PHY 742 Quantum Mechanics II 1-1:50 AM MWF via video link:

https://wakeforest-university.zoom.us/my/natalie.holzwarth
Extra notes for Lecture 34

A short introduction to the quantum theory of superconductivity

Bardeen, Cooper, Scrieffer, Phys. Rev. 108, 1175 (1957)

- 1. Cooper pairs
- 2. Gap equation
- 3. Estimate of T_c

Some of the slides contain materials from the textbook, Solid State Physics; Second Edition by Giuseppe Grosso and Giuseppe Pastori Parravicini (Academic Press, 2014)

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 1

We will go over some of the concepts of this famous paper.

21	Mon: 03/23/2020	Chap. 17	Quantization of the Electromagnetic Field	#17	03/25/2020
22	Wed: 03/25/2020	Chap. 17	Quantization of the Electromagnetic Field	#18	03/27/2020
23	Fri: 03/27/2020	Chap. 17	Quantization of the Electromagnetic Field	#19	03/30/2020
24	Mon: 03/30/2020	Chap. 18	Photons and atoms		
25	Wed: 04/01/2020	Chap. 10	Multiparticle systems	#20	04/03/2020
26	Fri: 04/03/2020	Chap. 10	Multiparticle systems	<u>#21</u>	04/06/2020
27	Mon: 04/06/2020	Chap. 10	Multielectron atoms	#22	04/08/2020
28	Wed: 04/08/2020	Chap. 10	Multielectron atoms		
	Fri: 04/10/2020	No class	Good Friday		
29	Mon: 04/13/2020	Chap. 10	Multielectron atoms	#23	04/15/2020
30	Wed: 04/15/2020		Hartree-Fock and other formalisms	<u>#24</u>	04/17/2020
31	Fri: 04/17/2020		Density functional theory		
32	Mon: 04/20/2020		Density functional theory for atoms		
33	Wed: 04/22/2020		Practial density functional theory		
34	Fri: 04/24/2020		Brief discussion of BCS theory of superconductivity		
35	Mon: 04/27/2020		Review		
36	Wed: 04/29/2020		Review		

Ongoing schedule

PHYSICAL REVIEW

VOLUME 108, NUMBER 5

DECEMBER 1, 1957

Theory of Superconductivity*

J. BARDEEN, L. N. COOFER,† AND J. R. SCHRIEFFER,‡
Department of Physics, University of Illinois, Urbana, Illinois
(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $(\hbar\omega)^*$, consistent with the isotope effect. A mutually orthogonal set of excited states in

one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5kT_{\rm e}$ at $T\!=\!0^{\rm T\!\!\! K}$ to zero at $T_{\rm e}$. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

Some of you may wish to read the paper which is available from zsr.wfu.edu and a pdf file is available on our webpage.

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

The Nobel Prize in Physics 1972



Photo from the Nobel Foundation archive.

John Bardeen

Prize share: 1/3



Photo from the Nobel Foundat archive. Leon Neil Cooper Prize share: 1/3



Photo from the Nobel Foundatio archive. John Robert Schrieffer

The Nobel Prize in Physics 1972 was awarded jointly to John Bardeen, Leon Neil Cooper and John Robert Schrieffer "for their jointly developed theory of superconductivity, usually called the BCS-theory."

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 4

Last time, we discussed the phenomenological theory of Fritz London which set up key aspects of the superconducting state. London established that there is a macroscopic current confined near the surface of the superconductor which screens out the B field within the material. BCS showed a model for the microscopic origin of this current.

