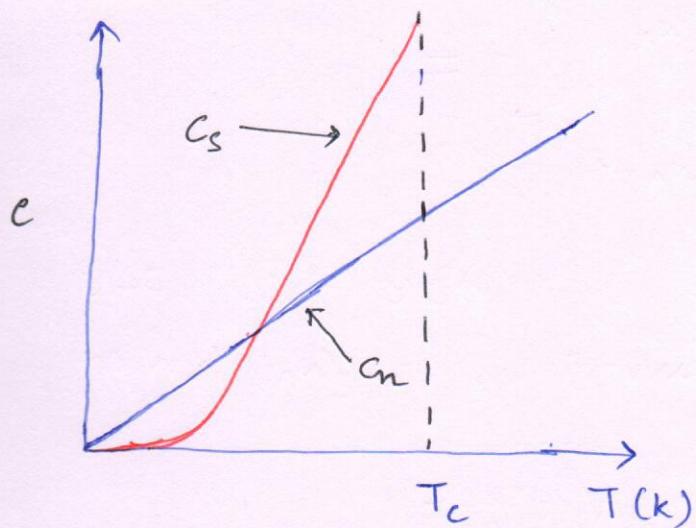


## Specific Heat Measurements

At low temperatures the specific heat of a normal metal has the form  $AT + BT^3$ .

Linear term ( $AT$ ) : Electronic excitation/contribution

Cubic term ( $BT^3$ ) : Lattice vibrations



As the temperature drops below  $T_c$  (in zero magnetic field) the specific heat jumps to a higher value and then slowly decreases, eventually falling well below the value one would expect for a normal metal.

In the superconducting state the linear electronic contribution to the specific heat is replaced by a term that vanishes much more rapidly at very low temperatures, having a dominant low temperature behavior of the form  $\exp(-\Delta/k_B T)$ . This is the characteristic thermal behavior of a system whose excited levels are separated from the ground state by an energy  $\Delta$ .

## Isotope Effect

Experiments on metals containing different isotopes of a particular elemental superconductor showed that the transition temperature changes with the mass of the crystal lattice ions. according to the relation

$$T_c \propto M^{-\alpha},$$

where  $\alpha \approx \frac{1}{2}$ .

This indicates that superconductivity involved a strong interaction (electron-phonon coupling) between the electrons and the lattice.

## Microscopic Description of Superconductivity

The experimental observations that have been discussed so far suggest that a description of superconductivity must embody the following features:

- It is a special state of electrons; i.e., it is more than just a perfectly conducting state.
- This special state is quantum mechanical in nature.
- An energy gap exists between the ground state and the states for the excited quasiparticles (electrons).
- The interaction between the electrons and the lattice vibrations is important in the mechanism of conventional superconductivity.

The central result of the BCS theory is that the energy gap is given by

$$E_g = 2\hbar\omega_D \exp\left(-\frac{\gamma_{\text{exp}}}{S(E=E_F)V}\right) \approx 3.5 k_B T_c,$$

where  $\omega_D$  is the Debye phonon frequency,  $\gamma_{\text{exp}}$  is a dimensionless constant that describes the strength of the electron-phonon interaction,  $S(E=E_F)$  denotes the density of single electron particle states at the Fermi level and  $V$  denotes the attractive electron-phonon interaction.

## Basic BCS results

- The special state of nearly  $10^{23}$  electrons/cm<sup>3</sup> can be described by quantum mechanical wave function  $\psi(\vec{r})$ .
- The electrons are bound in pairs, the so called Cooper pairs.

The electrons with opposite momenta ( $+\vec{p}$ ) and ( $-\vec{p}$ ) and opposite spins ( $\uparrow$ ) and ( $\downarrow$ ) are bound by an energy  $\Delta_0$  related to the superconducting band gap.

Sources

## Electron Pairs

- Electrons in normal metals: essentially perfect Fermi gas behavior.
- Superconductors

The ground state of the electrons can not be the Fermi degenerate ground state if there is even a very weak net attractive interaction between them.

The electrons instead form pairs, cooper pairs, which are the basic entities of the superconducting state.

Direct interaction between electrons:

repulsive screened coulomb electrostatic force.

- So, how does an attractive force between them arise?
- How a very weak attraction between electrons can lead to the formation of pairs.

