7.2 : Superconductivity

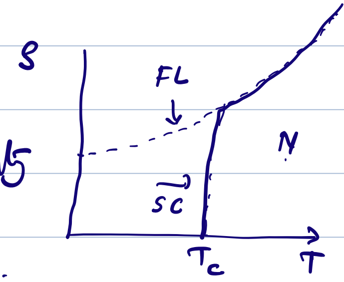
1. Physical Properties of Superconductivity.
2. Cooper pair
3. BCS Theory
4. Superfluid density, Meissner Effect.

Refs: 1. P. Phillips.
2. M. Tinkham, Introduction to Superconductivity.

Superconductivity, as we probably know by now, is a state of a metal at low temperature, where the resistivity becomes absolutely zero. It was discovered in the lab of Kammerling Onnes in Leiden in 1911 in Hg-element. There are many other properties of this state which make this phase a unique one, as we will discuss in this course. The theory for the superconductivity is also unique - very different from magnetism, density wave order etc and the theory came in 1957, called the BCS theory. It turns out any Fermi-liquid metal is unstable to an attractive potential, and becomes superconductor, but the transition temperature changes from material to material. In 1987, a new family of superconductors - namely high-Tc or unconventional superconductors are discovered in copper oxide material. In 2007, a iron-arsenic based unconventional superconductors are also discoverd. By now, there are more unconventional superconductor families are known. It is suspected that the mechanism of superconductivity in the unconventional superconductors which will not be discussed in this course.

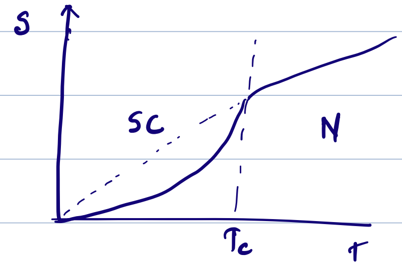
Experimental Properties of Superconductors:

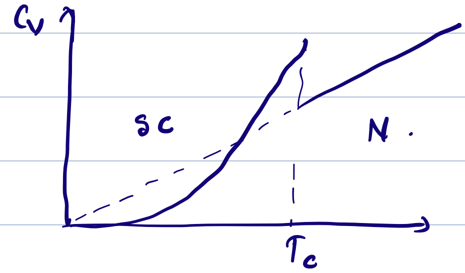
(a) Zero-resistance: The main signature of superconductivity is the complete vanishing of resistance below a characteristic temperature T_c. This is not a coincidence of a perfect conductor without any scattering process, but a new state of matter where all conduction electrons go to a macroscopic ("collective") state which can avoid "all" scattering process - saying that there is no other states in the nearby energy where the electrons can scatter to. So, there must be a finite gap between the superconducting ground state and the excited state. Indeed there is a finite gap as obtained from the specific heat data and also in the density of states measured in the scanning tunneling microscopy (STM) data, and others.



The non-superconducting state is called the normal state.

(b) Energy Gap: In the superconducting (SC) state, the entropy decreases continuously but has a "kink" at T_c, signalling that the specific heat must have a jump at T_c. This is the criterion for a 2nd order phase transition - to a macroscopically ordered state.





The specific heat has a exponential growth at low-temperature · which is a signature of an energy gap, denoted by Δ.
This can be obtained as follows

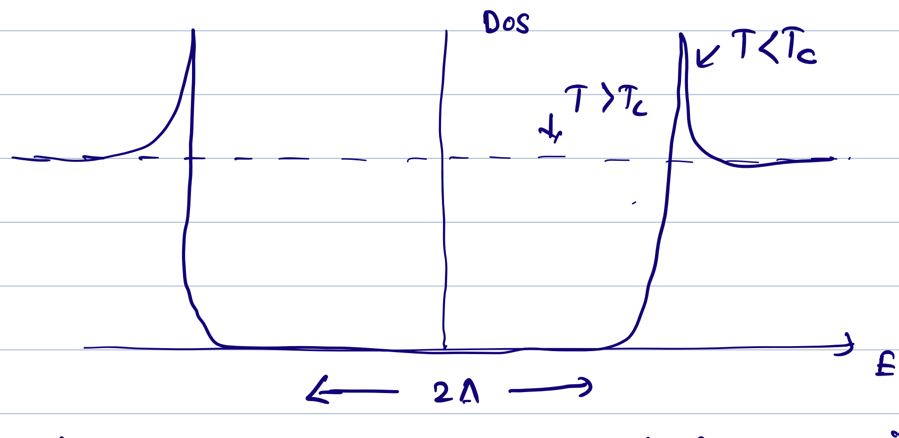
$$C_V = \frac{\partial}{\partial T}\int \frac{\varepsilon_k \, d\varepsilon_k}{(e^{\beta(\varepsilon_k-\mu)}+1)} \xrightarrow{T\to 0} \frac{\partial}{\partial T}\int \varepsilon_k \, e^{-\beta(\varepsilon_k-\mu)} d\varepsilon_k$$

If $\varepsilon_k - \mu \approx \Delta$, a gap in the single particle state near the fermi level, then we get

$$C_V \sim e^{-\beta\Delta}.$$

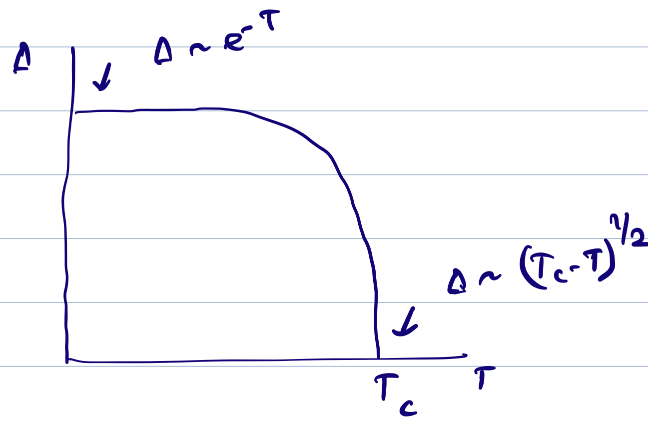
- The formation of a single particle gap at the Fermi level generally means the electrons near the fermi level has formed a bound state of some sort - and Δ is the energy cost to break the bound state. The bound state formation lower the total energy (Free energy) of the ground state.

  The gap manifests in the density of states



All the electrons near the fermi level, are now "condensed"/ formed bound state and goes to the coherence peak just above the 2Δ energy gap.