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

Notion of a Cooper pair

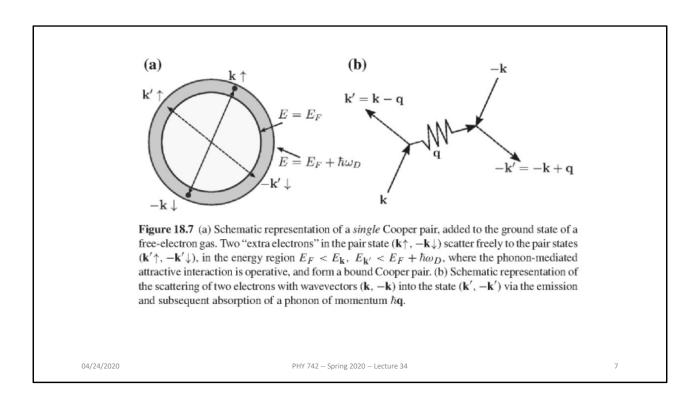
Starting with a material with all the states filled up to the Fermi level, we focus attention on a pair of states which have a net attractive interaction $U(r_1, r_2)$:

$$\left[\frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + U(\mathbf{r}_1, \mathbf{r}_2)\right] \psi(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2) = E \psi(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2)$$

$$\psi(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2) = \phi(\mathbf{r}_1,\mathbf{r}_2)\chi(\sigma_1,\sigma_2)$$

The thinking is that the interaction is related to lattice vibrations and had an energy $\hbar\omega_D$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34



Not sure that this helps... The thinking is that the pair of states are very close to the Fermi level.

Properties of pair wavefunction

$$\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \phi(\mathbf{r}_1, \mathbf{r}_2)\chi(\sigma_1, \sigma_2)$$
Note: $\sigma = \alpha \equiv \uparrow$

$$\sigma = \beta \equiv \downarrow$$

Spin part:

$$\chi^{(S=0)} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)].$$
or
$$\chi^{S=0}(\sigma_1, \sigma_2) = -\chi^{S=0}(\sigma_2, \sigma_1)$$

$$\Rightarrow \phi^{S=0}(\mathbf{r}_1, \mathbf{r}_2) = \phi^{S=0}(\mathbf{r}_2, \mathbf{r}_1)$$

Spin part: Note that:
$$\chi^{(S=0)} = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]. \qquad \chi^{S=0}(\sigma_1, \sigma_2) = -\chi^{S=0}(\sigma_2, \sigma_1)$$
 or
$$\Rightarrow \phi^{S=0}(\mathbf{r}_1, \mathbf{r}_2) = \phi^{S=0}(\mathbf{r}_2, \mathbf{r}_1)$$
 Note that:
$$\chi^{(S=1)} = \begin{cases} \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)]. & \chi^{S=1}(\sigma_1, \sigma_2) = \chi^{S=1}(\sigma_2, \sigma_1) \\ \beta(1)\beta(2), & \chi^{S=1}(\mathbf{r}_1, \mathbf{r}_2) = -\phi^{S=1}(\mathbf{r}_2, \mathbf{r}_1) \end{cases}$$

$$\Rightarrow \phi^{S=1}(\mathbf{r}_1, \mathbf{r}_2) = -\phi^{S=1}(\mathbf{r}_2, \mathbf{r}_1)$$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

The pair of electrons can have total spin 0 or 1 which determines the spatial symmetry to be symmetric or antisymmetric, respectively.

Here are some possible functional forms for the spatial part of the Cooper pair. Which of these are associated with S=0 and which are associated with S=1?

1.
$$\phi(\mathbf{r}_1, \mathbf{r}_2) = A\cos(k(\mathbf{r}_1 - \mathbf{r}_2))$$

2.
$$\phi(\mathbf{r}_1, \mathbf{r}_2) = A \sin(k(\mathbf{r}_1 - \mathbf{r}_2))$$

04/24/2020

PHY 742 -- Spring 2020 -- Lecture 34

9

Properties of pair wavefunction – continued

Assume that the electron pair can be represented by a linear combination of plane wave states of wavevectors k and -k:

$$\phi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\mathbf{k}} g(\mathbf{k}) \frac{1}{V} e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)}$$

What is g(k)?

Note that:

$$g^{S=0}(\mathbf{k}) = g^{S=0}(-\mathbf{k})$$

$$g^{S=1}(\mathbf{k}) = -g^{S=1}(-\mathbf{k})$$

Note that the states composing Cooper pairs are supposed to exist in the energy range $E_F \le E_{\mathbf{k}} \le E_F + \hbar \omega_D$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

It will be convenient to express the spatial part in terms of the Fourier representation.

