10.2 Microscopic Theory

BCS Theory 1957

John Bardeen   Leon N. Cooper   Robert P. Schrieffer

BCS ground state

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

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

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

Pauli matrices

application of generation and annihilation operators

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

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

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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 $T = 0$

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

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

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

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

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

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

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

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

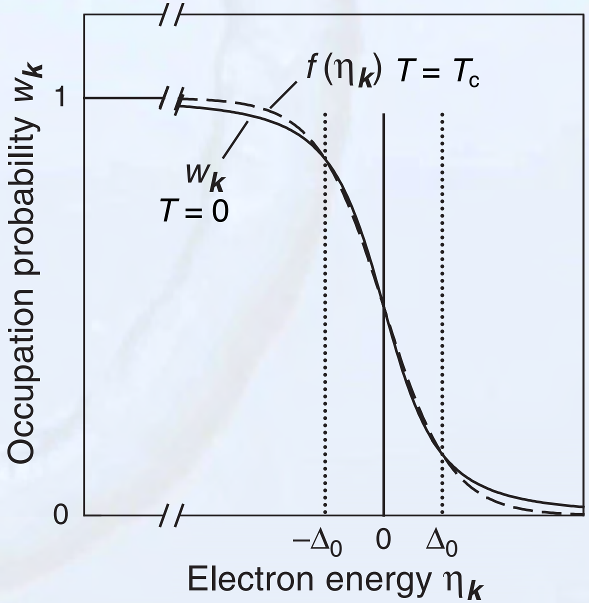
$$E_{\boldsymbol{k}}^2 = \eta_{\boldsymbol{k}}^2 + \Delta_0^2$$

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

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



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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

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

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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 $\boldsymbol{k}'$

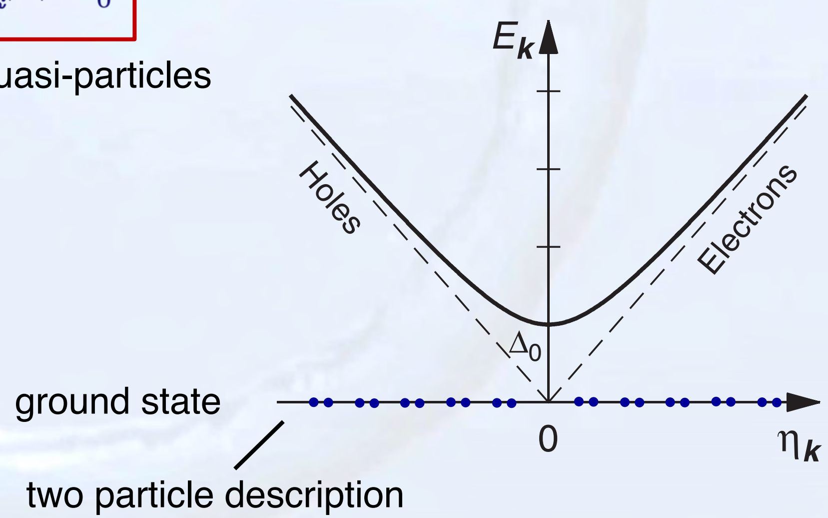
two quasi-particles

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: $\delta E_{\min} = 2\Delta_0$



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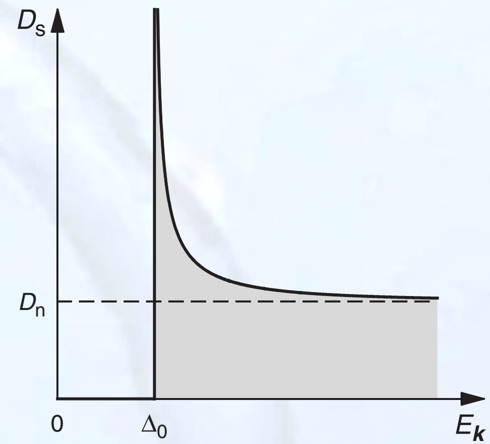
Density of states of quasi-particles

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

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

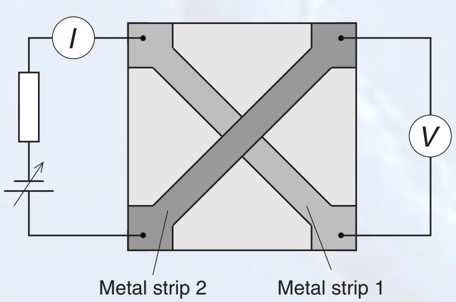
$$D_\mathrm{s}(E_{\boldsymbol{k}}) = D_\mathrm{n}(\eta_{\boldsymbol{k}})\,\frac{\mathrm{d}\eta_{\boldsymbol{k}}}{\mathrm{d}E_{\boldsymbol{k}}} = \begin{cases} D_\mathrm{n}(E_\mathrm{F})\,\dfrac{E_{\boldsymbol{k}}}{\sqrt{E_{\boldsymbol{k}}^2 - \Delta_0^2}} & \text{for} \quad E_{\boldsymbol{k}} > \Delta_0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