- Electrons in metals can be imagined to be zipping through the lattice at something like the Fermi velocity.
- Suppose that one electron passes through the lattice. The ions are attracted to the electrons but, owing to their large mass, move very slowly compared to the much lighter electrons.
- By the time ions respond the electron is long gone, but it polarizes the positive ion cores and leaves a lattice distortion in the immediate vicinity of the electron trail.
- If another electron enters this region before the lattice relaxes, its energy will be lowered because the lattice is already polarized by the first electron.
- This mechanism thus provides an attractive interaction between the two electrons.
- Imagine: The first electron created a phonon, which was absorbed by the second one.  
The interaction is strongest if the two electrons traverse exactly the same path, that is if they have, say, equal and opposite momenta.  
(Be carefull before you take it literally, but it does give some idea.)

- Weak attractive interactions between particles do not, in general, lead to the formation of bond pairs.
- Then why do electrons form pairs under the weak and the subtle interaction discussed above.

We will try to answer this.

- Consider a perfect Fermi gas in its ground state
  - isolate two electrons from this
  - examine the effect ~~of~~ on them of an attractive interaction between them discussed above.
- Ultimately find:
  - their state is changed regardless of how weak the interaction
  - the many-electron ground state we assumed to start with is metastable when there is any net attractive interaction.

## Set up the machinery

→ In the absence of the interaction the two chosen electrons are in momentum eigenstates in the Fermi sea.

- choose electrons at the Fermi surface with momenta  $\vec{q}$  and  $-\vec{q}$   
(the magnitude of each is  $q_F$  (the Fermi value))
- Thus, their centre of mass is at rest.  
So now if they do form a Bose-like bond pair, it will be in the zero-momentum condensate of the Bose system.
- We expect the interaction to be strongest for a pair with equal and opposite momenta.

→ The spatial wavefunction of the pair,  $\psi = \psi(|\vec{r}_2 - \vec{r}_1|)$ , where  $\vec{r}_2$  and  $\vec{r}_1$  are positions of the two electrons, obeys the Schrödinger equation

$$\boxed{-\frac{\hbar^2}{2m} [\nabla_1^2 + \nabla_2^2] \psi + V(|\vec{r}_2 - \vec{r}_1|) \psi = (\epsilon + 2\epsilon_F) \psi},$$

where  $V$  is the potential acting between them.

$E_F = \frac{k^2 q_F^2}{2m}$  is the energy of each electron in the ground state when  $N=0$ .

\*  $\rightarrow \epsilon$  is the energy of the pair relative to the non-interacting state.

If  $\epsilon < 0 \Rightarrow$  the pair is bound

the ordinary Fermi-degenerate g.s. is metastable.

$\rightarrow$  Note that the wavefunction of the pair must be "anti-symmetric".

The spatial part is symmetric, so in addition to specifying that the pair have opposite momenta, they must have opposite spins.

e.g.  $\vec{q} \uparrow$  and  $-\vec{q} \downarrow$  ( $+\vec{q}$ , spin up;  $-\vec{q}$ , spin down)

Now what is the effect of all the other electrons that are present?

They try to keep these two electrons from occupying any states below the Fermi surface.

We will show this in  $\vec{q}$  space (wave number space)  
 so let us switch to it.

→ Write the pair wavefunction as a linear combination of momentum eigenstates

$$\psi(\vec{r}) = \sum_{\vec{q}} g_{\vec{q}} e^{i\vec{q} \cdot \vec{r}},$$

where we have (from opposite momentum states)

$$e^{i\vec{q}_1 \cdot \vec{r}_2} e^{i(-\vec{q}_1) \cdot \vec{r}_1} = e^{i\vec{q}_1 \cdot (\vec{r}_2 - \vec{r}_1)} = e^{i\vec{q} \cdot \vec{r}}.$$

(Important side info): If  $V=0$ , then only one of  $g_{\vec{q}}$  would be non-zero. The electrons would be in the momentum eigenstates of the perfect Fermi gas.

So what is the effect of  $V$ ? ( $V \neq 0$ )

This potential scatters the pair, with some probability, into other states, e.g.

from  $\vec{q}, -\vec{q}$  into  $\vec{q}', -\vec{q}'$ .

This process mixes some amplitude for the state  $(\vec{q}', -\vec{q}')$  into the wave function.

Thus, more than one of  $g_{\vec{q}}$  will be nonzero.

→ No scattering can take place into states below the Fermi surface, for they are fully occupied.

