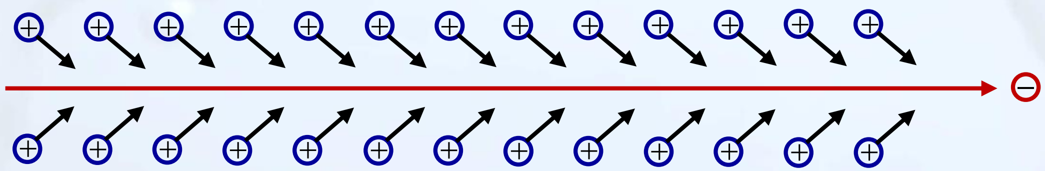
10.2 Microscopic Theory

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



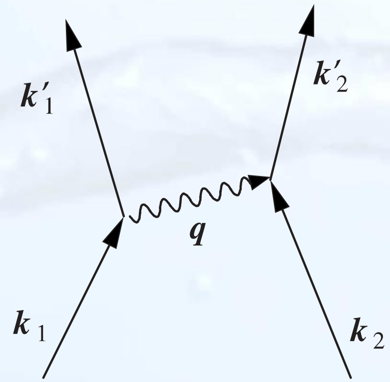
estimated distance between electron and positive charge density maximum

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

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

10.2 Microscopic Theory

Cooper pairs



Leon N. Cooper

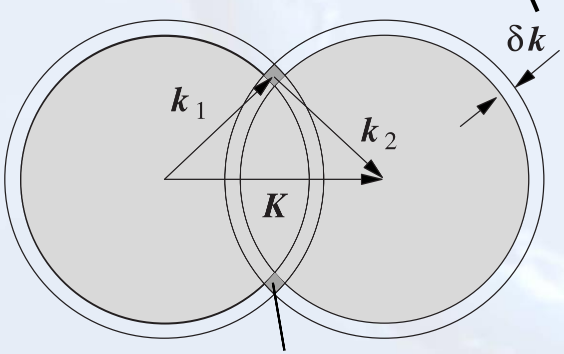
$$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}'_1 + \boldsymbol{k}'_2 = \boldsymbol{K}$$

center of mass motion

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

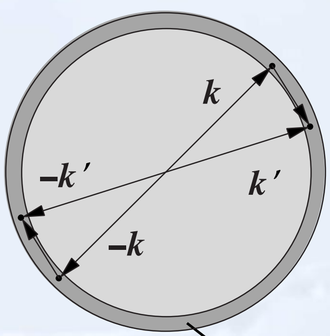
$\boldsymbol{K} \neq 0$

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



phase space

$\boldsymbol{K} = 0$



phase space

$\longrightarrow$ 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

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

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 $D(E) \approx D(E_\mathrm{F})$ $\longrightarrow$ $1 = \mathcal{V}_0 \frac{D(E_\mathrm{F})}{2} \int\limits_{E_\mathrm{F}}^{E_\mathrm{F}+\hbar\omega_\mathrm{D}} \frac{\mathrm{d}z}{2z - E}$

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 $T_\mathrm{c} \cong 1$ 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

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

Pauli matrices

application of generation and annihilation operators

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

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

10.2 Microscopic Theory

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 $T = 0$

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

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 $u_{\boldsymbol{k}}$

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

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

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

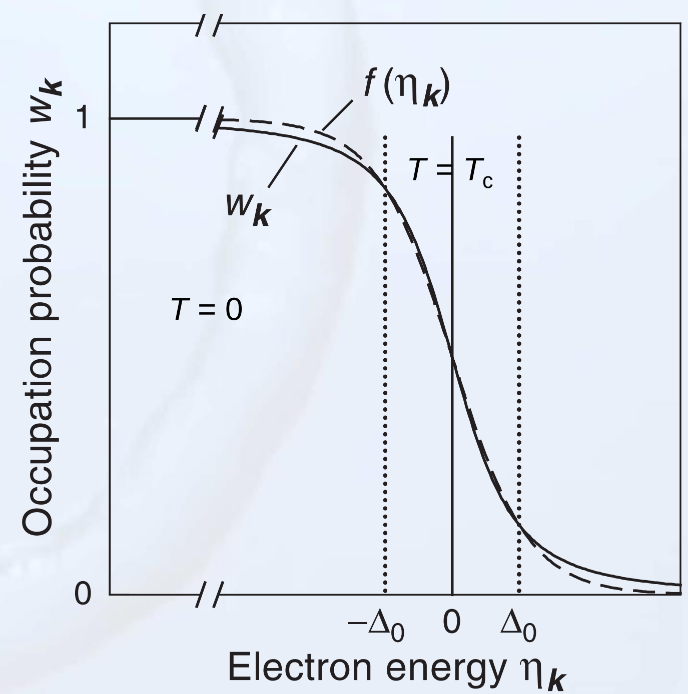
$$v_{\boldsymbol{k}}^2 = \frac{1}{2}\left(1 - \frac{\eta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)$$

