PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 37

Superconductivity (Chap. 18 in GGGPP)

Other references: Schrieffer, Theory of Superconductivity, W. A. Benjamin, Inc. (1964)

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

1. **Review of T=0 analysis**
2. **Temperature dependence of superconductivity**
3. **Course evaluation forms**

Slides contain materials from GGGPP text.

23	Fri, 10/23/2015	Chap. 11	Optical and transport properties of metals	#21
24	Mon, 10/26/2015	Chap. 11	Optical and transport properties of metals	#22
25	Wed, 10/28/2015	Chap. 11	Transport in metals	#23
26	Fri, 10/30/2015	Chap. 12	Optical properties of semiconductors and insulators	
27	Mon, 11/02/2015	Chap. 7 & 12	Excitons	#24
28	Wed, 11/04/2015	Chap. 9	Lattice vibrations	#25
29	Fri, 11/06/2015	Chap. 9	Lattice vibrations	#26
30	Mon, 11/09/2015	Chap. 13	Defects in semiconductors	#27
31	Wed, 11/11/2015	Chap. 14	Transport in semiconductors	#28
32	Fri, 11/13/2015	Chap. 15	Electron gas in Magnetic fields	#29
33	Mon, 11/16/2015	Chap. 15	Electron gas in Magnetic fields	Prepare presentation.
34	Wed, 11/18/2015	Chap. 17	Magnetic ordering in crystals	Prepare presentation.
35	Fri, 11/20/2015	Chap. 18	Superconductivity	Prepare presentation.
36	Mon, 11/23/2015	Chap. 18	Superconductivity	Prepare presentation.
	Wed, 11/25/2015		*Thanksgiving Holiday*	
	Fri, 11/27/2015		*Thanksgiving Holiday*	
37	Mon, 11/30/2015	Chap. 18	Superconductivity	Prepare presentation.
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	

**Note: The final exam has the take-home form similar to that of the mid-term. In order to accommodate your schedules, it will be available on 12/04 and will be due before 9 AM on 12/14.

PHY 752 Presentation Schedule

Wednesday, December 2, 2015

	Presenter	Title of presentation
10:00-10:25	Larry Rush	First Principles Investigation of the geometrical and electrochemical properties of Na4P2S6 and Li4P2S6
10:25-10:50	Katelyn Goetz	Poole-Frenkel Effect in an Ambipolar Material

Friday, December 4, 2015

	Presenter	Title of presentation
10:00-10:25	Gabriel Marcus	Thermoelectric Materials
10:25-10:50	Nathan Beets	Magnetic fields in the Electron Gas

Some guidelines about the presentations

1. In your presentations, please make sure to acknowledge all of your sources.
2. We have allotted 25 minutes including questions for each presentation.
3. In order to encourage participation, points will be awarded for questions from the audience.
4. For efficiency, you may wish to email me your talk an use my computer for the presentation.
5. At the end each session, please email me your presentations and any supplementary materials.

PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

Theory of Superconductivity*

J. BARDEEN, L. N. COOPER,† 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 $(\hbar\omega)^2$, 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 $3.5kT_c$ at $T=0°K$ to zero at T_c. 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.

At T=0 K, a pair of electrons with a net attractive interaction are found to be stable:

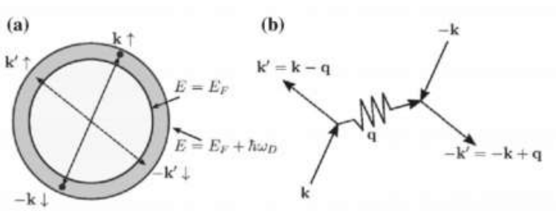

Figure 18.7 (a) Schematic representation of a *single* Cooper pair, added to the ground state of a free-electron gas. Two "extra electrons" in the pair state ($\mathbf{k}\uparrow, -\mathbf{k}\downarrow$) scatter freely to the pair states ($\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow$), in the energy region $E_F < E_{\mathbf{k}}, E_{\mathbf{k}'} < E_F + \hbar\omega_D$, where the phonon-mediated attractive interaction is operative, and form a bound Cooper pair. (b) Schematic representation of the scattering of two electrons with wavevectors ($\mathbf{k}, -\mathbf{k}$) into the state ($\mathbf{k}', -\mathbf{k}'$) via the emission and subsequent absorption of a phonon of momentum $\hbar\mathbf{q}$.

Variational determination of the ground-state wavefunction in the BCS model

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} \left(c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} + c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\downarrow} \right) + \sum_{\mathbf{kk'}} U_{\mathbf{kk'}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k'}\downarrow} c_{\mathbf{k'}\uparrow}.$$

independent particle states — Cooper-pair interaction

Consider a ground state wavefunction of the form

$$|\Psi_S\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right) |0\rangle .$$

$$u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$$

probability amplitude for forming Cooper pair

Variational determination of the ground-state wavefunction in the BCS model -- continued

Need to minimize the expectation value:

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

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

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

After some algebra:

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

Variational determination of the ground-state wavefunction in the BCS model -- continued