This can be specified by writing

$$g_{\vec{q}} = 0 \quad (\text{for all } q < q_F).$$

→ Substitute all this in the Schrödinger eqn. that we wrote earlier.

$$\frac{\hbar^2}{2m} \sum_{\vec{q}} g_{\vec{q}} (2q^2) e^{i\vec{q} \cdot \vec{r}} + V(\vec{r}) \sum_{\vec{q}} g_{\vec{q}} e^{i\vec{q} \cdot \vec{r}}$$

$$= (\varepsilon + 2\varepsilon_F) \sum_{\vec{q}} g_{\vec{q}} e^{i\vec{q} \cdot \vec{r}}.$$

(divide by the volume  $V=L^3$ , multiply by  $e^{-i\vec{q}' \cdot \vec{r}}$  and integrate over volume).

$$\Rightarrow \boxed{\frac{\hbar^2}{m} g_{\vec{q}} + \sum_{\vec{q}'} g_{\vec{q}'} V_{\vec{q}\vec{q}'} = (\varepsilon + 2\varepsilon_F) g_{\vec{q}}} \quad | \text{Bethe-Goldstone equation}$$

where

$$V_{\vec{q}\vec{q}'} = \frac{1}{L^3} \int V(\vec{r}) e^{i(\vec{q}-\vec{q}') \cdot \vec{r}} d^3 r$$

and

$$\frac{1}{L^3} \int e^{i(\vec{q}-\vec{q}') \cdot \vec{r}} d^3 r = \delta_{\vec{q}\vec{q}'}$$

So,  $V_{\vec{q}\vec{q}'}$  is the matrix element for scattering the pair from pair state  $\vec{q}$  ( $\vec{q}_1 \uparrow, -\vec{q}_1 \downarrow$ ) to pair state  $\vec{q}'$ .

What happens to the pair that started out in state  $\vec{q}$ ,

Under the interaction  $V_{\vec{q}\vec{q}'}$ , ?

Of course, to answer this we have to know the interaction. But we already know its general/ qualitative nature, don't we.

Where is the energy for the interaction going to come from?

It is going to come from the energy involved in the lattice distortions — energy in the phonon spectrum of the solid.

Now what is the largest interaction energy possible from the lattice distortions?

This must be the energy of the highest-frequency phonon in the spectrum,  $\boxed{\sim \hbar \omega_D}$ , where  $\omega_D$  is the Debye frequency.

Therefore, in general under simple circumstances, the potential  $V$  cannot scatter a pair from the state  $\vec{q}$  to the state  $\vec{q}'$ , if these states are separated by more than  $\hbar \omega_D$  in energy? Why?

Thus, we expect that  $V_{\vec{q}\vec{q}'}$  will be non zero only for states within  $\hbar\omega_D$  of the Fermi surface.

Recall,  $\epsilon_F \gg \hbar\omega_D$ . (go & check)

Therefore, the states from which and into which electrons are scattered by the potential  $V(r)$  are all of nearly the same energy.

The states  $\vec{q}$  &  $\vec{q}'$  really differ only in the directions of the  $\vec{q}$  vectors.

Let us simplify our life and assume that the potential is "isotropic" — independent of the direction,

$\Rightarrow V_{\vec{q}\vec{q}'}$  is just a constant in a narrow shell above the Fermi surface.

$$V_{\vec{q}\vec{q}'} = -V, \text{ if } \begin{cases} \frac{\hbar^2 q^2}{2m} < \epsilon_F + \hbar\omega_D \\ \text{and} \\ \frac{\hbar^2 q'^2}{2m} < \epsilon_F + \hbar\omega_D \end{cases}$$

$$= 0, \text{ otherwise,}$$

where  $V > 0$  so that  $V_{\vec{q}\vec{q}'} = -V$  is an attractive potential.

Therefore, the Schrödinger equation in wave number space can be written as

$$\frac{\hbar^2 q^2}{m} g_{\vec{q}} - V \sum_{\vec{q}'} g_{\vec{q}'} = (\varepsilon + 2\varepsilon_F) g_{\vec{q}},$$

where the sum extends only over states in the interacting shell.

Rearrange the terms,

$$\left( \frac{\hbar^2 q^2}{m} - \varepsilon - 2\varepsilon_F \right) g_{\vec{q}} = V \sum_{\vec{q}'} g_{\vec{q}'} = -D.$$

Note that  $V \sum_{\vec{q}'} g_{\vec{q}'}$  is independent of  $\vec{q}$  and is a constant equal to  $-D$ .