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

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

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 $T = 0$ resembles the Fermi function at $T = T_c$
- to form Cooper pairs, electrons accept their kinetic energy @ T_c and don't lower it further, as they can lower their potential energy even more

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

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

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

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

explains isotope effect

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

10.2 Microscopic Theory

Excitation of BCS ground state

ground state: $W_0 = -2\sum_{\boldsymbol{k}} E_{\boldsymbol{k}} v_{\boldsymbol{k}}^4$

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

breaking of one Cooper pair:

$(\boldsymbol{k}' \uparrow, -\boldsymbol{k}' \downarrow)$

- electron with $\boldsymbol{k}$ plus hole with $-\boldsymbol{k}'$
- electron with $-\boldsymbol{k}$ plus hole with $\boldsymbol{k}'$

two quasi-particles

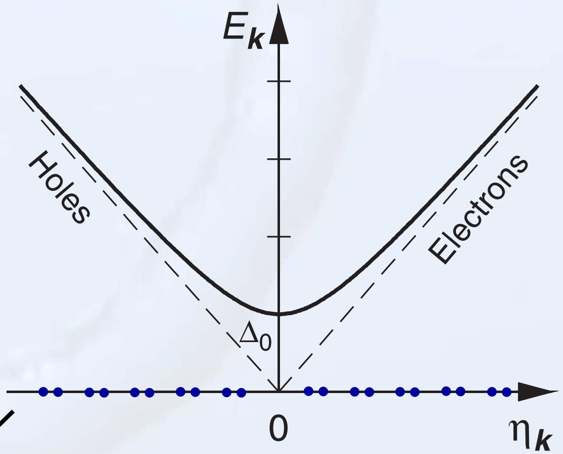
energy of remaining Cooper pairs $W_1 = -2\sum_{\boldsymbol{k}\neq\boldsymbol{k}'} E_{\boldsymbol{k}} v_{\boldsymbol{k}}^4$

energy difference: $\delta E = W_1 - W_0 = \boxed{2E_{\boldsymbol{k}'} = 2\sqrt{\eta_{\boldsymbol{k}'}^2 + \Delta_0^2}}$

dispersion of quasi-particles

→ even if unpaired electrons have no kinetic energy ($\eta_{\boldsymbol{k}'} = 0$) to break a Cooper pair one must invest $2\Delta_0$

→ energy gap: $\delta E_{\min} = 2\Delta_0$



ground state

two particle description

10.2 Microscopic Theory

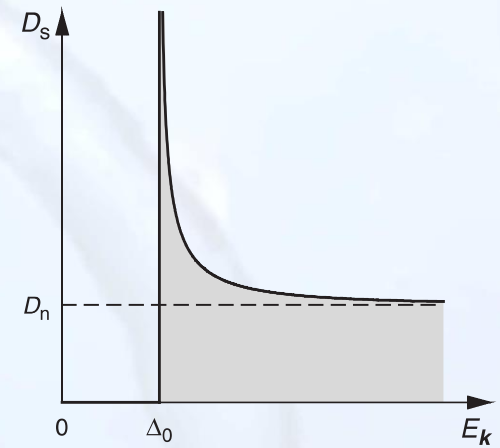
Density of states of quasi-particles

$D_\mathrm{n}(\eta_{\boldsymbol{k}}) \longleftrightarrow D_\mathrm{s}(E_{\boldsymbol{k}})$ each state in normal conductor is uniquely connected with one in the superconductor

