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

Plan for Lecture 36

Superconductivity (Chap. 18 in GGGPP)

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

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

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

Some 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	

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Theory of Superconductivity*

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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.

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 $U(\mathbf{r}_1,\mathbf{r}_2)$:

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

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

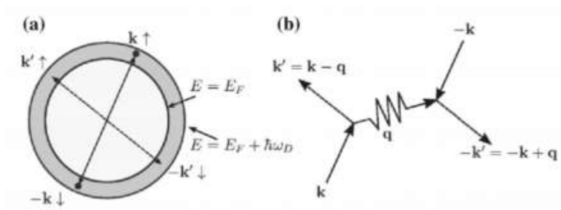

Figure 18.7 (a) Schematic representation of a *single* Cooper pair, added to the ground state of a free-electron gas. Two "extra electrons" in the pair state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ scatter freely to the pair states $(\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)$, in the energy 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 $\hbar\mathbf{q}$.

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

$$\chi^{(S=1)}=\begin{cases}\alpha(1)\alpha(2),\\ \frac{1}{\sqrt{2}}[\alpha(1)\beta(2)+\beta(1)\alpha(2)],\\ \beta(1)\beta(2).\end{cases}$$

Note that:

$$\chi^{S=0}(\sigma_1,\sigma_2)=-\chi^{S=0}(\sigma_1,\sigma_2)$$
$$\Rightarrow\phi^{S=0}(\mathbf{r}_1,\mathbf{r}_2)=\phi^{S=0}(\mathbf{r}_2,\mathbf{r}_1)$$

Note that:

$$\chi^{S=1}(\sigma_1,\sigma_2)=\chi^{S=1}(\sigma_1,\sigma_2)$$
$$\Rightarrow\phi^{S=1}(\mathbf{r}_1,\mathbf{r}_2)=-\phi^{S=1}(\mathbf{r}_2,\mathbf{r}_1)$$

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**:

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

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 $E_F \le E_{\mathbf{k}} \le E_F + \hbar\omega_D$

Define Fourier transform of interaction potential:

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

V volume of sample composed of N unit cells

Ω volume of unit cell

Equation satisfied by pair amplitude functions:

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

Cooper pair equations -- continued

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

Simplified model for interaction:

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

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

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

$\Rightarrow$ Cooper pair states can only be singlet states

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:

$$1 = U_0 \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}} - E_{\rm pair}} \qquad E_F < E_{\mathbf{k}} < E_F + \hbar\omega_D.$$

$$1 = U_0 \frac{1}{N}\int_{E_F}^{E_F+\hbar\omega_D} D_0(E)\frac{1}{2E - E_{\rm pair}}\, dE,$$

Density of states (one electron basis)

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.

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

Second quantization

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

Note that the Cooper pair singlet state can be written

$$\psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \sum_{\mathbf{k}} g(\mathbf{k})\frac{1}{\sqrt{2}}\frac{1}{V}\left[e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\alpha(1)\beta(2) - e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\beta(1)\alpha(2)\right]$$

$$\equiv \sum_{\mathbf{k}} g(\mathbf{k})\, c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|0\rangle.$$

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

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

independent particle states   Cooper-pair interaction

Consider a ground state wavefunction of the form

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

$$u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$$

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

Need to minimize the expectation value:

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

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

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

After some algebra:

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

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

Convenient transformation:

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

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

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

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

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

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

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

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

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

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

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:

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

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

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