- As we increase temperature, the bound state of electrons weakens – the number of electrons go to the bound state decreases, which essentially decreases the energy gap also in a self-consistent way. Therefore, both the coherence peak height in the above density of state as well as the gap between the coherence peaks decreases. The Δ vs T plot goes like



The gap has an exponentially slow dependence at $T \to 0$, while it has a powerlaw dependence near T_c, with a mean field exponent of $1/2$. In simple metals the experimental value of exponent matches quite well with this mean-field exponent – suggesting that the mean-field theory works quite well here.

There is also a "universal like" ratio of $2\Delta / k_B T_c \sim 3.5$ that is observed in most metallic superconductors – which is also obtained within the weak coupling BCS theory. This ratio – called the BCS ratio, increases if the electron-phonon coupling increases, and often taken as a measure of the electron-phonon coupling constant's strength.

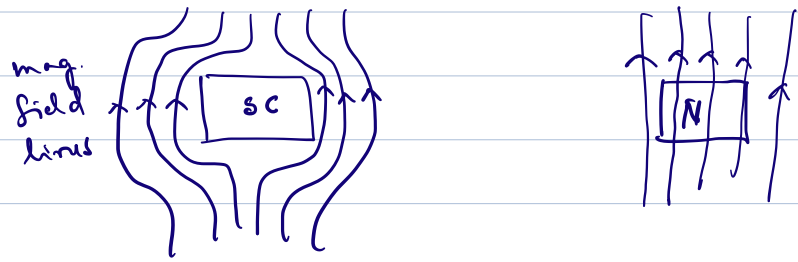
- Due to the energy gap in the electronic structure, the particle-hole continuum is also gapped by 2Δ. Therefore, much like the plasmon case, there will not be any photon absorption for frequency $\omega < 2\Delta$. Similarly, the phonon's decay process is determined by the particle-hole continuum (ultrasonic attenuation) which will not occur for phonon frequency $\omega_p < 2\Delta$. For $T_c \sim 10\,K$, $\Delta \sim 1\,meV$, which translates into infrared frequency region $\omega \sim 10^{12}\,s^{-1}$.

(c) Isotope Effect

Experimentally, it was found that as the nucleus mass is changed by substituting the isotope of an element, which changes the phonon frequency $\omega_q \sim \sqrt{K_q/M}$, the superconducting transition temperature T_c changes as $T_c \propto 1/\sqrt{M} \propto \omega_D$. This provided an important clue that electron-phonon coupling played a key role in the mechanism of superconductivity.

(d) Meissner Effect (Diamagnetism).

Another most important feature of superconductivity is the complete exclusion of the magnetic field from the interior of a superconductor - this means the superconductivity is a diamagnet and diamagnetism vanishes as superconductivity vanishes.



$T < T_c$ $\qquad$ $T > T_c$

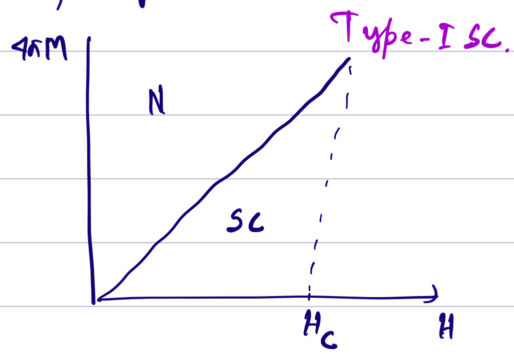
If B is the total magnetic field in a material, in response to an applied field of $\vec{H}$, then

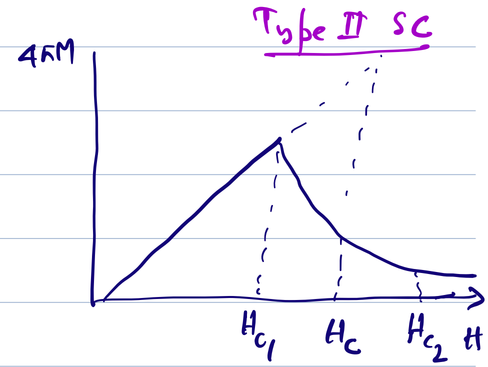
$$\vec{B} = \vec{H} + 4\pi \vec{M} = 0.$$

So, $\vec{M} = -\dfrac{\vec{H}}{4\pi}$ is the induced magnetization.

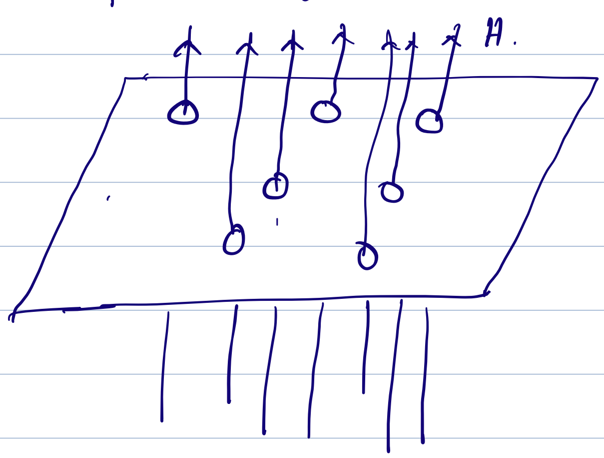
This phenomena was discovered by Meissner and Ochsenfeld, and called the Meissner effect.

In fact, the magnetic field penetrates inside the material a bit, and there is a distance - called the penetration depth λ_L, which measures the distance from the surface of the material upto which the magnetic field penetrates inside the system. The penetration depth is inversely proportional to the SC gap (actually it turns out to be $\lambda \propto 1/\Delta^2$), and hence as superconductivity weakens, i.e., the gap decreases, the penetration depth increases, and at T_c, $\Delta \to 0$, $\lambda \to L$, the system size. As magnetic field strength increases, the SC gap Δ decreases. So there is a critical magnetic field, called H_c, above which superconductivity is completely zero.





In fact, there are two types of superconductors - called Type I and Type II. The above description holds for the Type-I SC. In some materials - especially in alloys or disorder superconductors there are two critical fields H_{c_1} & H_{c_2}. The material shows the usual Meissner effect upto H_{c_1}, and above it, the magnetization does not sharply vanish to zero but smoothly decreases to zero at some higher critical field H_{c_2}. Between H_{c_1} and H_{c_2}, the magnetic field penetrates through the inside of the material, but superconductivity is not yet destroyed. The magnetic field in fact makes holes through the material and passes through them - they are called vortex or Abrikosov vortex (1957), and the rest of the material remains superconducting. All unconventional superconductors are Type-II.