$\Longrightarrow$ $D_\mathrm{s}(E_{\boldsymbol{k}})\,\mathrm{d}E_{\boldsymbol{k}} = D_\mathrm{n}(\eta_{\boldsymbol{k}})\,\mathrm{d}\eta_{\boldsymbol{k}}$

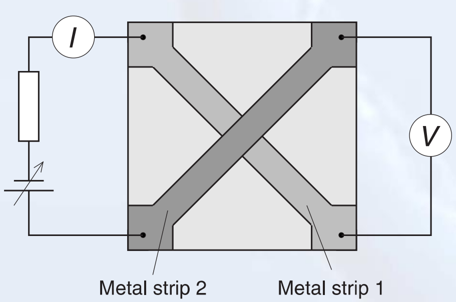
$$D_\mathrm{s}(E_{\boldsymbol{k}}) = D_\mathrm{n}(\eta_{\boldsymbol{k}})\,\frac{\mathrm{d}\eta_{\boldsymbol{k}}}{\mathrm{d}E_{\boldsymbol{k}}} = \begin{cases} D_\mathrm{n}(E_\mathrm{F})\,\dfrac{E_{\boldsymbol{k}}}{\sqrt{E_{\boldsymbol{k}}^2 - \Delta_0^2}} & \text{for} \quad E_{\boldsymbol{k}} > \Delta_0 \\ 0 & \text{for} \quad E_{\boldsymbol{k}} < \Delta_0 \end{cases}$$

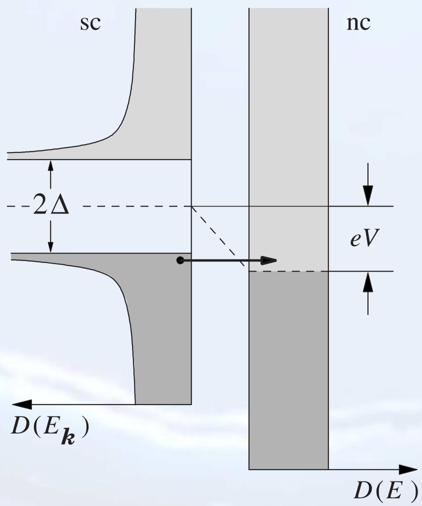
singularity at $E_{\boldsymbol{k}} = \Delta_0$

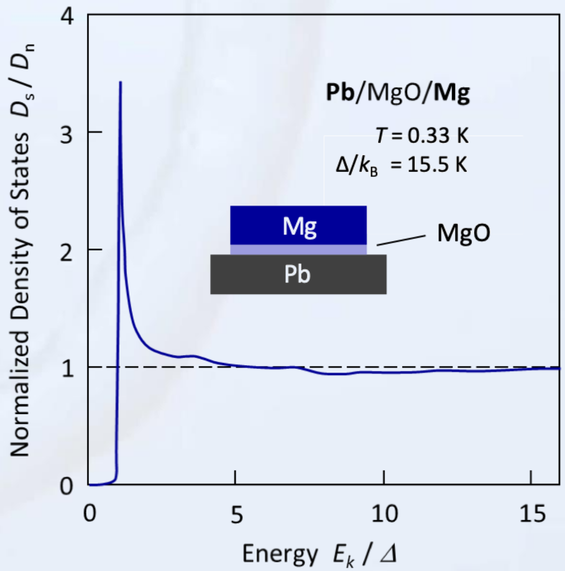


experimental observation using superconducting tunnel junctions

schematic setup







10.2 Microscopic Theory

BCS state at finite temperatures

Cooper pairs ⟶ quasi-particles ⟶ BCS state weakens ⟶ energy gap decreases

BCS theory in weak coupling limit

$$\left.\begin{aligned} \Delta_0 &= 2\,\hbar\omega_{\mathrm{D}}\,\mathrm{e}^{-2/\mathcal{V}_0\,D(E_{\mathrm{F}})} \\ k_{\mathrm{B}}T_{\mathrm{c}} &= 1.14\,\hbar\omega_{\mathrm{D}}\,\mathrm{e}^{-2/\mathcal{V}_0 D(E_{\mathrm{F}})} \end{aligned}\right\}$$