In fact, we can write the above equation as two equations

$$D = -V \sum_{\vec{q}'} g_{\vec{q}'},$$

and

$$g_{\vec{q}} = \frac{D}{\varepsilon + 2\varepsilon_F - (\hbar^2 q^2/m)}.$$



Substitute the  $g_{\vec{q}}$  expression from below the second eqn. into the first equation.

We obtain

$$D = -V \sum_{\vec{q}} \frac{D}{\epsilon + 2\epsilon_F - (\hbar^2 q^2/m)},$$

Note that we have changed the dummy variable from  $\vec{q}'$  to  $\vec{q}$ .

Define

$$\xi = \frac{\hbar^2 q^2}{2m} - \epsilon_F,$$

so. (after canceling D from both sides)

$$1 = V \sum_{\vec{q}} \frac{1}{2\xi - \epsilon}.$$

$\xi$  is the energy of a single electron relative to the Fermi energy.

Note the above sum is to be carried out for values of  $\xi$  between zero and  $\hbar\omega_D$ .

Change the sum to an integral,

$$1 = V \int_0^{\hbar\omega_D} \frac{P(\xi) d\xi}{2\xi - \epsilon}$$

$P(\xi)$  is the usual single particle density of states except that  $\xi$  is the energy above the Fermi level,

$$\text{so } P(0) = \frac{4\pi\sqrt{2} L^3 m^{3/2}}{(2\pi\hbar)^3} \epsilon_F^{Y_2}.$$

Now in the narrow band between  $\epsilon_F$  and  $\epsilon_F + \hbar\omega_D$ ,  $S(\xi)$  hardly changes at all.

We can take

$$S(\xi) \approx S(0).$$

So,

$$\begin{aligned} I &= V S(0) \int_0^{\hbar\omega_D} \frac{d\xi}{2\xi - \epsilon} \\ &= \frac{1}{2} V S(0) \int_{-\epsilon}^{2\hbar\omega_D - \epsilon} \frac{dx}{x} \\ &= \frac{1}{2} V S(0) \ln \left( \frac{\epsilon - 2\hbar\omega_D}{\epsilon} \right). \end{aligned}$$

Solve for  $\epsilon$ ,

$$\boxed{\epsilon = \frac{2\hbar\omega_D}{1 - e^{2/S(0)V}}}.$$

If the potential  $V$  is weak (i.e. small  $V$ ), the exponential in the denominator will be large, and we can write

$$\boxed{\epsilon = -2\hbar\omega_D \exp\left(-\frac{2}{S(0)V}\right)}.$$

The energy of the pair is lower than it was in the pure Fermi ground state by this amount.

- The pair is not bound in the ordinary sense, since its overall energy,  $2\epsilon_F + \epsilon$ , is still quite positive, but it is quasi-bound, with energy lower than  $2\epsilon_F$ .
- The above calculation does not describe the <sup>superconducting</sup> ground state.
- It only tells us that the normal ground state is unstable if there is even a weak attractive potential between the electrons.
- Why discriminate!  
If there is an attractive potential acting between any one pair, it will act between all such pairs, changing their states as well as that of the pair we have isolated.
- So the Fermi sea will no longer be present in its unaltered form, and so the final state of the pair, which depended on the presence of the unperturbed Fermi sea, cannot be the one found above.
- In order to find the superconducting ground, a method of treating all the electrons together must be found, while using the <sup>same</sup> interaction as above.

## The BCS Ground State

Our toyst with the Fermi ground state showed that it is unstable under an attractive interaction acting between pairs of electrons of opposite momentum and spin,  $\vec{q}\uparrow$  and  $-\vec{q}\downarrow$ .

We are still in search of a new superconducting ground state.

We will now use the techniques that are usually used to examine the equilibrium states of thermodynamic system when interactions are included

We will use the following free energy (potential)

$$\Omega = E - TS - \mu N,$$

where the variables have their standard meaning.

We will put the Cooper interactions into the Fermi gas problem and find the distribution of particles among the single-particle states that minimizes  $\Omega$ .

- $\Omega$  will be minimized for a system at fixed  $T$ ,  $V$  and  $\mu$ .
- System is in a particle bath, so that  $N$  may change but  $\mu$  remains fixed
- The constant temperature in the problem is  $T=0$ .

