10.2 Microscopic Theory

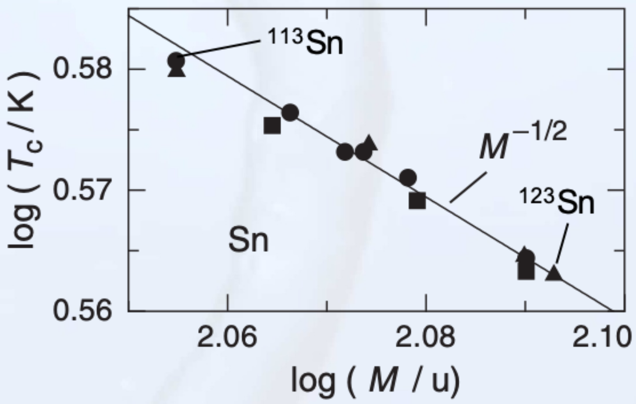
superconductivity occurs in many different materials

low transition temperatures ⟶ small energy differences matter ⟷ electrons have Fermi energy !

1950 Fröhlich ⟶ interaction between electrons and lattice can mediate attraction between electrons
(Bardeen)

Isotope effect, discovered 1950

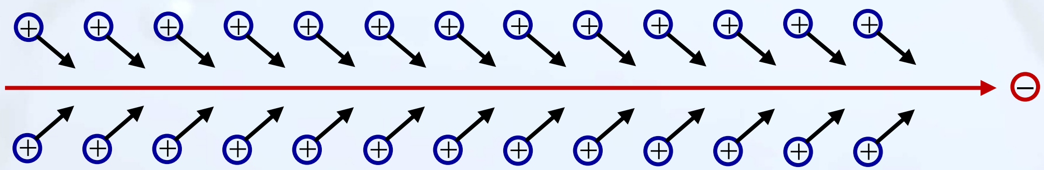
- T_c depends on atomic mass $T_c \propto 1/\sqrt{M}$
- for m = 113 u … 123 u T_c = 3.8 K … 3.66 K
- lattice properties are important for superconductivity



10.2 Microscopic Theory

schematic picture

- electron passes through lattice and attracts positive ions
- positive charge density maximum occurs long after electron has passed
- a second electron is attracted, but Coulomb repulsion is small since it is far away from first electron



estimated distance between electron and positive charge density maximum

$$s = v_{\mathrm{F}} t \approx 10^8 \times 10^{-13}\,\mathrm{cm} = 1000\,\mathrm{\AA}$$

time for ions to react $1/\omega_{\mathrm{D}}$

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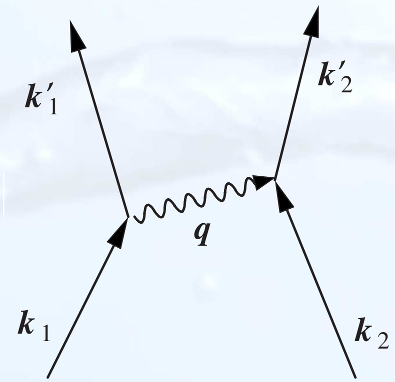
Cooper pairs



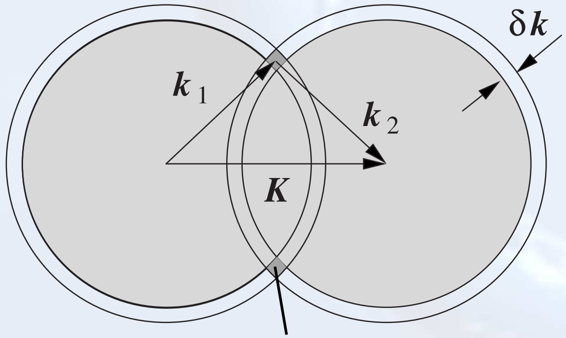
Leon N. Cooper

$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}'_1 + \boldsymbol{k}'_2 = \boldsymbol{K}$ — center of mass motion

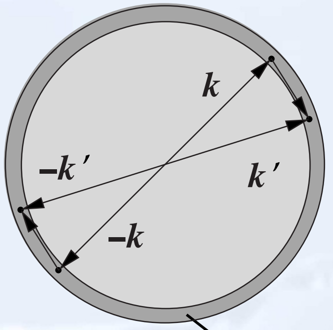
for $\hbar\boldsymbol{K} = 0$ phase space maximum ⟶ $\boldsymbol{k}_1 = -\boldsymbol{k}_2 = \boldsymbol{k},$

