \tag{A3}$$

It's not difficult to see from Eq. (A1) that

$$\frac{1}{i}\frac{\partial}{\partial\theta}|\lambda\rangle = \hat{n}|\lambda\rangle. \tag{A4}$$

Therefore $\hat{n} \simeq \frac{1}{i}\frac{\partial}{\partial\theta}$, and just like the uncertainty relation, we have

$$\Delta n \Delta\theta \geq \frac{1}{2}. \tag{A5}$$

That is, one cannot fix the values of n and θ simultaneously.

Note: The relation $\hat{n} \simeq \frac{1}{i}\frac{\partial}{\partial\theta}$ cannot be exact. If it is, then

$$[\hat{n}, \hat{\theta}] = \frac{1}{i}, \tag{A6}$$

which leads to

$$(n - n')\langle n|\hat{\theta}|n'\rangle = \frac{1}{i}\delta_{nn'}. \tag{A7}$$

This leads to contradiction when $n = n'$. That is why there can be no angle (or phase) operator in quantum mechanics. However, for a system with large n, when the fluctuation (uncertainty) is of little significance, the angle operator can be used in an approximate manner.

2. BCS coherent state

If we consider the Cooper pair as a single entity and define

$$b_k^\dagger = c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger, \tag{A8}$$

then

$$[b_k, b_{k'}^\dagger] = (1 - \hat{n}_{k\uparrow} - \hat{n}_{-k\downarrow})\,\delta_{kk'}. \tag{A9}$$

Therefore, the new entity is not exactly a boson with the usual commutation relation. Also, $\left(b_k^\dagger\right)^2 = 0$, so it still has the fermion character.

How did Schrieffer arrive at the BCS wave function in Eq. (21)? He pictured the BCS state as a coherent state of Cooper pairs and wrote

$$\begin{aligned} |\Psi_{BCS}\rangle &= e^{\sum_k \alpha_k b_k^\dagger}|0\rangle \\ &= \prod_k e^{\alpha_k b_k^\dagger}|0\rangle \quad \text{due to Eq. (A9)} \\ &= \prod_k \left(1+\alpha_k b_k^\dagger\right)|0\rangle. \end{aligned} \tag{A10}$$

After suitable normalization, we then have the BCS state in Eq. (21)

When expanded in states with n Cooper pairs, we have

$$|\Psi_{BCS}\rangle = \sum_{n=0}^{M} a_n e^{in\phi}|n\rangle. \tag{A11}$$

This is sharply peaked around $\bar{n}$. Similar to Eq. (A4), one has

$$\frac{1}{i}\frac{\partial}{\partial\phi}|\Psi_{BCS}\rangle = \hat{n}|\Psi_{BCS}\rangle. \tag{A12}$$

Also,

$$\langle\Psi_{BCS}(\phi')|\Psi_{BCS}(\phi)\rangle = \sum_{n_p=0}^{M} e^{in(\phi-\phi')}|a_n|^2. \tag{A13}$$

For a macroscopic system, due to the rapid oscillation of $e^{i\bar{n}(\phi-\phi')}$, this product drops rapidly to zero as soon as $\phi \neq \phi'$.

APPENDIX B: CONNECTION WITH SPONTANEOUS SYMMETRY BREAKING (SSB)

1. SSB in a ferromagnet (FM)

The following ferromagnetic Heisenberg Hamiltonian is invariant under SO(3) rotations,

$$H = -\sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{B1}$$

However, its ground state is a ferromagnetic state,

$$|\Psi_0\rangle = |\uparrow\uparrow\uparrow\cdots\uparrow\rangle, \tag{B2}$$

which only has SO(2) symmetry (around the magnetization axis). So the symmetry of the ground state is *not* the same as that of the Hamiltonian. This is called **Spontaneous Symmetry Breaking** (SSB).

The manifold of the FM ground state is

$$SO(3)/SO(2) = S^2, \quad \text{a sphere.} \tag{B3}$$

The magnetization $\mathbf{m}$ of a ground state points to a particular point on this sphere. It costs no energy to globally rotate $\mathbf{m}$ around S^2, so the excitation energy of a spin wave approaches zero (gapless) at long wavelength limit. This is a special case of the Goldstone theorem.

Goldstone theorem states that, if a continuous symmetry (with a group manifold G) is broken (to a smaller manifold H), then there will be *gapless* excitations. These gapless excitations are called the **Nambu-Goldstone mode** (NG mode). The number of Nambu-Goldstone modes is equal to, or less than, dim G − dim H (Nayak's lecture note). For example (h is an external magnetic field),

- FM: SO(3) → SO(2), # of NG mode = 1.
- AFM: SO(3) → SO(2), # of NG mode = 2.
- FM+h: SO(2) → SO(2), # of NG mode = 0.

2. SSB in a BCS state

The BCS Hamiltonian in Eq. (32) conserves charge,

$$[H_{BCS}, \hat{N}] = 0, \tag{B4}$$

where $\hat{N} = \sum_{ks} c^\dagger_{ks} c_{ks}$, which is a generator of U(1) symmetry (see below). However, the BCS ground state does not conserve charge,

$$\langle \Psi_{BCS} | c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} | \Psi_{BCS} \rangle \neq 0. \tag{B5}$$

So the U(1) symmetry is broken (to Z_2, to be precise).

If $|\Psi_{BCS}\rangle$ has a global phase ϕ, i.e.,

$$|\Psi_{BCS}(\phi)\rangle = \prod_k \left(u_k + |v_k| e^{i\phi} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right) |\mathbf{0}\rangle, \tag{B6}$$

then

$$e^{i\chi\hat{N}}|\Psi_{BCS}(\phi)\rangle = |\Psi_{BCS}(\phi + 2\chi)\rangle. \tag{B7}$$

So $e^{i\chi\hat{N}}$ is the generator of a U(1) symmetry. The rotated coherent state overlaps little with $|\Psi_{BCS}(\phi)\rangle$ (See App. A). A ground state picks up a particular phase ϕ_0, and slight deviation from this point costs no energy (gapless phase mode).

In reality, there is no gapless phase mode in a superconductor. This NG mode would couple with a massless photon field (U(1) gauge field), so that the former disappears, and the latter becomes massive. This is called the **Anderson-Higgs mechanism**. A massive photon has three degrees of freedom, which is equal to the original degrees of freedom (one from the NG mode, two from the massless photon). Massive longitudinal photons are plasmons (with an energy gap), and massive transverse photons cause the Meissner effect. More discussions on this topic can be found in Ref. 6.

Prob. 1 Calculate

$$\sum_{k_1 k_2} \langle \Psi_G | c^\dagger_{k_1\uparrow} c_{k_1\uparrow} c^\dagger_{k_2\uparrow} c_{k_2\uparrow} | \Psi_G \rangle$$

and

$$\sum_{k_1 k_2} \langle \Psi_G | c^\dagger_{k_1\uparrow} c_{k_1\uparrow} c^\dagger_{k_2\downarrow} c_{k_2\downarrow} | \Psi_G \rangle,$$

where

$$|\Psi_G\rangle = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right) |\mathbf{0}\rangle.$$

Prob. 2 Show that

$$\langle \Psi_G | c^\dagger_{k_1\uparrow} c^\dagger_{-k_1\downarrow} c_{-k_2\downarrow} c_{k_2\uparrow} | \Psi_G \rangle = u_{k_1} v^*_{k_1} u^*_{k_2} v_{k_2}.$$

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