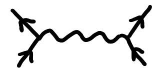
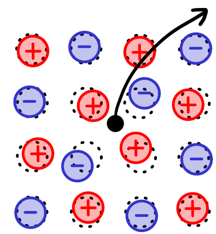
Superconductivity

① Overview of BCS theory

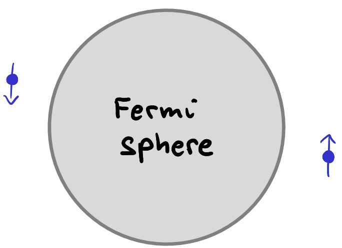
- Fröhlich – effective e–e interaction mediated by phonons



$$H_{int} = \frac{1}{2} \sum_{\substack{kk'q \\ \sigma\sigma'}} |M_q|^2 \left(\frac{1}{\varepsilon_k - \varepsilon_{k+q} - \hbar\omega_q} - \frac{1}{\varepsilon_k - \varepsilon_{k+q} + \hbar\omega_q} \right) \hat{c}^{+}_{k+q\sigma} \hat{c}^{+}_{k'-q\sigma'} \hat{c}_{k'\sigma'} \hat{c}_{k\sigma}$$



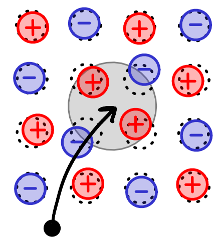
- Cooper problem – two electrons above frozen Fermi sphere



trial state $|\Psi\rangle = \sum_k g_k c^{+}_{k\uparrow} c^{+}_{-k\downarrow} |F\rangle$

variational optimization → bound state

$$E_{bound} = 2E_F - 2\hbar\omega_D \exp\left[- \frac{2}{V\mathcal{N}(E_F)} \right]$$



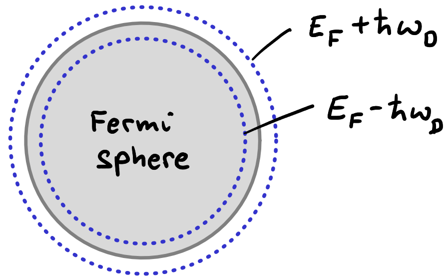
→ FS unstable against formation of Cooper pairs

- simplified BCS interaction – keeps only scattering of singlet zero-momentum pairs

$$H_{int} = \sum_{kk'} V_{kk'} \, c^{+}_{k\uparrow} c^{+}_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

→ attractive interaction for electron pairs near Fermi energy

$$V_{kk'} = -V \, w_k w_{k'} \qquad w_k = \begin{cases} 1 & |\varepsilon_k - \mu| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

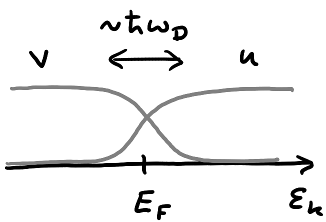


reduced BCS Hamiltonian (ε_k measured from μ)

$$H_{BCS} = \sum_{k\sigma} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma} + \sum_{kk'} V_{kk'} \, c^{+}_{k\uparrow} c^{+}_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

- Schrieffer's trial Ansatz

$$|\Psi_{BCS}\rangle = \prod_k \left(u_k + v_k c^{+}_{k\uparrow} c^{+}_{-k\downarrow} \right) |vac\rangle$$



- mean-field decoupling & Bogoliubov-Valatin

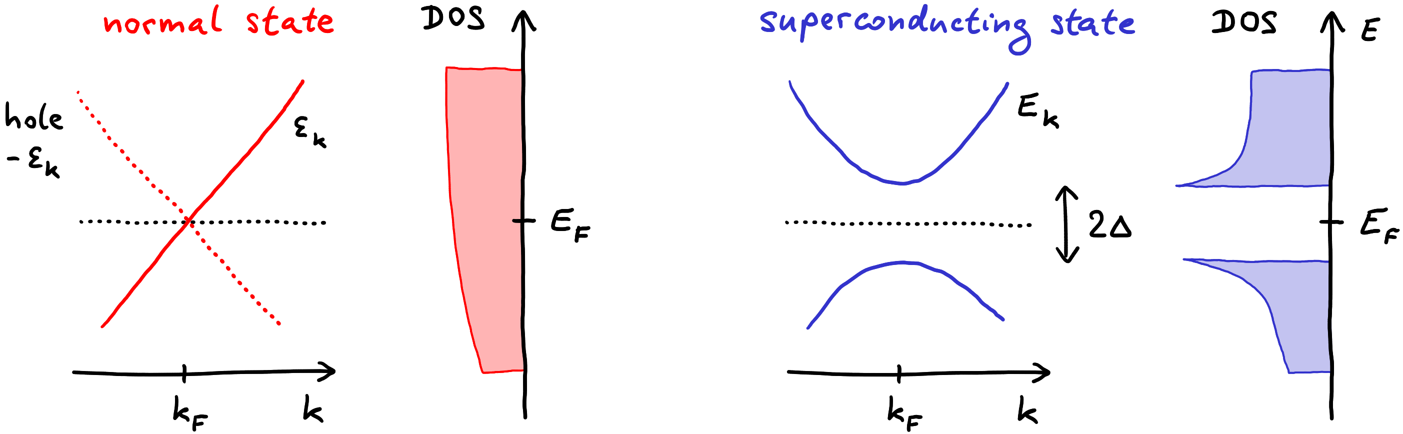
$$\Delta_k = -\sum_{k'} V_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle \qquad \text{SC gap}$$

$$H_{MF} = \sum_k E_k \left(b^{+}_{k\uparrow} b_{k\uparrow} + b^{+}_{k\downarrow} b_{k\downarrow} \right)$$