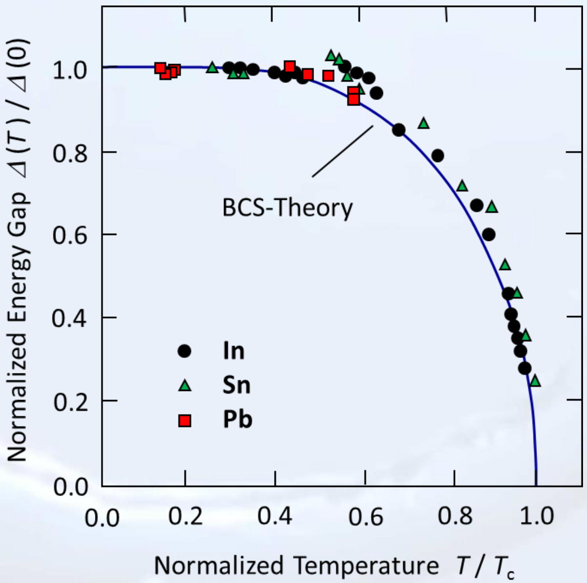
$$\Delta_0 = 1.76\,k_{\mathrm{B}}T_{\mathrm{c}}$$

	Al	Cd	Hg	In	Nb	Pb	Zn
$\Delta_0/(k_{\mathrm{B}}T_{\mathrm{c}})$	1.7	1.6	2.3	1.8	1.9	2.15	1.6

weak coupling regime does not really apply

energy gap at finite temperatures can be calculated numerically.
An approximation close to Tc is:

$$\frac{\Delta(T)}{\Delta_0} = 1.74\sqrt{1-\frac{T}{T_{\mathrm{c}}}}$$



10.3 Macroscopic Quantum State

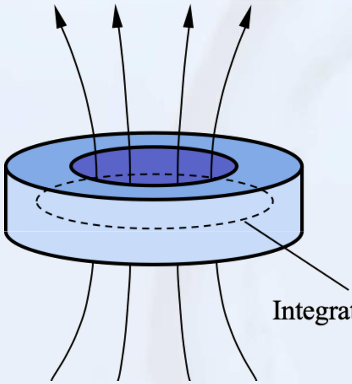
Macroscopic wave function $\Psi = \Psi_0\, \mathrm{e}^{\mathrm{i}\varphi(\boldsymbol{r})}$ → flux quantization

$|\Psi_0|^2 = n_\mathrm{s}$ → Josephson effect

a) flux quantization

phase $\varphi(\boldsymbol{r})$ is well defined in entire superconducting system

consider superconducting ring in magnetic field



phase difference along a path $\Delta\varphi = \int_1^2 \mathrm{grad}\,\varphi(\boldsymbol{r}) \cdot \mathrm{d}\boldsymbol{s}$

closed loop $\boldsymbol{r}_1 = \boldsymbol{r}_2 \longrightarrow \Delta\varphi = 2\pi p$

quantum mechanical current density $\boldsymbol{j} = \mathrm{i}\dfrac{\hbar q}{2M}\left(\Psi^\star\nabla\Psi - \Psi\nabla\Psi^\star\right) - \dfrac{q^2}{M}\boldsymbol{A}\,\Psi^\star\Psi$

with $q = -2e$ and $M = 2m$ $\longrightarrow$ $\mu_0\lambda_\mathrm{L}^2\boldsymbol{j} = \left(\dfrac{\hbar}{e}\nabla\varphi - 2\boldsymbol{A}\right)$

integration along closed contour line L

$$\mu_0\lambda_\mathrm{L}^2 \oint_L \boldsymbol{j}\cdot\mathrm{d}\boldsymbol{s} = \frac{\hbar}{e}\oint_L \nabla\varphi\cdot\mathrm{d}\boldsymbol{s} - 2\underbrace{\oint_L \boldsymbol{A}\cdot\mathrm{d}\boldsymbol{s}}_{\int_\Sigma \boldsymbol{B}\cdot d\boldsymbol{f} = \Phi}$$