We will still deal with electron pairs of opposite  $\vec{q}$  and spin

But now we must consider an antisymmetrized wave function of the  $N$  electron system, all together at one time.

In our endeavour to do so we will avoid the usage of second quantization techniques. So things may look cumbersome at times, but then we can save time that will go into educating or re-educating ourselves about the same.

Let us set up the machinery/notation that we will use to represent the above <sup>desired</sup> ground state.

$|0\rangle \equiv$  a pair state is ~~either~~ unoccupied,

$|1\rangle \equiv$  a pair state is occupied.

Note that a state is available for occupation by a single electron in the perfect Fermi gas that has

{ momentum  $\hbar\vec{q}$   
energy  $\hbar^2\vec{q}^2/2m$   
. spin up }.

and another state with

{ momentum  $-\hbar\vec{q}$   
energy  $\hbar^2\vec{q}^2/2m$   
. spin down }.

$|0\rangle \Rightarrow$  both states are empty,

$|1\rangle \Rightarrow$  both states are occupied.

Sometimes we will use subscript  $\vec{q}$  to indicate that it is the pair  $(\vec{q}\uparrow, -\vec{q}\downarrow)$ .

- The wave function of the  $N$  electron system is

$$|\psi\rangle = \prod_{\vec{q}} (a_{\vec{q}}|0\rangle + b_{\vec{q}}|1\rangle)$$

where  $a_{\vec{q}}$  and  $b_{\vec{q}}$  are just numbers.

→ They give the amplitudes for the pair state  $\vec{q}$  to be empty or full.

→ In the noninteracting ground state,

$$\begin{cases} b_{\vec{q}} = 1 \text{ and } a_{\vec{q}} = 0 & \text{for all states up to the Fermi level.} \\ b_{\vec{q}} = 0 \text{ and } a_{\vec{q}} = 1 & \text{for all states above the Fermi level.} \end{cases}$$

→ Also, for any state  $\vec{q}$ ,

$$\langle 0|0\rangle = 1,$$

$$\langle 1|1\rangle = 1,$$

$$\langle 0|1\rangle = 0.$$

→ Products commute when they refer to different states:

$$(a_{\vec{q}}|0\rangle_{\vec{q}} + b_{\vec{q}}|1\rangle_{\vec{q}})(a_{\vec{q}'}|0\rangle_{\vec{q}'} + b_{\vec{q}'}|1\rangle_{\vec{q}'}) = (a_{\vec{q}}|0\rangle_{\vec{q}} + b_{\vec{q}}|1\rangle_{\vec{q}})(a_{\vec{q}'}|0\rangle_{\vec{q}'} + b_{\vec{q}'}|1\rangle_{\vec{q}}).$$

→ The probability that a state is occupied:  $b_{\vec{q}}^2$   
 unoccupied:  $a_{\vec{q}}^2$

and so, we always have

$$a_{\vec{q}}^2 + b_{\vec{q}}^2 = 1.$$

→ Since  $b_{\vec{q}}^2$  is the probability of finding a pair in state  $\vec{q}$ ,

so

$$N = 2 \sum_{\vec{q}} b_{\vec{q}}^2.$$

→ Normalization of the overall state

$$\begin{aligned} \langle \Psi | \Psi \rangle &= \prod_{\vec{q}} (\langle 0|a_{\vec{q}} + \langle 1|b_{\vec{q}}) \prod_{\vec{q}'} (a_{\vec{q}'}|0\rangle + b_{\vec{q}'}|1\rangle) \\ &= \dots (\langle 0|a_k + \langle 1|b_k)(a_k|0\rangle + b_k|1\rangle) \dots \\ &= \dots (a_k^2 \langle 0|0\rangle + b_k^2 \langle 1|1\rangle + a_k b_k \langle 0|1\rangle + a_k b_k \langle 1|0\rangle) \dots \\ &= \dots (a_k^2 + b_k^2) \dots \\ &= \dots (1) \dots \end{aligned}$$

(same is true for any  $k$  state).

$$\Rightarrow \langle \Psi | \Psi \rangle = 1.$$

## Manybody Hamiltonian

- For the kinetic energy component, define an operator

(  $\mathcal{H}_{0\vec{q}}$  which has the following properties

$$\left\{ \begin{array}{l} \mathcal{H}_{0\vec{q}} |1\rangle_{\vec{q}} = \frac{\hbar^2 q^2}{m} |1\rangle_{\vec{q}} \\ \text{and } \mathcal{H}_{0\vec{q}} |0\rangle_{\vec{q}} = 0. \end{array} \right.$$

$\mathcal{H}_{0\vec{q}}$  does not act on any state other than  $|\vec{q}\rangle$ .