It was F. London and H. London brothers explained this phenomena in 1934, which is called the London equation. They argued that in a superconductor, since there is no resistance, the Ohm's law $\vec{J} = \sigma \vec{E}$ must be violated. Ohm's law is based on dissipative force $\vec{F} \propto \vec{v}$ argument. London assumed that rather Newton's law, which is based on energy, momentum conservation, is valid. So, the electromagnetic force

$$\vec{F} = -e\vec{E} = m\frac{d\vec{v}}{dt}$$

$$= \frac{m}{ne}\frac{d\vec{J}}{dt} \qquad [\because \vec{J} = ne\vec{v}].$$

$$\Rightarrow \frac{d\vec{J}}{dt} = -\frac{ne^2}{m}\vec{E} \qquad ---(1)$$

(This gives for $\vec{E}=0$, $\vec{J} \neq 0$ but $\vec{J} =$ constant as in Newton's law)

[One can also derive eq (1) using the continuity equation by assuming that all the charge particle density $n(t)$ oscillated at the plasma frequency $w_p = \sqrt{\frac{4\pi ne^2}{m}}$, or, $n(t) = n(0)\, e^{-iw_p t}$. Then from the continuity equation we have $\vec{\nabla}\cdot\vec{J} = -\frac{\partial \rho}{\partial t} = -e\frac{\partial n}{\partial t}$ $i w_p n(t)$. Now, the Gauss law gives $\vec{\nabla}\cdot\vec{E} = 4\pi n(t)$

Then we get
$$\vec{\nabla}\cdot\left(\frac{d\vec{J}}{dt}\right) = -w_p^2\, n(t)$$
$$= -w_p^2 \cdot \frac{1}{4\pi}\vec{\nabla}\cdot\vec{E}$$
$$\Rightarrow \frac{d\vec{J}}{dt} = -\frac{ne^2}{m}\vec{E} + \text{constant}. \quad]$$

Next we take $\vec{\nabla}\times$ on both sides of eq (1) and used Maxwell's equations:

$$\frac{d}{dt}(\vec{\nabla}\times\vec{J}) = -\frac{ne^2}{m}(\vec{\nabla}\times\vec{E})$$

$$\Rightarrow \frac{d}{dt}(\underbrace{\vec{\nabla}\times\vec{\nabla}\times\vec{B}}_{\nabla(\cancel{\nabla\cdot B})^{0} - \nabla^2 B}) = -\frac{4\pi ne^2}{mc^2}\left(-\frac{\partial B}{\partial t}\right) \qquad \left[\because \vec{\nabla}\times\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t},\ \vec{\nabla}\times\vec{B} = \frac{4\pi}{c}\vec{J}\right].$$

$$\Rightarrow \quad \nabla^2 B = \frac{1}{\lambda^2} \vec{B}. \quad , \text{where} \quad \boxed{\lambda^{-1} = \sqrt{\frac{4\pi n e^2}{mc^2}} = \omega_p / c.} \quad -(28).$$

$$\Rightarrow \quad B(r) = B(0)\, e^{-r/\lambda} \quad --(26).$$

London's prediction of the penetration depth matches remarkably with experiments despite not assuming any mechanism of superconductivity. In fact, after the discovery of the BCS theory in 1957, the expression for the penetration depth was reproduced to be the same where $n = n_e = \rho_s$ is called the superfluid density i.e., the Cooper pair density, and $e \to 2e$ for it. The cooper pair density is proportional to the sc gap Δ, and hence we get $\lambda^2 \propto 1/\Delta^2$. Since λ is related to the plasma frequency expression for Cooper pair as $\omega_p = \lambda c$, therefore, as if all cooper pair collectively oscillates at the plasma frequency at the speed of light with the wave length λ.

(e) Supercurrent, phase velocity and Josephson Effect:

The understanding of phase stiffness of Cooper pair and the Josephson current (Josephson experiment) came after the BCS theory, we discuss this important effect now for the completeness of the experimental fact.

Whereas an electron's velocity is determined by the group velocity of its wavefunction, the Cooper pair's velocity is defined by the phase velocity wavefunction. The reason is that superconductivity breaks the gauge symmetry of the theory, and all Cooper pairs acquire a uniform and fixed phase in its wavefunction. The phase (ϕ) of a wavefunction and its amplitude, i.e. probability density or number of particles (N) follow the uncertainty principle:

$$\Delta N \, \Delta\phi \geq \hbar/2.$$

Therefore, as the phase becomes fixed in the SC state, the number of Cooper pair in this state becomes arbitrary. This is like the bosonic situation, but a Cooper pair is not quite a boson as we will see later.

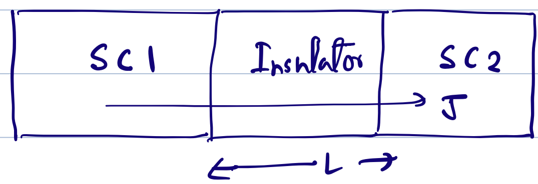
In what follows, as one tries to change the phase of the Cooper pair in space with some perturbation (such as electric field), the system tries to oppose it and as a result one has a phase velocity which gives the persistent current.

This can be understood as follows.

$$\Psi(r) = \text{wavefunction of a Cooper pair}$$
$$= |\Psi|\, e^{i\theta(r)} = |\Psi|\, e^{i\theta(0) + \frac{\partial\theta}{\partial r} r} = |\Psi|\, e^{i\theta_0} e^{i p\cdot r}$$

where θ_0 is the phase coherence of the SC state, and $p = \frac{\partial \theta}{\partial r}$ is the phase momentum.