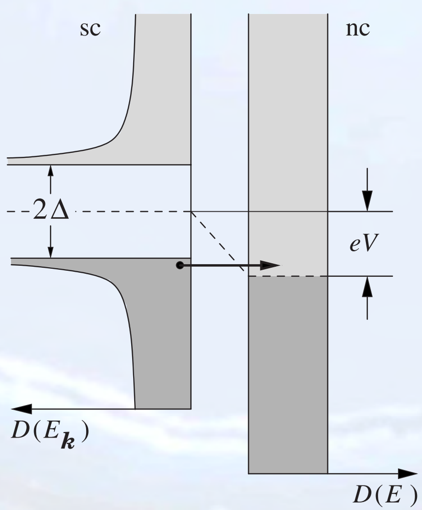
singularity at $E_{\boldsymbol{k}} = \Delta_0$

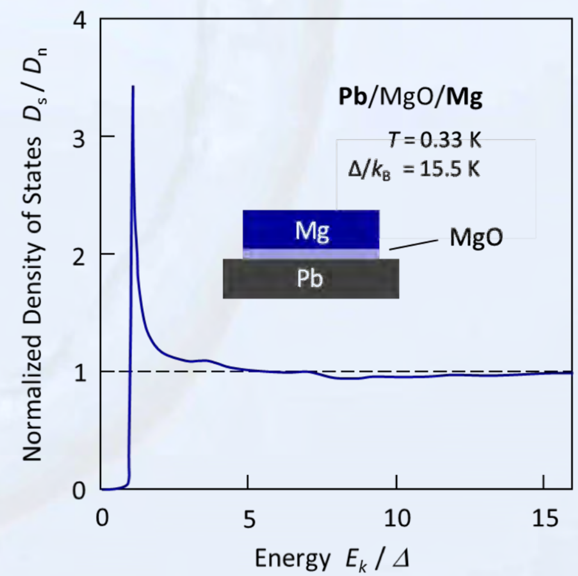


experimental observation using superconducting tunnel junctions

schematic setup







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BCS state at finite temperatures

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

BCS theory in weak coupling limit

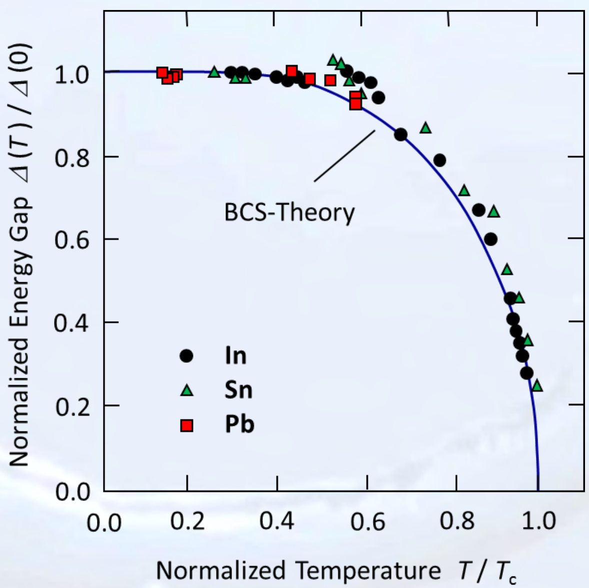
$$\left.\begin{aligned} \Delta_0 &= 2\,\hbar\omega_D\, e^{-2/\mathcal{V}_0\, D(E_F)} \\ k_B T_c &= 1.14\,\hbar\omega_D\, e^{-2/\mathcal{V}_0 D(E_F)} \end{aligned}\right\} \quad \Delta_0 = 1.76\, k_B T_c$$