So, the kinetic energy of the system is described by the operator

$$\boxed{\mathcal{H}_0 = \sum_{\vec{q}} \mathcal{H}_{0\vec{q}}}.$$

The kinetic energy of the system is given by

$$\langle \psi | \mathcal{H}_0 | \psi \rangle = \prod_{\vec{q}} (\langle 0 | a_{\vec{q}} + \langle 1 | b_{\vec{q}}) \left( \sum_{\vec{q}'} \mathcal{H}_{0\vec{q}'} \right) \prod_{\vec{q}''} (a_{\vec{q}''} |0\rangle + b_{\vec{q}''} |1\rangle).$$

$$= \sum_{\vec{q}} b_{\vec{q}}^2 \frac{\hbar^2 q^2}{m}.$$

## • Potential energy component

Let the operator  $\hat{V}_{\vec{q}\vec{q}'}$  scatters pairs from state  $\vec{q}$  to another  $\vec{q}'$ .

→ It always acts on two pair states at a time.

$$\hat{V}_{\vec{q}\vec{q}'} |10\rangle_{\vec{q}} |11\rangle_{\vec{q}'} = V_{\vec{q}\vec{q}'} |11\rangle_{\vec{q}'} |10\rangle_{\vec{q}} .$$

So, the operator has scattered, with strength  $V_{\vec{q}\vec{q}'}$  (just a number), an occupied state  $\vec{q}$  to an empty state  $\vec{q}'$ .

→ If it does not find both  $\vec{q}$  occupied and  $\vec{q}'$  empty, it gives zero:

$$\hat{V}_{\vec{q}\vec{q}'} |10\rangle_{\vec{q}'} |10\rangle_{\vec{q}} = 0$$

$$\hat{V}_{\vec{q}\vec{q}'} |11\rangle_{\vec{q}'} |11\rangle_{\vec{q}} = 0$$

$$\hat{V}_{\vec{q}\vec{q}'} |11\rangle_{\vec{q}'} |10\rangle_{\vec{q}} = 0.$$

Thus, the potential energy of the system (owing to this interaction only) is described by

$$H_I = \sum_{\vec{q}\vec{q}'} \hat{V}_{\vec{q}\vec{q}'} .$$

The potential energy Hamiltonian is the interaction between all pairs of pair states.

(Here the double sum does not count each pair twice, since the interaction goes one way - from  $\vec{q}$  to  $\vec{q}'$ , not reverse).

→ Potential energy

$$\langle \psi | \mathcal{H}_1 | \psi \rangle = \prod_{\vec{q}} (\langle 0 | a_{\vec{q}} + \langle 1 | b_{\vec{q}}) \left( \sum_{\vec{q}\vec{q}''} \hat{V}_{\vec{q}\vec{q}''} \right) \prod_{\vec{q}''} (a_{\vec{q}''}|0\rangle + b_{\vec{q}''}|1\rangle)$$

Consider one of the terms

$$\dots (\langle 0 | a_{\vec{q}} + \langle 1 | b_{\vec{q}}) (\langle 0 | a_{\vec{q}'} + \langle 1 | b_{\vec{q}'}) \hat{V}_{\vec{q}\vec{q}'} (a_{\vec{q}'}|0\rangle + b_{\vec{q}'}|1\rangle) \dots \times (a_{\vec{q}}|0\rangle + b_{\vec{q}}|1\rangle) \dots$$

→ All other terms in the two products, of the form

$$\dots (\langle 0 | a_{\vec{k}} + \langle 1 | b_{\vec{k}}) \dots (a_{\vec{k}}|0\rangle + b_{\vec{k}}|1\rangle) \dots$$

commute with everything but their opposite numbers, coming together to give the factor one.