$\boldsymbol{K} \neq 0$

$\delta k = (m\omega_{\mathrm{D}}/\hbar k_{\mathrm{F}})$



$\boldsymbol{K} = 0$



⟶ Cooper pair state $(\boldsymbol{k}, -\boldsymbol{k})$

in addition: $L = 0$

10.2 Microscopic Theory

stationary Schrödinger equation for two interacting particles

$$\left[-\frac{\hbar^2}{2m}(\Delta_1+\Delta_2)+\mathcal{V}(\boldsymbol{r}_1,\boldsymbol{r}_2)\right]\psi(\boldsymbol{r}_1,\boldsymbol{r}_2)=E\psi(\boldsymbol{r}_1,\boldsymbol{r}_2)$$

electron-phonon interaction

two-particle wave function

$$\psi(\boldsymbol{r}_1,\boldsymbol{r}_2)=\frac{1}{V}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{r}_1}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_2\cdot\boldsymbol{r}_2}=\frac{1}{V}\,\mathrm{e}^{\boldsymbol{k}\cdot\boldsymbol{r}}=\Psi(\boldsymbol{r})$$

$$\boldsymbol{r}=(\boldsymbol{r}_1-\boldsymbol{r}_2)$$

electrons are scattered constantly into new pair states

$$\longrightarrow\quad \Psi(\boldsymbol{r})=\sum_{\boldsymbol{k}}A_{\boldsymbol{k}}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$$

probability to find a particular pair state

$$A_{\boldsymbol{k}}\begin{cases}\neq 0 & \text{for}\quad k_\mathrm{F}<k<\sqrt{2m(E_\mathrm{F}+\hbar\omega_\mathrm{D})/\hbar^2}\\ =0 & \text{otherwise}\,.\end{cases}$$

insert $\Psi(\boldsymbol{r})$, multiplying with $\exp(-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r})$ and integrate

$$\longrightarrow\quad \frac{\hbar^2k^2}{m}A_{\boldsymbol{k}}+\frac{1}{V}\sum_{\boldsymbol{k}'}A_{\boldsymbol{k}'}\mathcal{V}_{\boldsymbol{k}\boldsymbol{k}'}=EA_{\boldsymbol{k}}$$

Fourier transform of electron-phonon interaction

10.2 Microscopic Theory

approximation for electron-phonon interaction

$$\mathcal{V}_{\boldsymbol{k}\boldsymbol{k}'} = \begin{cases} -\mathcal{V}_0 & \text{for} \quad E_\mathrm{F} < \epsilon_{\boldsymbol{k}}, \epsilon_{\boldsymbol{k}'} < E_\mathrm{F} + \hbar\omega_\mathrm{D} \\ 0 & \text{otherwise} \end{cases}$$

$$\longrightarrow \quad \left(\frac{\hbar^2 k^2}{m} - E\right) A_{\boldsymbol{k}} = \frac{\mathcal{V}_0}{V} \sum_{\boldsymbol{k}'} A_{\boldsymbol{k}'}$$

with $z = \hbar^2 k^2 / 2m$ $\longrightarrow$ $A_{\boldsymbol{k}} = \frac{\mathcal{V}_0}{V} \frac{1}{2z - E} \sum_{\boldsymbol{k}'} A_{\boldsymbol{k}'}$

with $\sum_{\boldsymbol{k}} A_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} A_{\boldsymbol{k}'}$ $\longrightarrow$ $1 = \frac{\mathcal{V}_0}{V} \sum_{\boldsymbol{k}} \frac{1}{2z - E}$

replacing the sum with an integral, and $D(E) \approx D(E_\mathrm{F})$ $\longrightarrow$ $1 = \mathcal{V}_0 \frac{D(E_\mathrm{F})}{2} \int_{E_\mathrm{F}}^{E_\mathrm{F}+\hbar\omega_\mathrm{D}} \frac{\mathrm{d}z}{2z - E}$

integration

$$\longrightarrow \quad \boxed{\delta E = E - 2E_\mathrm{F} = \frac{2\,\hbar\omega_\mathrm{D}}{1 - \exp[4/\mathcal{V}_0 D(E_\mathrm{F})]} \approx -2\,\hbar\omega_\mathrm{D}\, \mathrm{e}^{-4/[\mathcal{V}_0 D(E_\mathrm{F})]}}$$

energy reduction per Cooper pair

$\mathcal{V}_0\, D(E_\mathrm{F}) \ll 1$ weak coupling

- for Cu, Ag, K, … $\mathcal{V}_0$ is small, because they are good conductors $\longrightarrow$ no superconductor since small δE
- Al has small $\mathcal{V}_0$, but high density of states at Fermi energy $\longrightarrow$ superconductor with $T_c \approx 1$ K