Define Fourier transform of interaction potential:

$$\begin{split} U_{\mathbf{k}\mathbf{k}'} &= \iint \frac{1}{V} e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} U(\mathbf{r}_1-\mathbf{r}_2) \frac{1}{V} e^{i\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{r}_2)} d\mathbf{r}_1 d\mathbf{r}_2 \\ &= \frac{1}{N\Omega} \int e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} U(\mathbf{r}) \, d\mathbf{r} \end{split}$$

V volume of sample composed of N unit cells

 Ω volume of unit cell

Equation satisfied by pair amplitude functions:

$$(2E_{\mathbf{k}} - E)g(\mathbf{k}) + \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'}g(\mathbf{k}') = 0$$
 $E_F < E_{\mathbf{k}}, E_{\mathbf{k}'} < E_F + \hbar\omega_D$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 11

Here is the equation that the unknow amplitude g(k) must satisfy. The initial states are below the Fermi level and scattered states are above the Fermi level.

Cooper pair equations -- continued

$$(2E_{\mathbf{k}} - E)g(\mathbf{k}) + \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'}g(\mathbf{k}') = 0$$
 $E_F < E_{\mathbf{k}}, E_{\mathbf{k}'} < E_F + \hbar\omega_D$

Simplified model for interaction:

$$U_{\mathbf{k}\mathbf{k}'} = -U_0/N$$

$$(2E_{\bf k}-E)g({\bf k})-U_0\frac{1}{N}\sum_{{\bf k}'}g({\bf k}')=0 \qquad E_F < E_{\bf k}, E_{{\bf k}'} < E_F + \hbar\omega_D; \quad U_0 > 0.$$

In this approximation, for triplet states $\sum_{\mathbf{k}} g^{S=1}(\mathbf{k}) = 0$

 \Rightarrow Cooper pair states can only be singlet states

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 12

Simplifying the interaction term to a constant. Why must Cooper pair states have singlet spin?

Cooper pair equations -- continued

Non-trivial solution for singlet state:

$$(2E_{\mathbf{k}} - E)g(\mathbf{k}) - U_0 \frac{1}{N} \sum_{\mathbf{k}'} g(\mathbf{k}') = 0$$

$$E_{pair}$$

Equation to determine eigenstate energy:

$$\begin{split} 1 &= U_0 \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}} - E_{\mathrm{pair}}} &\quad E_F < E_{\mathbf{k}} < E_F + \hbar \omega_D. \\ 1 &= U_0 \frac{1}{N} \int_{E_F}^{E_F + \hbar \omega_D} D_0(E) \frac{1}{2E - E_{\mathrm{pair}}} \, dE, &\quad \text{into the result?} \end{split}$$

Density of states (one electron basis)

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 13

How does the derivation of the eigenstate energy equation work?

Cooper pair equations -- continued

$$1 = U_0 \, n_0 \int_{E_F}^{E_F + \hbar \omega_D} \frac{1}{2E - E_{\rm pair}} \, dE = \frac{1}{2} U_0 \, n_0 \, \ln \frac{2E_F + 2\hbar \omega_D - E_{\rm pair}}{2E_F - E_{\rm pair}}$$

where
$$n_0 \equiv \frac{D_0(E_F)}{N} = \frac{3}{4} \frac{Z}{E_F}$$
 denoting Fermi level DOS for a single spin for simple metal of valence Z

 $\Delta_b = 2E_F - E_{\rm pair} = \hbar \omega_D \frac{e^{-1/U_0 \, n_0}}{\sinh[1/U_0 n_0]} \approx 2\hbar \omega_D \exp[-2/U_0 n_0].$

Shows that a singlet Cooper pair is more stable than the independent particle system even for small U_0 .

What justifies this conclusion?

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

Why do we conclude that the Cooper pair is more stable?