Josephson showed that Cooper pair can tunnel from one superconductor to another even with an insulator between them,

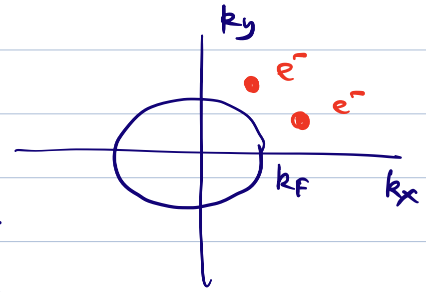


We understand this phenomena as follows. SC1 & SC2 are two different samples of the same superconducting material. As we cool down them, both becomes superconducting, but despite the two material being the same, they will condensate into some phase ϕ_1 & ϕ_2 which do not need to be same. Note that ϕ_1 is fixed for the entire SC1 material, and ϕ_2 the same for SC2, but $\phi_1 \neq \phi_2$. Therefore, there will be momentum generated between the superconductor as $p = \frac{\phi_1 - \phi_2}{L}$. ($\hbar = 1$). This generates a spontaneous current between the two superconductors, without any external potential, even through the insulator. One can show that that the current, called the Josephson current, oscillates with the phase difference as

$$J = J_0 \sin(\phi_1 - \phi_2).$$

The Cooper Problem:

Leon Cooper solved an interesting problem in 1956, a year before the BCS theory, called the Cooper problem or Cooper instability. We learned in the Fermi Liquid chapter that a Fermi surface is stable to any repulsive (density-density) interaction due to exclusion principle. This turns out not to be the case for an attractive interaction as pointed out by Cooper. He showed that a Fermi surface is unstable to any infinitesimally small attractive interaction which results in a bound state formation of two electrons. What happen to the exclusion principle here? It turns out that the single electron picture breaks down here, and one has a many body state where any number of electron pair can occupy - as if the electrons pair obey bosonic statistics. In reality that is not quite true, as we will see in the BCS theory, but all electrons pair (Cooper pair) has the same microscopic (global) phase, and according to the uncertainty principle of $\Delta N \, \Delta\phi \gtrsim \hbar/2$, since $\Delta\phi = 0$, $\Delta N \to \infty$, and hence this new state can host any number of Cooper pairs. Therefore, this new state is often called condensation of Cooper pairs.



We imagine a given Fermi surface in any dimension at any filling factor. Then we add two test electrons, subject to an interaction $V(\vec{r}_1 - \vec{r}_2)$ between them.
The two particle wavefunction is split into space and spin part as

$$\Psi_{s_1 s_2}(r_1, r_2) = \phi(r_1, r_2)\, \chi_{s_1 s_2} \quad \text{---(3)}$$

$$\left[-\frac{\hbar^2}{2m}\left(\nabla_1^2+\nabla_2^2\right)+V(r_1-r_2)\right]\phi(r_1,r_2)\,\chi_{s_1 s_2}=E\,\phi(r_1,r_2)\,\chi_{s_1 s_2} \quad -(4)$$

Since the interaction only depends on the relative coordinates, we should go to the center of mass and relative coordinates as

$\bar{R}=(r_1+r_2)/2$, $\bar{r}=\bar{r}_1-\bar{r}_2$, where the Schrödinger eqn decouples

$$\left[-\frac{\hbar^2}{2m^*}\nabla_R^2-\frac{\hbar^2}{2\mu}\nabla_r^2+V(r)\right]\Phi(R)\,\phi(r)=E\,\Phi(R)\,\phi(r).$$

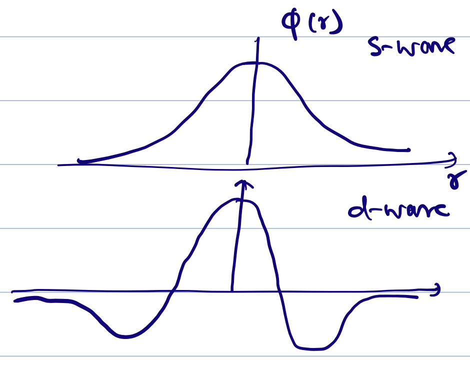
($m^*=2m$ and $\mu=m/2$ are the total and reduced masses). The center of mass has no potential, so, it has the plane wave solution $\Phi(R)=\frac{1}{\sqrt{V}}e^{i\bar{K}\cdot\bar{R}}$. The remaining Schrödinger equation is

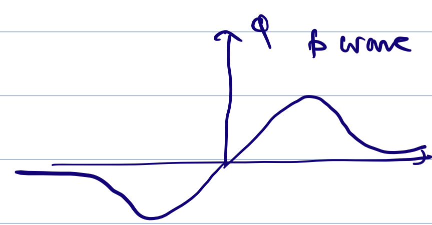
$$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2+V(r)\right]\phi(r)=\left(E+\frac{\hbar^2K^2}{2m}\right)\phi(r) \quad -(4)$$

The lowest energy corresponds to $K=0$, ie, the individual momentum of the two particles are <u>opposite</u> to each other.

The remaining part of the wave function is $\phi(r_1-r_2)\,\chi_{s_1,s_2}$. Since the total wave function must be antisymmetric, now we have two options: → spatial part symmetric $\phi(r)=\phi(-r)$ and spin part antisymmetric, ie, a singlet $(\uparrow\downarrow-\downarrow\uparrow)/2$. This gives a s-wave spin singlet superconductor.

→ spatial part antisymmetric and spin part symmetric. This gives p-wave spin triplet superconductor.





• Now given that the attractive potential is symmetric $V(r) = V(-r)$, and spherically symmetric, so, these angular momentum states are the eigen state of the Hamiltonian. Also note that as the attractive potential is maximum at $r \to 0$, so, the wavefunction must be more localized at $r \to 0$. Therefore, the s-wave spin singlet wavefunction wins here.

we fourier transform $\phi(r) = \frac{1}{\sqrt{N}} \sum_{k} \phi_k \, e^{i\vec{k}.\vec{r}}$ --(5)

which diagonalize the Hamiltonian as $\left[V_{kk'} = \int V(r) \, e^{-i(k-k')r} d^3r \right]$

$$(2\varepsilon_k - E)\,\phi_k = -\sum_{k'} V_{kk'}\,\phi_{k'} \quad \text{--- (6a)}$$

If we define $\Delta_k = (2\varepsilon_k - E)\,\phi_k$ = SC gap, condensation energy, or Cooper pair bound state energy, then eq (6a) turns into a self-consistent gap equation:

$$\boxed{\Delta_k = -\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{(2\varepsilon_{k'} - E)}} \quad \text{-- (6b).}$$

since E is the energy for the Cooper pair formation, therefore, a Cooper pair bound state exists if $E < 2\varepsilon_k$. Now from eq (6b), RHS $\Delta_k > 0$, and hence this equation has a finite root for Δ_k if the interaction $V_{kk'}$ is attractive to these two electrons with energy ε_k & ε_{-k}. We often introduce this approximation for isotropic interaction as

$$V_{kk'} = \begin{cases} -V_0 & \text{for } k, k' > k_F, \\ 0 & \text{otherwise} \end{cases} \quad \text{--(7a)}$$

we also introduce a s-wave (singlet) pairing, i.e, an isotropic pairing $\Delta_k = \Delta_0$. With these two approximations we obtain the criterion for the formation of a Cooper pair bound state on a Fermi sea as

$$\boxed{1 = V_0 \sum_k \frac{1}{2\varepsilon_k - E}} \quad \text{-- (7b)}$$

(This is analogous to the Stoner criterion for FM, and can be called Cooper criterion for SC instability).