$\boldsymbol{j} = 0$

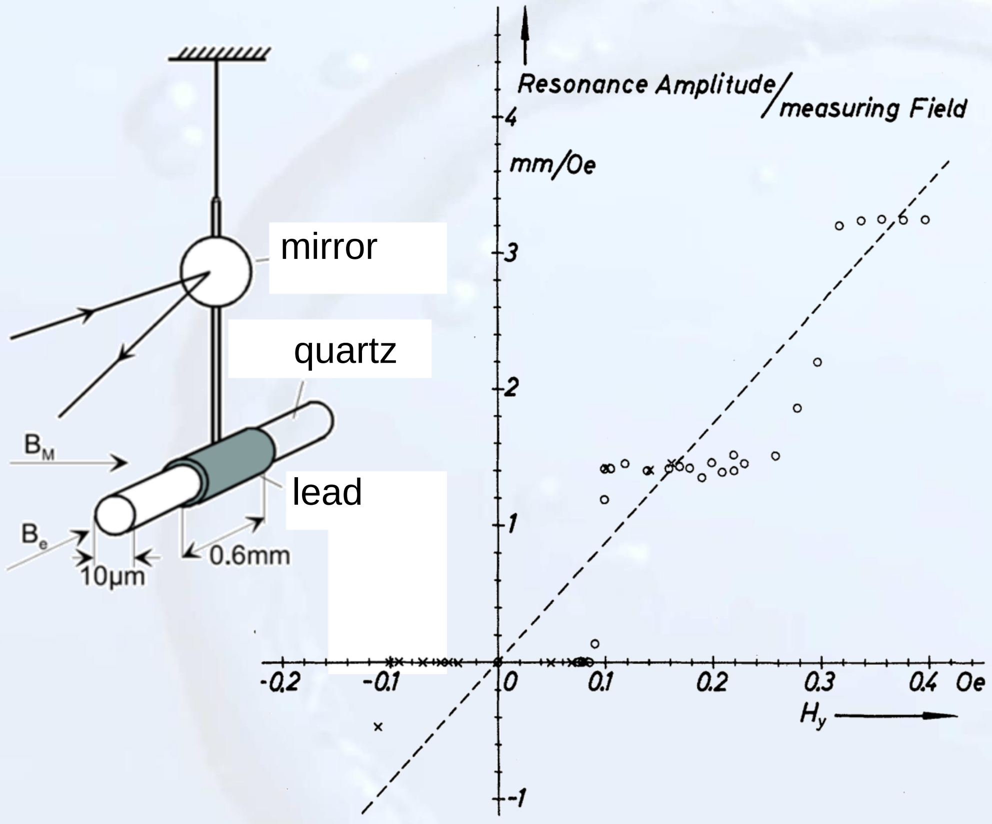
$\int_\Sigma \boldsymbol{B}\cdot d\boldsymbol{f} = \Phi$ Stokes theorem

$$\boxed{\Phi = p\,\frac{h}{2e} = p\,\Phi_0}$$

magnetic flux enclosed by the ring is quantized

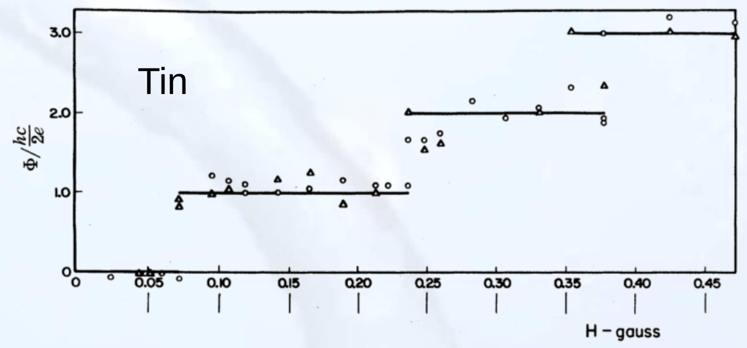
10.3 Macroscopic Quantum State

Experimental observation of flux quantization 1961



Doll and Näbauer

Deaver and Fairbank



modern measurement