Second quantization

$$\left\{c_{\mathbf{k}\sigma},c_{\mathbf{k}'\sigma'}\right\} = \left\{c_{\mathbf{k}\sigma}^{\dagger},c_{\mathbf{k}'\sigma'}^{\dagger}\right\} = 0, \qquad \left\{c_{\mathbf{k}\sigma},c_{\mathbf{k}'\sigma'}^{\dagger}\right\} = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}.$$

Note that the Cooper pair singlet state can be written

$$\psi(\mathbf{r}_{1}\sigma_{1}, \mathbf{r}_{2}\sigma_{2}) = \sum_{\mathbf{k}} g(\mathbf{k}) \frac{1}{\sqrt{2}} \frac{1}{V} \left[e^{i\mathbf{k}\cdot(\mathbf{r}_{1}-\mathbf{r}_{2})} \alpha(1)\beta(2) - e^{-i\mathbf{k}\cdot(\mathbf{r}_{1}-\mathbf{r}_{2})} \beta(1)\alpha(2) \right]$$
$$= \sum_{\mathbf{k}} g(\mathbf{k}) c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} |0\rangle,$$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

It is convenient to use second quantization

Consider a ground state wavefunction of the form

$$|\Psi_{\mathcal{S}}\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger}\right) |0\rangle \,,$$

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1 \qquad \text{probability amplitude for forming Cooper pair}$$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

Hamiltonian of the BCS model. The parameters u and v will be determined variationally.

Need to minimize the expectation value:

$$W_S = \langle \Psi_S | H_{\rm BCS} | \Psi_S \rangle$$

$$H_{BCS} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \left(c_{\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\uparrow} + c_{-\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\uparrow} \right) + \sum_{\mathbf{k}\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \right)$$

$$\varepsilon_{\mathbf{k}} = E_{\mathbf{k}} - \mu = (\hbar^2 \mathbf{k}^2 / 2m) - \mu$$

Here μ is essentially E_{F} .

After some algebra:

$$W_S = \langle \Psi_S | H_{\rm BCS} | \Psi_S \rangle = 2 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}$$

04/24/2020

PHY 742 -- Spring 2020 -- Lecture 34

17

Writing out the energy to be determined variationally.

Convenient transformation:

$$\begin{cases} u_{\mathbf{k}} = \cos \theta_{\mathbf{k}} & \Longrightarrow \sin 2\theta_{\mathbf{k}} = 2u_{\mathbf{k}}v_{\mathbf{k}}; \quad \cos 2\theta_{\mathbf{k}} = u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2. \\ W_S = 2 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \sin^2 \theta_{\mathbf{k}} + \frac{1}{4} \sum_{\mathbf{k}\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k}'} \\ \frac{\partial W_S}{\partial \theta_{\mathbf{k}}} = 0 & \Longrightarrow 2\varepsilon_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} + \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} \cos 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k}'} = 0 \\ & \Longrightarrow 2\varepsilon_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} \left(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 \right) u_{\mathbf{k}'} v_{\mathbf{k}'} = 0 \end{cases}$$

Define: $\Delta_{\bf k} = -\sum_{\substack{{\bf k}'\\ {\rm PHY}\,742\,-\,Spring\,2020\,-\,Lecture\,34}} U_{{\bf k}{\bf k}'} u_{{\bf k}'} v_{{\bf k}'}.$

Clever tricks and notations.

04/24/2020

In terms of the "gap parameter" the variational equations become:

$$2\varepsilon_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} - \Delta_{\mathbf{k}}\left(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2\right) = 0.$$

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left[1 + \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}} \right] \quad \text{ and } \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left[1 - \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}} \right].$$

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2}}$$

04/24/2020

PHY 742 -- Spring 2020 -- Lecture 34

19

In the end, we have an integral equation for the gap parameter.