- Now, we can perform this integral exactly for a tight-binding band ε_k, having a finite bandwidth. Keeping in mind the attractive potential comes from the electron-phonon coupling and that phonon has a finite bandwidth upto which electrons feel the attractive interaction, so we restrict our energy integration upto the phonon bandwidth. BCS put the phonon bandwidth cutoff to be the Debye frequency ω_D. In the presence case, we simply treat ω_D as some energy cut off upto which the interaction is attractive and above it $V=0$.

Now, convert the momentum summation to momentum integral $\sum_k \to V\int \frac{d^3k}{(2\pi)^3} \to \int d(\varepsilon)\, d\varepsilon$, where $d(\varepsilon)$ is the density of states, then we have

$$1 = V_0 \int_0^{\omega_D} \frac{d(\varepsilon)\, d\varepsilon}{2\varepsilon - E}$$

As often we will assume the density of state is peaked at ε_F and replace $d(\varepsilon) \simeq d(\varepsilon_F)$. And also we are here interested in the condensation energy for two electrons added to a Fermi sea of many electrons. Therefore, the integration extends from $\varepsilon = \varepsilon_F$ to $\varepsilon_F + \hbar\omega_D$. as the energy for other electrons fro $\varepsilon = 0$ to $\varepsilon = \varepsilon_F$ remain unchanged. So, we obtain

$$1 = V_0 d(\varepsilon_F) \int_{\varepsilon_F}^{\varepsilon_F + \omega_D} \frac{d\varepsilon}{(2\varepsilon - E)}$$

$$= \frac{V_0 d(\varepsilon_F)}{2} \ln \frac{2\varepsilon_F - E}{2(\varepsilon_F + \omega_D) - E}$$

$$\Rightarrow \boxed{E \approx 2\varepsilon_F - \underbrace{2\omega_D e^{-\frac{2}{V_0 d(0)}}}_{\Delta.}}$$

The first term $2\varepsilon_F$ is the energy of the Fermi sea, and the 2nd term is the condensation energy Δ. We introduce the superconducting coupling constant $\lambda = V_0 d(\varepsilon_F)$. Then the SC gap at $T=0$ is determined by three parameters ω_D, $V_0 < 0$ and $d(\varepsilon_F)$ as

$$\boxed{\Delta = 2\omega_D e^{-2/\lambda}} \quad — (8).$$

We notice that for any infinitesimally small λ, we have a superconductivity $(\Delta \neq 0)$, i.e., for any infinitesimally small $(V_0 > 0)$ attractive potential, and for any finite carrier density $d(\varepsilon_F) > 0$, i.e., any metal of how low the carrier density is, it is unstable to superconductivity.

We started with two test electrons added to a Fermi sea, with a plane wave wave function. This is equivalent to two electrons taken out of a Fermi sea, but now they are subjected to an attractive interaction. We see that they from a bound state. The wave function of a bound state cannot be a plane wave, but has a decay part parameterized as e^{-r/ξ_g}, where ξ_g is called the SC coherence length. Remarkably, it turns out that the coherence length

$$\xi_g \sim \frac{\hbar v_F}{\Delta} \sim \frac{\epsilon_F}{\Delta} k_F^{-1} \sim 10^3\text{-}10^4 \, A^0 .$$

is much larger than the interatomic distance. Therefore, the Cooper pairs are very robust in a metal.

⊛ The BCS Theory :

Bardeen, Cooper and Schrieffer (BCS) developed the microscopic theory for superconductivity in 1957. They built on the Cooper's work as discussed above and used the electron-phonon coupling induced attractive potential, that we obtained using the 2nd order perturbation theory before, to develop a mean field theory.

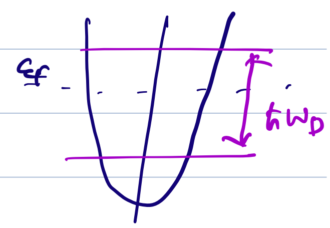
We start with the electron-phonon coupling mediated two-body interaction Hamiltonian that we derived before:

$$H = \sum_{k} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kk'q} V_{kk'} c^\dagger_{k\sigma} c^\dagger_{k'\sigma'} c_{k'-q\sigma'} c_{k+q\sigma} \qquad \text{—(9a)}$$

where

$$V_{k,k}(q) = |g(q)|^2 \frac{2\hbar\omega_q}{(\varepsilon_k - \varepsilon_{k+q})^2 - (\hbar\omega_q)^2} + V_{ee}(q), \qquad \text{—(9b)}$$

and $V_{ee}(q)$ is the Coulomb repulsion between electrons. Using TF screened coulomb interaction $V_{ee}(q) = 4\pi e^2/(q^2 + q_{TF}^2)$, an effective attractive interaction $V_{kk'}(q) < 0$ occurs when the electron-phonon coupling dominates over the repulsion term. This happens for electrons close to the fermi level, with $|\varepsilon_k - \varepsilon_{k+q}| \leq \hbar\omega_D$ where $\hbar\omega_D$ stands for the phonon bandwidth, which we often denote by $\hbar\omega_D$ (like the Debye frequency).



It is customary to make the assumption that

$$V_{kk'}(q) = -V_0 \quad \text{for } |\varepsilon_k - \varepsilon_{k+q}| \leq \hbar\omega_D$$
$$= 0 \quad \text{otherwise}$$