10.2 Microscopic Theory

BCS Theory 1957

BCS ground state

pair state $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)$ → $|1\rangle_{\boldsymbol{k}}$ occupied
→ $|0\rangle_{\boldsymbol{k}}$ unoccupied

John Bardeen Leon N. Cooper Robert P. Schrieffer

spin analog representation

$$|1\rangle_{\boldsymbol{k}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\boldsymbol{k}} \qquad |0\rangle_{\boldsymbol{k}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\boldsymbol{k}}$$

generation and annihilation of Cooper pairs

$$\sigma_{\boldsymbol{k}}^{+} = \frac{1}{2}(\sigma_{\boldsymbol{k}}^{x} + \mathrm{i}\sigma_{\boldsymbol{k}}^{y}) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_{\boldsymbol{k}} \qquad \sigma_{\boldsymbol{k}}^{-} = \frac{1}{2}(\sigma_{\boldsymbol{k}}^{x} - \mathrm{i}\sigma_{\boldsymbol{k}}^{y}) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_{\boldsymbol{k}}$$

Pauli matrices

application of generation and annihilation operators

$$\sigma_{\boldsymbol{k}}^{+}|1\rangle_{\boldsymbol{k}} = 0 \qquad \sigma_{\boldsymbol{k}}^{+}|0\rangle_{\boldsymbol{k}} = |1\rangle_{\boldsymbol{k}}$$

$$\sigma_{\boldsymbol{k}}^{-}|1\rangle_{\boldsymbol{k}} = |0\rangle_{\boldsymbol{k}} \qquad \sigma_{\boldsymbol{k}}^{-}|0\rangle_{\boldsymbol{k}} = 0$$

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general representation of one Cooper pair

$$|\psi\rangle_{\boldsymbol{k}} = u_{\boldsymbol{k}}|0\rangle_{\boldsymbol{k}} + v_{\boldsymbol{k}}|1\rangle_{\boldsymbol{k}}$$

real coefficients
- probability that a pair state is occupied $w_{\boldsymbol{k}} = v_{\boldsymbol{k}}^2$
- probability that a pair state is unoccupied $u_{\boldsymbol{k}}^2 = 1 - w_{\boldsymbol{k}}$

BCS ground state $T = 0$

$$|\Psi\rangle = \prod_{\boldsymbol{k}} |\psi\rangle_{\boldsymbol{k}} = \prod_{\boldsymbol{k}} \left(u_{\boldsymbol{k}}|0\rangle_{\boldsymbol{k}} + v_{\boldsymbol{k}}|1\rangle_{\boldsymbol{k}} \right)$$

Hamiltonian

$$\eta_{\boldsymbol{k}} = \hbar^2 k^2/2m - E_{\mathrm{F}}$$

$$\mathcal{H} = \sum_{\boldsymbol{k}} 2\eta_{\boldsymbol{k}}\, \sigma_{\boldsymbol{k}}^+ \sigma_{\boldsymbol{k}}^- - \frac{\mathcal{V}_0}{V} \sum_{\boldsymbol{k},\boldsymbol{k}'} \sigma_{\boldsymbol{k}}^+ \sigma_{\boldsymbol{k}'}^-$$

kinetic energy — potential energy: electron-phonon interaction

expectation value

$$W_0 = \langle \Psi|\mathcal{H}|\Psi\rangle \longrightarrow W_0 = \sum_{\boldsymbol{k}} 2 v_{\boldsymbol{k}}^2 \eta_{\boldsymbol{k}} - \frac{\mathcal{V}_0}{V} \sum_{\boldsymbol{k}',\boldsymbol{k}} v_{\boldsymbol{k}} u_{\boldsymbol{k}'} u_{\boldsymbol{k}} v_{\boldsymbol{k}'}$$

10.2 Microscopic Theory

Minimizing W_0 with respect to $v_{\boldsymbol{k}}$ and $u_{\boldsymbol{k}}$

$$\longrightarrow \quad 2u_{\boldsymbol{k}}v_{\boldsymbol{k}}\eta_{\boldsymbol{k}} - \Delta_0(u_{\boldsymbol{k}}^2 - v_{\boldsymbol{k}}^2) = 0$$

$$\Delta_0 = \frac{\mathcal{V}_0}{V}\sum_{\boldsymbol{k}'} u_{\boldsymbol{k}'}v_{\boldsymbol{k}'}$$

$$u_{\boldsymbol{k}}^2 = \frac{1}{2}\left(1 + \frac{\eta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)$$