Simplified model

$$\begin{split} U_{\mathbf{k}\mathbf{k}'} &= \begin{cases} -U_0/N & \text{if } |\varepsilon_{\mathbf{k}}|, |\varepsilon_{\mathbf{k}'}| < \hbar\omega_D \quad (U_0 > 0), \\ 0 & \text{otherwise,} \end{cases} \\ \Delta_{\mathbf{k}} &= \begin{cases} \Delta_0 & \text{if } |\varepsilon_{\mathbf{k}}| < \hbar\omega_D, \\ 0 & \text{otherwise.} \end{cases} \\ 1 &= \frac{1}{2}U_0\frac{1}{N}\sum_{\mathbf{k}'}\frac{1}{\sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_0^2}} \quad \text{with} \quad -\hbar\omega_D < \varepsilon_{\mathbf{k}'} < \hbar\omega_D. \end{split}$$

$$\mbox{Using DOS:} \qquad 1 = \frac{1}{2} U_0 n_0 \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_0^2}} \, ,$$

04/24/2020

PHY 742 -- Spring 2020 -- Lecture 34

Make a simplified model for the interaction term in order to solve the equation.

$$1 = \frac{1}{2} U_0 n_0 \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_0^2}} = U_0 n_0 \sinh^{-1} \frac{\hbar\omega_D}{\Delta_0}$$

Solving for the gap parameter:

$$\Delta_0 = \frac{\hbar \omega_D}{\sinh{(1/U_0 n_0)}} \approx 2\hbar \omega_D \exp[-1/U_0 n_0]$$

Estimating the ground state energy of the superconducting state:

$$W_S - W_N = 2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'} - 2\sum_{\mathbf{k}}^{k < k_F} \varepsilon_{\mathbf{k}}.$$

04/24/2020

PHY 742 -- Spring 2020 -- Lecture 34

21

Estimating the ground state energy of the superconducting state – continued

Using the variational solution and integrating the DOS:

$$\begin{split} W_S - W_N &= D_0(E_F) \int_{-\hbar\omega_D}^{\hbar\omega_D} \left(\varepsilon - \frac{2\varepsilon^2 + \Delta_0^2}{2\sqrt{\varepsilon^2 + \Delta_0^2}} \right) d\varepsilon - D_0(E_F) \int_{-\hbar\omega_D}^0 2\varepsilon \, d\varepsilon. \\ W_S - W_N &= D_0(E_F) \left[-\hbar\omega_D \sqrt{\hbar^2 \omega_D^2 + \Delta_0^2} + \hbar^2 \omega_D^2 \right]. \\ &\thickapprox - \frac{1}{2} D_0(E_F) \Delta_0^2 \end{split}$$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

Here we assume that the gap parameter is smaller that the phonon energy.

Effects of temperature:

Thermal average of Cooper pair operator:

$$a_{\mathbf{k}} = \left\langle c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} \right\rangle_{T}$$

Define

$$c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}=a_{\mathbf{k}}+\left(c_{\mathbf{k}\uparrow}^{\dagger}c_{-\mathbf{k}\downarrow}^{\dagger}-a_{\mathbf{k}}\right),$$
 average

Now we need to consider how temperature affects the analysis.

04/24/2020

PHY 742 -- Spring 2020 -- Lecture 34

Modified Gap relationship

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} [1 - 2f(w_{\mathbf{k}'})] \quad \text{with} \quad w_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}.$$

Fermi-Dirac distribution

$$f(E) = \frac{1}{e^{\beta E} + 1} \quad \Longrightarrow \quad 1 - 2f(E) = \tanh\frac{\beta E}{2},$$

Modified Gap equation

$$\boxed{\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2}} \tanh \frac{\beta \sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2}}{2}}.$$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 2

Introducing the Fermi-Dirac distribution

Simplified model

$$U_{\mathbf{k}\mathbf{k}'} = \begin{cases} -U_0/N & \text{if } |\varepsilon_{\mathbf{k}}|, |\varepsilon_{\mathbf{k}'}| < \hbar\omega_D & (U_0 > 0), \\ 0 & \text{otherwise,} \end{cases}$$

$$1 = \frac{1}{2} U_0 n_0 \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh \frac{\beta \sqrt{\varepsilon^2 + \Delta^2}}{2},$$

Determine the critical temperature such that $\Delta(T_c) = 0$:

$$1 = U_0 n_0 \int_0^{\hbar \omega_D} \frac{1}{\varepsilon} \tanh \frac{\varepsilon}{2k_B T_c} d\varepsilon,$$