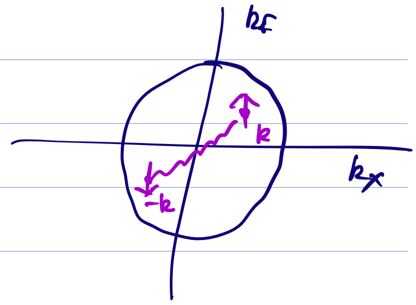
Mean-field Theory: Based on the Cooper result, we look for a mean field order for the two electron to form a bound state, called the Cooper pair such that there is a finite expectation value (we assume a singlet pairing with zero center of mass momentum:

$$\langle \Psi_{sc} | \underbrace{c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}}_{b_k \text{ (define)}} | \Psi_{sc} \rangle = \Psi^\dagger \neq 0, \quad \text{--(10)}$$

where $|\Psi_{sc}\rangle$ is the new ground state wavefunction in the sc state. Note that the sc operparameter does not conserve electron-number, and the sc wavefunction must be invariant for any number of Cooper pair. We know one such wavefunction for boson - which takes the coherent linear superposition of states with any number of bosons. We seek for such a wavefunction here in which two electrons of opposite momentum and opposite spin can simple "disappear" i.e, condense and the wavefunction remains invariant. Inspire by bosonic case, we think of a wavefunction as

$$|\Psi_{sc}\rangle = \Big(\alpha^{(0)}_k + \sum_{|k| \leq k_F} \alpha^{(1)}_k b_k + \sum_{|k| \neq |k'| \leq k_F} \alpha^{(2)}_{kk'} b_k b_{k'} + \cdots \Big)|0\rangle \quad \text{--(11)}$$

where 1st term corresponds to no Cooper pair with probability amplitude $|\alpha^{(0)}|^2$, 2nd term creates a Cooper pair at k, by taking two electrons from k & $-k$ and form a bound state, and so on.



The problem with this wave function is that it has macroscopically large number of variational parameters $\alpha^{(2)}$ to minimize to obtain such a wave function. BCS assumed that the two Cooper pairs b_k & $b_{k'}$ are like non-interacting, so that $\alpha^{(2)}_{kk'}$ can be approximated as a product of the two probability amplitude, i.e., $\alpha^{(2)}_{kk'} = \alpha^{(1)}_k \alpha^{(1)}_{k'}$. Then we have two variational parameters $\alpha_k^{(0)}$ & $\alpha_k^{(1)}$ which are tradinally denoted by $\alpha_k^{(0)} = u_k$ & $\alpha_k^{(1)} = v_k$. Then eq(11a) can be expressed concisely as

$$|\Psi_{BCS}\rangle = \prod_k \left(u_k + v_k C^{\dagger}_{k\uparrow} C^{\dagger}_{-k\downarrow}\right)|0\rangle . \quad \text{--- (11b)}.$$

- Next we apply the standard mean-field theory that we shift the operator b_k with respect to its mean value in the above ground state as $b_k \to \langle b_k\rangle + b_k$, where the new operator b_k gives the fluctuation of b_k with respect to its mean value, i.e. the electrons released from the Cooper pair condensate.

  We substitute $k' = -k$ and $k' + q \to k'$ in eq(9a). Then doing the mean field decomposition we get

$$H = \sum_{k\sigma} \varepsilon_k C^{\dagger}_{k\sigma} C_{k\sigma} - V_0 \sum_{kk'} \left(\langle b^{\dagger}_k\rangle + b^{\dagger}_k\right)\left(\langle b_{k'}\rangle + b_{k'}\right)$$

$$= \sum_{k\sigma} \varepsilon_k C^{\dagger}_{k\sigma} C_{k\sigma} - V_0 \sum_{kk'} \Big[\langle b^{\dagger}_k\rangle b_{k'} + \langle b_{k'}\rangle b^{\dagger}_k + \langle b^{\dagger}_k\rangle\langle b_{k'}\rangle - O(b^2)\Big].$$

Next we define the SC order parameter

$$\Delta_k = \sum_{kk'} V_{kk'} \langle b_{k'} \rangle$$

$$= -V_0 \sum_{k'} \langle b_{k'} \rangle \qquad \text{— (12)}$$

(Notice that for isotropic potential, the k-dependence on the L.H.S drops out. This is consistent with our assumption of s-wave pair).

Substituting the order parameter in the Hamiltonian we have the mean-field BCS Hamiltonian (sometimes called Bogoliubov - de - Gennes (BdG) Hamiltonian) as

$$\boxed{H = \sum_{k\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{k} \left[\Delta_k c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} + \Delta^{*}_{k} c_{-k\downarrow} c_{k\uparrow} \right] - \frac{\Delta_0^2}{V_0}} \qquad \text{-- (13)}$$

(Although k-dependence in Δ_k is dropped out for the s-wave pairing, we have kept it for now for generality).

The last term is the ground state energy of the SC condensate. The first two terms are the quasiparticle excitations that come out from the superconducting ground state.

- **Bogoliubov diagonalization:**

Now to obtain the eigenstates of the Hamiltonian we play the same trick, we define a suitable spinor, write the Hamiltonian in a matrix form in this spinor basis and diagonalize it. In the 2nd term we have $c^\dagger c^\dagger$ & c.c. So, to get a matrix form, we need to have a spinor which mixes c & $c^\dagger$. Such a spinor is called Nambu spinor:

$$\Psi_{k\sigma} = \begin{pmatrix} c_{k\sigma} \\ c^\dagger_{-k\sigma} \end{pmatrix}.$$

Then we get $H_k = \langle \Psi_k | H | \Psi_k \rangle$

$$= \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta_k^\dagger & -\varepsilon_k \end{pmatrix} \qquad = \begin{array}{c|cc} & c_{k\uparrow} & c^\dagger_{-k\downarrow} \\ \hline c^\dagger_{k\uparrow} & \varepsilon_k & \Delta_k \\ c_{-k\downarrow} & \Delta_k^\dagger & -\varepsilon_k \end{array}$$

Notice that we get $-\varepsilon_k$ because explicitly this term corresponds to $-\varepsilon_{-k}\, c_{-k\downarrow} c^\dagger_{-k\downarrow} = \varepsilon_k\, c^\dagger_{-k\downarrow} c_{-k\downarrow}$.

- The spinor has both electron ($c^\dagger$) and hole (c) state, much like the Dirac spinor. So, one would expect a particle-hole symmetric energy eigenstate. Indeed the SC Hamiltonian has particle-hole symmetry.
- We can diagonalize this matrix as before and write the eigenvectors in a similar canonical transformation form.

We write

$$H_k = \varepsilon_k \sigma_z + \mathrm{Re}\,\Delta_k \sigma_x - \mathrm{Im}\,\Delta_k \sigma_y$$

where σ_μ are Pauli matrices in the Nambu basis (not to think of them as spin-1/2 case).