	Al	Cd	Hg	In	Nb	Pb	Zn
$\Delta_0/(k_B T_c)$	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

$$\frac{\Delta(T)}{\Delta_0} = 1.74\sqrt{1-\frac{T}{T_c}}$$



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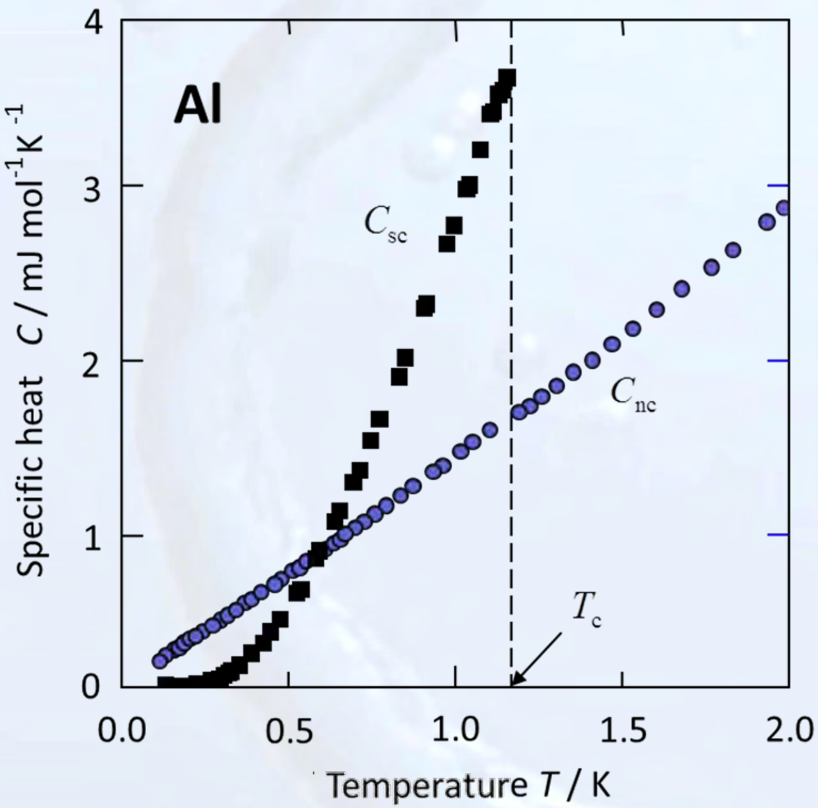
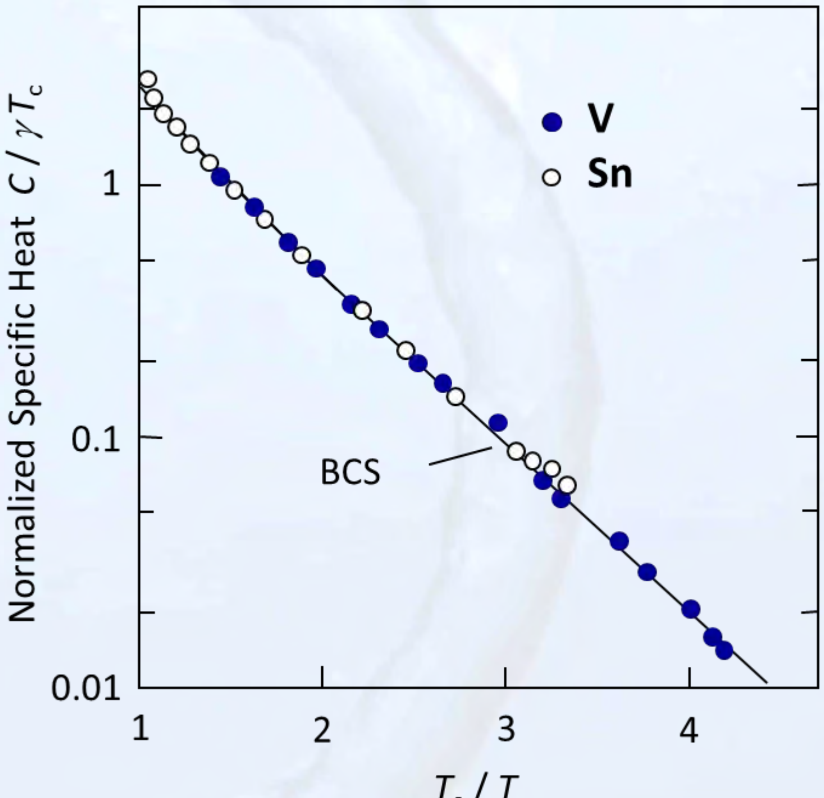
Specific heat: $$\frac{C_\mathrm{s}}{\gamma T_\mathrm{c}} = 1.34\left(\frac{\Delta_0}{k_\mathrm{B}T}\right)^{3/2} \mathrm{e}^{-\Delta_0/k_\mathrm{B}T}$$





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Ultraound absorption

$$\frac{\alpha_\mathrm{s}}{\alpha_\mathrm{n}} = \frac{2}{\mathrm{e}^{\Delta(T)/k_\mathrm{B}T} + 1}$$