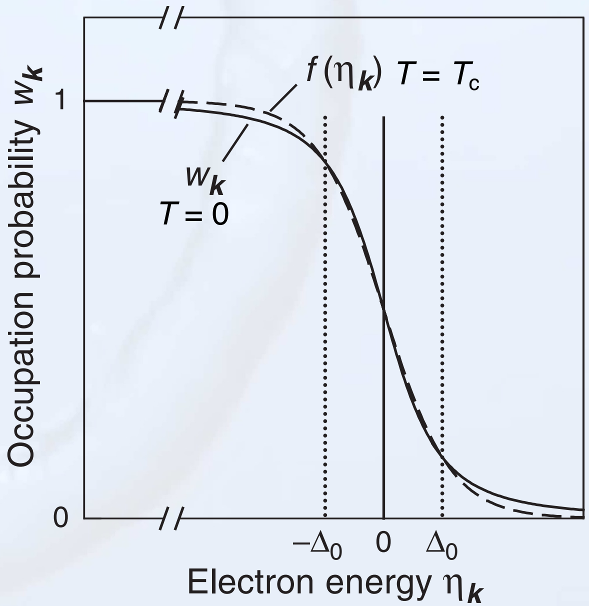
$$v_{\boldsymbol{k}}^2 = \frac{1}{2}\left(1 - \frac{\eta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)$$

$$E_{\boldsymbol{k}}^2 = \eta_{\boldsymbol{k}}^2 + \Delta_0^2$$

$$\longrightarrow \quad W_0 = \sum_{\boldsymbol{k}} \eta_{\boldsymbol{k}}\left(1 - \frac{\eta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right) - \frac{\Delta_0^2\, V}{\mathcal{V}_0}$$

probability that a pair state is occupied

$$w_{\boldsymbol{k}} = v_{\boldsymbol{k}}^2 = \frac{1}{2}\left(1 - \frac{\eta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right) = \frac{1}{2}\left(1 - \frac{\eta_{\boldsymbol{k}}}{\sqrt{\eta_{\boldsymbol{k}}^2 + \Delta_0^2}}\right)$$



- occupation of a pair at $T = 0$ resamples the Fermi function at $T = T_c$
- when forming Cooper pairs electrons gain kinetic energy

10.2 Microscopic Theory

condensation energy

$W_0^\mathrm{n} = 2\sum_{|k|<k_\mathrm{F}} \eta_{\boldsymbol{k}}$ normal state internal energy

$$\frac{W_\mathrm{con}}{V} = \frac{W_0 - W_0^\mathrm{n}}{V} = -\frac{1}{4} D(E_\mathrm{F})\, \Delta_0^2$$

$$\Delta_0 = \frac{\mathcal{V}_0}{V}\sum_{\boldsymbol{k}} u_{\boldsymbol{k}} v_{\boldsymbol{k}} = \frac{1}{2}\frac{\mathcal{V}_0}{V}\sum_{\boldsymbol{k}} \frac{\Delta_0}{E_{\boldsymbol{k}}} = \frac{1}{2}\frac{\mathcal{V}_0}{V}\sum_{\boldsymbol{k}} \frac{\Delta_0}{\sqrt{\eta_{\boldsymbol{k}}^2 + \Delta_0^2}}$$

replace sum by integral

$$\rightarrow \quad 1 = \frac{\mathcal{V}_0}{2}\int_{-\hbar\omega_\mathrm{D}}^{\hbar\omega_\mathrm{D}} \frac{D(E_\mathrm{F})}{2}\frac{\mathrm{d}\eta}{\sqrt{\eta^2+\Delta_0^2}} = \frac{\mathcal{V}_0\, D(E_\mathrm{F})}{2}\,\mathrm{arc\,sinh}\left(\frac{\hbar\omega_\mathrm{D}}{\Delta_0}\right)$$

$$\rightarrow \quad \boxed{\Delta_0 = \frac{\hbar\omega_\mathrm{D}}{\sinh\left[\frac{2}{\mathcal{V}_0\, D(E_\mathrm{F})}\right]} \approx 2\,\hbar\omega_\mathrm{D}\,\mathrm{e}^{-2/\mathcal{V}_0\, D(E_\mathrm{F})}}$$

$\mathcal{V}_0\, D(E_\mathrm{F}) \ll 1$ weak coupling

explains isotope effect

$$T_\mathrm{c} \propto \omega_\mathrm{D} \propto M^{-1/2}$$