Then the eigenvalues of such a Hamiltonian gives

$$E_k^{\pm} = \pm\sqrt{\epsilon_k^2 + (\mathrm{Re}\,\Delta_k)^2 + (\mathrm{Im}\,\Delta_k)^2}$$

$$= \pm\sqrt{\epsilon_k^2 + |\Delta_k|^2} = \pm E_k \quad \cdots (14).$$

We denote the corresponding eigenvectors as

$$\phi_k^+ = \begin{pmatrix} u_k \\ -v_k \end{pmatrix}, \quad \phi_k^- = \begin{pmatrix} v_k^* \\ u_k^* \end{pmatrix}$$

where we obtain $u_k = \frac{1}{\sqrt{2}}\left(1 + \frac{\epsilon_k}{E_k}\right)$, $v_k = \frac{1}{\sqrt{2}}\left(1 - \frac{\epsilon_k}{E_k}\right)$ (15)

with $|u_k|^2 + |v_k|^2 = 1$, which comes from the normalization.
Using the eigenvector we construct the unitary matrix

$$U_k = \begin{pmatrix} u_k & v_k^* \\ -v_k & u_k^* \end{pmatrix},$$

which rotates the Nambu spinor into something called Bogoliubov quasiparticles $\gamma_{k\uparrow}$, $\gamma^{+}_{-k\downarrow}$ which are obtained as

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^+_{-k\downarrow} \end{pmatrix} = U_k^{-1} \begin{pmatrix} c_{k\uparrow} \\ c^+_{-k\downarrow} \end{pmatrix}$$

$$\Rightarrow \quad \boxed{\begin{aligned} \gamma_{k\uparrow} &= u_k^* c_{k\uparrow} + v_k c^+_{-k\downarrow} \\ \gamma^+_{-k\downarrow} &= -v_k c_{k\uparrow} + u_k^* c^+_{-k\downarrow} \end{aligned}} \quad \begin{aligned} &\cdots (16a) \\ &\cdots (16b) \end{aligned}$$

• Two important points :

(a) The Bogoliubov quasiparticles arise from the linear superposition of an electron (c^{+}) and a hole (c). So, they are neither an electron nor an hole, and the charge of this quasiparticle is not well-defined and not integer as in the case for electron ($-e$) and hole ($+e$). The charge density of the Bogoliubov quasiparticle is defined as

$$\rho_{k\uparrow} = |u_k|^2 e + |v_k|^2 (-e)$$
$$= (|u_k|^2 - |v_k|^2) e,$$

which can vanish when $|u_k|^2 = |v_k|^2$. This can happen when $\xi_k = 0$, i.e., at the Fermi level. Such a state is called Majorana fermion.

(b) Although one does include the spin index $\uparrow, \downarrow$ in the Bogoliubov quasiparticle, but notice that on the R.H.S its a linear superposition of $\uparrow$ & $\downarrow$ spins of electrons and hole. So, the spin of the Bogoliubov quasiparticle is also not well defined. (In fact, one should not include a spin index in the Bogoliubov quasiparticle state, but all books do and we hence keep the spin index).

H.W. (i) show that the Bogoliubov quasiparticles obey fermion statistics.

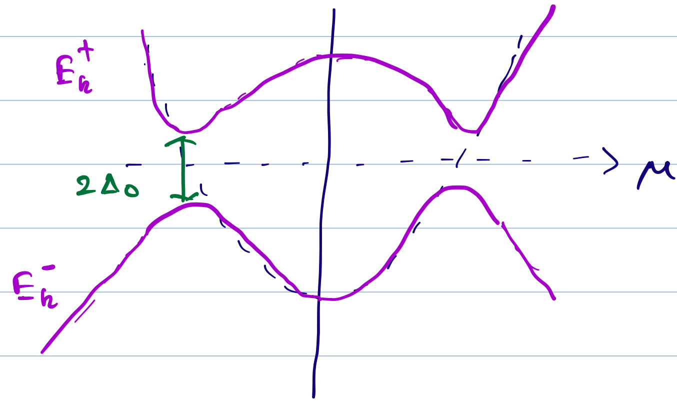
(ii) show that the Cooper pairs b_k, b_k^{+} do not obey fermion or boson statistics but a spin-1/2 algebra. Sometimes its called the pseudo spin.

⊛ The diagonal mean-field Hamiltonian is

$$H_{MF} = \sum_{k,\nu=\pm} E_k^{\nu} \gamma_{k\nu}^{\dagger} \gamma_{k\nu} - \frac{\Delta_0^2}{V_0} \quad \text{-- (17)}$$

$\nu = \pm \,(\Rightarrow\, \uparrow,\downarrow$ for $\gamma_{k\uparrow,\downarrow})$.

The superconducting quasiparticle dispersion looks like:



Here the gap opens at all fermi-momentum, unlike in the SDW case where the gap opens at the mag. BZ boundary.

- As before, the SC gap has to be computed self-consistently because the gap enters in the wavefunction with which the expectation value of the order parameter is also computed. From eq(12)

$$\Delta = - V_0 \sum_k \langle c_{-k\downarrow} c_{k\uparrow} \rangle$$

$$= - V_0 \sum_k \langle (-v_k^* \gamma_{k\uparrow}^{\dagger} + u_k \gamma_{-k\downarrow}) (u_k \gamma_{k\uparrow} + v_k^* \gamma_{-k\downarrow}^{\dagger}) \rangle$$

$$= - V_0 \sum_k \Big[-u_k v_k^* \langle \gamma_{k\uparrow}^{\dagger} \gamma_{k\uparrow} \rangle + u_k v_k^* \langle \gamma_{-k\downarrow} \gamma_{-k\downarrow}^{\dagger} \rangle - v_k^{*2} \langle \gamma_{k\uparrow}^{\dagger} \gamma_{-k\downarrow}^{\dagger} \rangle + u_k^2 \langle \gamma_{-k\downarrow} \gamma_{k\uparrow} \rangle \Big]$$

Now, $\langle \gamma_{-k\downarrow} \gamma_{k\uparrow} \rangle = \langle \gamma_{k\downarrow}^{\dagger} \gamma_{-k\uparrow}^{\dagger} \rangle = 0$ as they do not conserve quasiparticle numbers in the state.

$\langle \gamma^{\dagger}_{k\uparrow} \gamma_{k\uparrow} \rangle = f(E_k)$

$\langle \gamma_{-k\downarrow} \gamma^{\dagger}_{-k\downarrow} \rangle = f(-E_k) = 1 - f(E_k)$

[Note that according to our definition $\gamma^{\dagger}_{k\uparrow}$ creates a quasiparticle in the E^{+}_{k} band while $\gamma_{-k\downarrow}$ creates a quasiparticle in the $E^{-}_{k} = -E_k$ band. Its actually a very confusing notation chosen in the literature. One could simply define the two quasiparticle creation operators as $\gamma^{\dagger}_{k\pm}$ for the two bands $E^{\pm}_{k} = \pm E_k$ and the results would remain the same.]