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 2

Evaluating expressions for simplified model

Evaluation of the integral

$$\begin{split} I(a) &= \int_0^a \frac{1}{x} \tanh x \, dx = \left[\tanh x \, \ln x\right]_0^a - \int_0^a \ln x \frac{1}{\cosh^2 x} \, dx \\ (\text{for } a \gg 1) &\approx \ln a - \int_0^\infty \ln x \, \frac{1}{\cosh^2 x} \, dx = \ln a + \ln \frac{4\gamma}{\pi} \quad \gamma = 1.78107 \dots \end{split}$$
 If $\frac{\hbar \omega_D}{2kT_c} >> 1$:
$$\int_0^{\hbar \omega_D/2k_BT_c} \frac{1}{x} \tanh x \, dx = \ln \left(\frac{2\gamma}{\pi} \frac{\hbar \omega_D}{k_BT_c}\right) \approx \ln \frac{1.13\hbar \omega_D}{k_BT_c} = \frac{1}{U_0n_0}. \end{split}$$

Then, in the weak coupling limit $U_0 n_0 \ll 1$ and $\hbar \omega_D / k_B T_c \gg 1$, we have $k_B T_c = 1.13 \, \hbar \omega_D \exp[-1/U_0 n_0]$.

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 26

Some arithmetic...

Numerical evaluation of integral:

$$\begin{split} 1 &= \frac{1}{2} U_0 n_0 \int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh \frac{\beta \sqrt{\varepsilon^2 + \Delta^2}}{2}. \\ &1 &= U_0 n_0 \int_0^{\hbar\omega_D} \frac{1}{\varepsilon} \tanh \frac{\varepsilon}{2k_B T_c} \, d\varepsilon, \end{split}$$

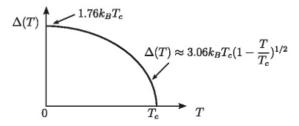


Figure 18.12 Behavior of the energy gap parameter $\Delta(T)$ for a superconductor in the BCS theory and in weak coupling limit.

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34 27

At the critical temperature, the gap is 0. Graph shows qualitative temperature dependence.

Estimation of critical magnetic field (BCS paper)

$$H_c^2/8\pi = F_n - F_s$$

Free energy of normal state

Free energy of superconducting state

After some approximations, etc.:
$$\frac{H_c^2}{8\pi} = N(0)(\hbar\omega)^2 \left\{ \left[1 + \left(\frac{\epsilon_0}{\hbar\omega} \right)^2 \right]^{\frac{1}{2}} - 1 \right\} - \frac{\pi^2}{3} N(0)(kT)^2 \\ \times \left\{ 1 - \beta^2 \int_0^\infty d\epsilon \left[\frac{2\epsilon^2 + \epsilon_0^2}{E} \right] f(\beta E) \right\}. \quad (3.38)$$

04/24/2020

PHY 742 -- Spring 2020 -- Lecture 34

Relationship to critical field.

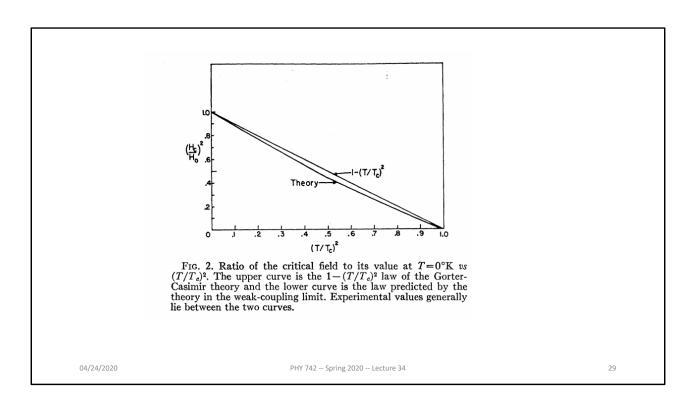


Figure from BCS theory showing agreement with experiment.

What do you think?

- 1. Full of admiration
- 2. Full of disgust
- 3. Not full
- 4. Want to read more
- 5. Never want to see this again

04/24/2020 PHY 742 -- Spring 2020 -- Lecture 34

30