Convenient transformation:

$$\begin{cases} u_{\mathbf{k}} = \cos\theta_{\mathbf{k}} \\ v_{\mathbf{k}} = \sin\theta_{\mathbf{k}} \end{cases} \implies \sin 2\theta_{\mathbf{k}} = 2u_{\mathbf{k}} v_{\mathbf{k}}; \quad \cos 2\theta_{\mathbf{k}} = u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2.$$

$$W_S = 2 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \sin^2\theta_{\mathbf{k}} + \frac{1}{4} \sum_{\mathbf{kk'}} U_{\mathbf{kk'}} \sin 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k'}}$$

$$\frac{\partial W_S}{\partial \theta_{\mathbf{k}}} = 0 \implies 2\varepsilon_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} + \sum_{\mathbf{k'}} U_{\mathbf{kk'}} \cos 2\theta_{\mathbf{k}} \sin 2\theta_{\mathbf{k'}} = 0$$

$$\implies 2\varepsilon_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \sum_{\mathbf{k'}} U_{\mathbf{kk'}} \left(u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 \right) u_{\mathbf{k'}} v_{\mathbf{k'}} = 0$$

Define: $\Delta_{\mathbf{k}} = -\sum_{\mathbf{k'}} U_{\mathbf{kk'}} u_{\mathbf{k'}} v_{\mathbf{k'}}.$

Variational determination of the ground-state wavefunction in the BCS model -- continued

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

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

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

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

Variational determination of the ground-state wavefunction in the BCS model -- continued

Simplified model

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

$$\Delta_{\mathbf{k}} = \begin{cases} \Delta_0 & \text{if } |\varepsilon_{\mathbf{k}}| < \hbar\omega_D, \\ 0 & \text{otherwise}. \end{cases}$$

$$1 = \frac{1}{2}U_0 \frac{1}{N}\sum_{\mathbf{k}'} \frac{1}{\sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_0^2}} \quad \text{with} \quad -\hbar\omega_D < \varepsilon_{\mathbf{k}'} < \hbar\omega_D.$$

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

Variational determination of the ground-state wavefunction in the BCS model -- continued

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

Solving for the gap parameter:

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

Estimating the ground state energy of the superconducting state:

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

Estimating the ground state energy of the superconducting state – continued

Using the variational solution and integrating the DOS:

$$W_S - W_N = D_0(E_F)\int_{-\hbar\omega_D}^{\hbar\omega_D}\left(\varepsilon - \frac{2\varepsilon^2+\Delta_0^2}{2\sqrt{\varepsilon^2+\Delta_0^2}}\right)d\varepsilon - D_0(E_F)\int_{-\hbar\omega_D}^{0} 2\varepsilon\, d\varepsilon.$$

$$W_S - W_N = D_0(E_F)\left[-\hbar\omega_D\sqrt{\hbar^2\omega_D^2+\Delta_0^2}+\hbar^2\omega_D^2\right].$$

$$\approx -\frac{1}{2}D_0(E_F)\Delta_0^2$$

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 fluctuations

Modified Gap relationship

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

Fermi-Dirac distribution

$$f(E) = \frac{1}{e^{\beta E} + 1} \implies 1 - 2f(E) = \tanh \frac{\beta E}{2}.$$

Modified Gap equation

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

Simplified model

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

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

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

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

Evaluation of the integral

$$I(a) = \int_0^a \frac{1}{x} \tanh x \, dx = \left[\tanh x \, \ln x\right]_0^a - \int_0^a \ln x \frac{1}{\cosh^2 x} \, dx$$

$$(\text{for } a \gg 1) \approx \ln a - \int_0^\infty \ln x \frac{1}{\cosh^2 x} \, dx = \ln a + \ln \frac{4\gamma}{\pi} \quad \gamma = 1.78107\ldots$$

If $\frac{\hbar\omega_D}{2kT_c} >> 1$:

$$\int_0^{\hbar\omega_D/2k_B T_c} \frac{1}{x} \tanh x \, dx = \ln\left(\frac{2\gamma}{\pi} \frac{\hbar\omega_D}{k_B T_c}\right) \approx \ln \frac{1.13\hbar\omega_D}{k_B T_c} = \frac{1}{U_0 n_0}.$$

Then, in the weak coupling limit $U_0 n_0 \ll 1$ and $\hbar\omega_D / k_B T_c \gg 1$, we have

$$k_B T_c = 1.13 \, \hbar\omega_D \exp[-1/U_0 n_0].$$

Numerical evaluation of integral:

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

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

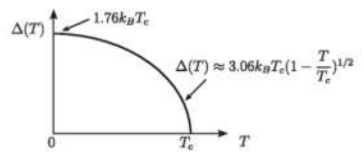

Figure 18.12 Behavior of the energy gap parameter $\Delta(T)$ for a superconductor in the BCS theory and in weak coupling limit.

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.:

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

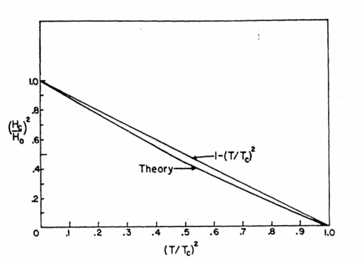

Fig. 2. Ratio of the critical field to its value at $T=0°K$ *vs* $(T/T_c)^2$. The upper curve is the $1-(T/T_c)^2$ law of the Gorter-Casimir theory and the lower curve is the law predicted by the theory in the weak-coupling limit. Experimental values generally lie between the two curves.