$$\rightarrow \hat{V}_{\vec{q}\vec{q}'} a_{\vec{q}'}|0\rangle, a_{\vec{q}'}|0\rangle_{\vec{q}} = 0, \dots$$

$$\hat{V}_{\vec{q}\vec{q}'} a_{\vec{q}'}|0\rangle, b_{\vec{q}'}|1\rangle_{\vec{q}} = \hat{V}_{\vec{q}\vec{q}'} a_{\vec{q}'} b_{\vec{q}'}|1\rangle_{\vec{q}},$$

this still gives zero when combined with the terms on the left, except for

$$\langle 0 | a_{\vec{q}} a_{\vec{q}'} | 1 | b_{\vec{q}} b_{\vec{q}'} \rangle = V_{\vec{q}\vec{q}'} a_{\vec{q}} b_{\vec{q}'} a_{\vec{q}'} b_{\vec{q}'}$$

(only this term <sup>contribution</sup> survives from every term in the double sum).

→ The potential energy of the system is

$$\boxed{\langle \psi | \mathcal{H}_1 | \psi \rangle = \sum_{\vec{q}\vec{q}'} V_{\vec{q}\vec{q}'} a_{\vec{q}} a_{\vec{q}'} b_{\vec{q}} b_{\vec{q}'}}.$$

→ Therefore, the energy of the system is given by

$$E = \sum_{\vec{q}} b_{\vec{q}}^2 \frac{\hbar^2 q^2}{m} + \sum_{\vec{q}, \vec{q}'} V_{\vec{q}\vec{q}'} a_{\vec{q}} a_{\vec{q}'} b_{\vec{q}} b_{\vec{q}'}.$$

→ To find the ground state  $\Omega$  must be minimized,  
since we have assumed  $T=0$ ,

$$\Omega = E - \mu N.$$

→ Therefore,

$$\Omega = \sum_{\vec{q}} \left( \frac{\hbar^2 q^2}{m} - \mu \right) b_{\vec{q}}^2 + \sum_{\vec{q}, \vec{q}'} V_{\vec{q}\vec{q}'} a_{\vec{q}} a_{\vec{q}'} b_{\vec{q}} b_{\vec{q}'}$$

$$= \sum_{\vec{q}} \left[ 2 \xi_{\vec{q}}^* b_{\vec{q}}^2 + \sum_{\vec{q}'} V_{\vec{q}\vec{q}'} a_{\vec{q}} a_{\vec{q}'} b_{\vec{q}} b_{\vec{q}'} \right],$$

where  $\xi_{\vec{q}} = \frac{\hbar^2 q^2}{2m} - \mu.$

$\xi_{\vec{q}}$  is the energy of one electron in the pair relative to the Fermi level.

→  $a_{\vec{q}}$  and  $b_{\vec{q}}$  are related:  $a_{\vec{q}}^2 + b_{\vec{q}}^2 = 1$ .  
So in order to deal with only one parameter, define the angle  $\theta_{\vec{q}}$  by  $\begin{cases} b_{\vec{q}} = \cos \theta_{\vec{q}} \\ a_{\vec{q}} = \sin \theta_{\vec{q}} \end{cases}$ .

→ So we have

$$\Omega = \sum_{\vec{q}} \left[ 2 \sum_{\vec{q}} \cos^2 \theta_{\vec{q}} + \frac{1}{4} \sum_{\vec{q}'} \sin 2\theta_{\vec{q}} \sin 2\theta_{\vec{q}'} \right].$$

(Note that  
 $\sin 2\theta = 2 \cos \theta \sin \theta$ )

→ Let us now minimize  $\Omega$  with respect to any one of the

$\theta_{\vec{q}}$ , say  $\theta_{\vec{k}}$ :

$$0 = \frac{\partial \Omega}{\partial \theta_{\vec{k}}} = -4 \sum_{\vec{K}} \cos \theta_{\vec{K}} \sin \theta_{\vec{K}} + \frac{1}{2} \cos 2\theta_{\vec{K}} \sum_{\vec{q}'} V_{\vec{q}\vec{K}} \sin 2\theta_{\vec{q}'} \\ + \frac{1}{2} \cos 2\theta_{\vec{K}} \sum_{\vec{q}} V_{\vec{q}\vec{K}} \sin 2\theta_{\vec{q}}.$$

$$= -2 \sum_{\vec{K}} \sin 2\theta_{\vec{K}} + \cos 2\theta_{\vec{K}} \sum_{\vec{q}} V_{\vec{q}\vec{K}} \sin 2\theta_{\vec{q}}$$

or,  $\left[ \tan 2\theta_{\vec{K}} = \frac{1}{2} \sum_{\vec{q}} V_{\vec{q}\vec{K}} \sin 2\theta_{\vec{q}} \right]$