Then we get

$$\boxed{\begin{aligned} \Delta &= -V_0 \sum_k u_k v_k^* \left[1 - 2f(E_k)\right] \\ &= -V_0 \sum_k \frac{\Delta}{2E_k} \tanh\left(\frac{\beta E_k}{2}\right). \end{aligned}} \quad \text{— (18)}$$

This is the self-consistent BCS gap equation. If there is a solution of $\Delta > 0$ for a given value of V_0 & band structure E_k, then superconductivity occurs. This equation is analogous to the Stoner instability for FM and exactly evaluates to the Cooper instability at $T=0$, where $\tanh\left(\frac{\beta E_k}{2}\right) \to 1$. We can evaluate it exactly for the constant potential V_0, in the limit of $T \to 0$ & $T \to T_c$.

- The integral we need to do is

$$\Delta = -V_0 \int_{-\infty}^{\infty} d(\varepsilon)\, d\varepsilon \, \frac{\Delta}{\sqrt{\varepsilon^2+\Delta^2}} \tanh\left(\frac{\beta}{2}\sqrt{\varepsilon^2+\Delta^2}\right).$$

The integral limit reduces from $-\omega_D$ to ω_D as $V_0 = 0$ outside the phonon frequency range. Since the integral is even in ε, we reduce it to from 0 to ω_D. Also we assume the density of states of electron is featureless in the range of ω_D that we approximate it as $d(\varepsilon) \approx d(0)$. So, we get

$$\Delta = -2\, d(0) V_0 \int_0^{\omega_D} d\varepsilon \, \frac{\Delta}{\sqrt{\varepsilon^2+\Delta^2}} \tanh\left(\frac{\beta}{2}\sqrt{\varepsilon^2+\Delta^2}\right) \quad \text{---}(19a)$$

$\lambda = d(0) V_0 =$ SC coupling constant.

- Now we take two limits:

$T \to 0$: $\beta \to \infty$. So, we take $\tanh \beta\sqrt{\varepsilon} \to 1$. Then we have

$$1 = -2\lambda \int_0^{\omega_D} \frac{1}{\sqrt{\varepsilon^2+\Delta^2}}\, d\varepsilon = -\lambda \log\left[\frac{\omega_D}{\Delta} + \sqrt{1+\left(\frac{\omega_D}{\Delta}\right)^2}\right]$$

$$\approx -\lambda \log\left(\frac{2\omega_D}{\Delta}\right)$$

$$\Rightarrow \boxed{\Delta = 2\omega_D\, e^{-1/\lambda}} \quad \text{---}(19b)$$

• $T = T_c$, $\Delta = 0$. So, we

$$1 = -2\lambda \int_0^{\omega_D} d\varepsilon \, \frac{\tanh(\beta_c \varepsilon/2)}{\varepsilon} \qquad \beta_c = 1/k_B T_c$$

$$= -2\lambda \int_0^{\beta_c \omega_D/2} dx \, \frac{\tanh x}{x}$$

$$= -2\lambda \left[\int_0^{\beta_c \omega_D/2} \operatorname{sech}^2(x) \log x \, dx + \tanh(x) \log(x) \Big|_0^{\beta_c \omega_D/2} \right.$$

$$= \gamma_E - \log\left(\frac{\pi}{4}\right) - \log(\beta_c \omega_D/2) = \log\left(2\beta_c \omega_D e^{\gamma_E}\right)$$

↑ Euler constant $\approx 0.577\ldots$

$$\Rightarrow \boxed{T_c = \frac{2\omega_D}{k_B} \frac{e^{\gamma_E}}{\pi} e^{-1/\lambda} \approx 1.13 \frac{\omega_D}{k_B} e^{-1/\lambda}} \quad \text{--- (19c)}$$

This is interesting that both Δ (at $T=0$) & T_c depends on ω_D & λ in a similar way, giving to a material independent value of the BCS ratio

$$\boxed{\frac{2\Delta}{k_B T_c} = \frac{4}{1.13} \approx 3.54} \quad \text{-- (19d)}$$

The important message of eq (19b) & (19c) is that for any infinitesimally small value of $\lambda = d(0) V_0$, we have a finite SC gap Δ & finite transition temperature. This is to say for any finite electron density at the Fermi surface ($d(0) \neq 0$) in metal, and for any finite value of attractive potential ($V_0 > 0$)

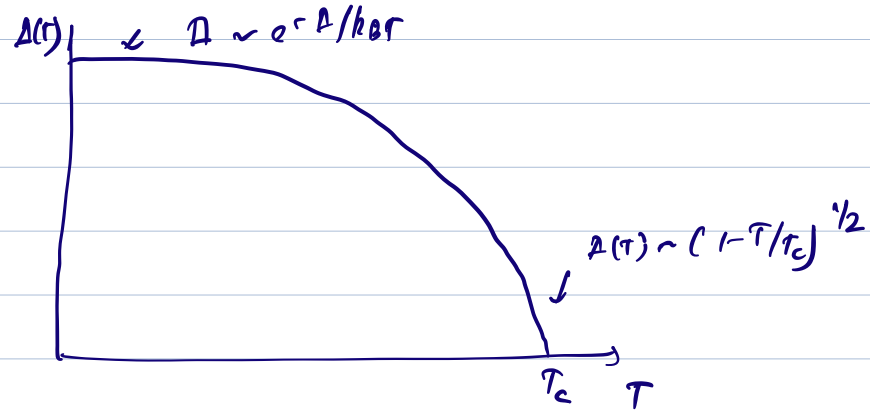
the Fermi surface is unstable to superconductivity.

- Near $T \to 0$, $\Delta(T)$ decreases exponentially slowly as as $\Delta(T) \simeq \Delta(0)\, e^{-\Delta/k_B T}$. On the other hand, near T_c, $\Delta(T)$ drops to zero with a vertical tangent, approximately as

$$\Delta(T) \simeq 1.74\,\Delta(0)\,(1 - T/T_c)^{1/2}$$

, with the mean field exponent of $1/2$.

- One can solve eq 19(?) numerically and the plot looks as



H.W. (1) Compute the Density of states in the superconducting state and show that it has a pole at $E = \pm\Delta$, which gives the "coherence peak" in the density of states

(2) Compute free-energy, entropy and specific heat in the superconducting state and compare them with the normal metal value. obtain the specific heat jump at $T = T_c$ and the entropy loss in the superconducting state.

(3) Compute Meissner effect, penetration depth and superfluid density for the BCS theory.