( $\vec{q}$  is a dummy variable above)

→ Define  $\Delta_{\vec{K}}$ ,

$$\Delta_{\vec{K}} = -\frac{1}{2} \sum_{\vec{q}} V_{\vec{q}\vec{K}} \sin^2 \theta_{\vec{q}}$$

so that

$$\boxed{\tan 2\theta_{\vec{K}} = -\frac{\Delta_{\vec{K}}}{\sum_{\vec{q}} V_{\vec{q}\vec{K}}}}.$$

→ Since  $\tan 2\theta_K$  is negative, either  $\sin 2\theta_K$  or  $\cos 2\theta_K$  must be negative.

If we choose cosine to be negative, then

$$\sin 2\theta_K = \frac{\Delta_K}{\sqrt{e_K^2 + \Delta_K^2}}$$

$$\cos 2\theta_K = -\frac{e_K}{\sqrt{e_K^2 + \Delta_K^2}}.$$

Why is this the correct choice of signs?

The above eqn. can be written as

$$b_K^2 - a_K^2 = -\frac{e_K}{\sqrt{e_K^2 + \Delta_K^2}}.$$

For states very far above the Fermi level, the weak interaction will make no difference, so in the

limit as  $e_K \rightarrow \infty$ ,  $b_K^2 \rightarrow 0$  and  $a_K^2 \rightarrow 0$ .

We expect very high energy states to be empty.

Finally we have

$$\Delta_K = -\frac{1}{2} \sum_{\vec{q}} V_{\vec{q}K} \frac{\Delta_{\vec{q}}}{\sqrt{e_{\vec{q}}^2 + \Delta_{\vec{q}}^2}}.$$

- The RHS of the previous equation depends on  $\vec{K}$  only through the interaction  $V_{\vec{q}\vec{k}}$ .
- The interaction can connect pair states that differ in energy by no more than  $\hbar\omega_D$  and it is angle independent.

$$\rightarrow \begin{cases} V_{\vec{q}\vec{k}} = -V & \text{if } |\xi_{\vec{q}}| \leq \hbar\omega_D \text{ & } |\xi_{\vec{k}}| \leq \hbar\omega_D \\ & \\ & = 0 \quad \text{otherwise.} \end{cases}$$

- In the earlier calculation, the interactions were restricted to a shell of states above the Fermi level.

Now there will be some amplitude for states to be available below the Fermi level as well.  
So the shell of interactions goes both above and below the Fermi level.

$$\rightarrow \Delta_{\vec{K}} = \frac{1}{2} V \sum_{\vec{q}} \frac{\Delta_{\vec{q}}}{\sqrt{\xi_{\vec{q}}^2 + \Delta_{\vec{q}}^2}}$$

Observe that the term on the RHS no longer depends on  $\vec{K}$ , so  $\Delta_{\vec{K}}$  does not depend on  $\vec{K}$ , nor does  $\Delta_{\vec{q}}$  depend on  $\vec{q}$ .

→ Therefore,

$$\Delta_0 = \frac{1}{2} V \sum_{\vec{q}} \frac{\Delta_0}{\sqrt{\xi_{\vec{q}}^2 + \Delta_0^2}}$$

Or.

$$1 = \frac{1}{2} V \sum_{\vec{q}} \frac{1}{\sqrt{\xi_{\vec{q}}^2 + \Delta_0^2}}$$

$$= \frac{1}{2} V \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{S(\xi) d\xi}{\sqrt{\xi^2 + \Delta_0^2}} .$$

Use  $S(\xi) \approx S(0)$  in the narrow shell of states within  $\hbar\omega_D$  of the Fermi level.

$$1 = \frac{S(0)V}{2} \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\xi}{\sqrt{\xi^2 + \Delta_0^2}}$$

$$= S(0)V \sinh^{-1} \left( \frac{\hbar\omega_D}{\Delta_0} \right) .$$

Solve for  $\Delta_0$ ,

$$\Delta_0 = \frac{\hbar\omega_D}{\sinh [1/(S(0)V)]}$$

$$\approx 2\hbar\omega_D e^{-1/(S(0)V)}$$

for small  $V$ .