$$E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2}$$

$u_k c_{k\uparrow} - v_k c^{+}_{-k\downarrow}$

- excitation spectrum



- selfconsistent equation for SC gap $\Delta_k = -\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}} [1 - 2n_F(E_{k'})]$ — $\tanh \frac{E_{k'}}{2k_BT}$

simplified for $V_{kk'} = -V w_k w_{k'}$

constant gap $\Delta_k = \Delta w_k$ obeying $1 = \underbrace{V \mathcal{N}(E_F)}_{\text{BCS } \lambda} \int_{-\hbar\omega_D}^{+\hbar\omega_D} d\xi \frac{1}{2\sqrt{\xi^2+\Delta^2}} \tanh \frac{\sqrt{\xi^2+\Delta^2}}{2k_BT}$

transition temperature $(\Delta \to 0)$

$$1 = V \sum_k w_k \frac{1}{2\varepsilon_k} \tanh \frac{\varepsilon_k}{2k_B T_c}$$

$$\frac{1}{\lambda} = \int_{-\hbar\omega_D}^{+\hbar\omega_D} d\xi \, \frac{1}{2\xi} \tanh \frac{\xi}{2k_B T_c}$$

$$k_B T_c = \frac{2\gamma}{\pi} \hbar\omega_D e^{-\frac{1}{\lambda}} \qquad \lambda = V \mathcal{N}(\varepsilon_F)$$

gap at zero temperature

$$\Delta(T=0) = 2\hbar\omega_D e^{-\frac{1}{\lambda}}$$

universal BCS ratio

$$\frac{2\Delta(T=0)}{k_B T_c} = \frac{2\pi}{\gamma} \approx 3.53$$

TABLE 8.2.† Measured values of $2\Delta(0)/kT_c$ (BCS theoretical value = 3.53)

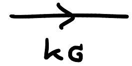
Superconductor	Tunnelling measurements	Thermodynamic measurements
Al	4.2 ± 0.6	3.53
	2.5 ± 0.3	
	2.8 — 3.6	
	3.37 ± 0.1	
Cd	3.2 ± 0.1	3.44
Ga		3.52, 3.50, 3.48
Hg (α)	4.6 ± 0.1	3.95
In	3.63 ± 0.1	3.65
	3.45 ± 0.07	
	3.61	
La	1.65 — 3.0 (fcc)	3.72 (fcc) (d-hcp)
	3.2	
Nb	3.84 ± 0.06	3.65
	3.6	
	3.6	
Pb	4.29 ± 0.04	3.95
	4.38 ± 0.01	
Sn	3.46 ± 0.1	3.61, 3.57
	3.10 ± 0.05	
	3.51 ± 0.18	
	2.8 — 4.06	
	3.1 — 4.3	
Ta	3.60 ± 0.1	3.63
	3.5	
	3.65 ± 0.1	
Tl	3.57 ± 0.05	3.63
	3.9	
V	3.4	3.50
Zn	3.2 ± 0.1	3.44

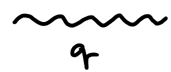
†Taken from Mersevey and Schwartz (1969), by courtesy of Marcel Dekker Inc.

② Propagator approach

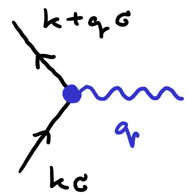
$$-\frac{1}{\hbar}\langle T\{\hat{c}^+_{k\sigma}(\tau)\,\hat{c}_{k\sigma}\}\rangle \qquad\qquad -\frac{1}{\hbar}\langle T\{(\hat{a}_q+\hat{a}^+_{-q})_\tau(\hat{a}_q+\hat{a}^+_{-q})_0\}\rangle$$

$$H = \sum_{k\sigma} \varepsilon_k\, c^+_{k\sigma}\hat{c}_{k\sigma} + \sum_q \omega_q\, a^+_q a_q$$

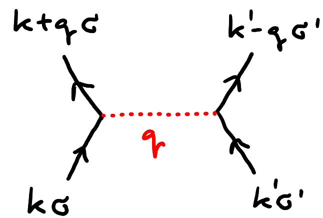
$\mathcal{G}_0$: 

$\mathcal{D}_0$: 

e-ph $$+\sum_{kq\sigma} M_{kq}\, c^+_{k+q\sigma}\hat{c}_{k\sigma}\,(a_q+a^+_{-q})$$



Coulomb $$+\frac{1}{2}\sum_{kk'q\sigma\sigma'} V_q\, c^+_{k+q\sigma} c^+_{k'-q\sigma'} c_{k'\sigma'} c_{k\sigma}$$

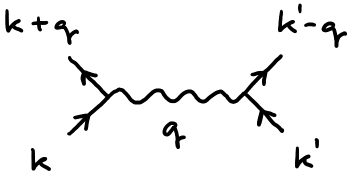


goals :

1) Cooper instability
2) electron propagation in SC state, excitation spectrum
3) analog of gap equation
~~4)~~ simultaneous treatment of e-ph and Coulomb

- effective e-e interaction mediated by phonons

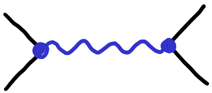
diagrammatic element:



$V_{eff}(q, i\nu) = |M_q|^2 \mathcal{D}(q, i\nu)$ & associated summations

bare: $|M_q|^2 \left(\frac{1}{i\nu - \hbar\omega_q} - \frac{1}{i\nu + \hbar\omega_q} \right)$

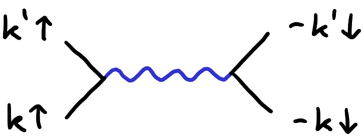
1) Eliashberg treatment - retardation effects included



$\rightarrow -|M_q|^2 \mathcal{D}(q, i\nu)$ or $-V_{eff}(q, i\nu)$ including Coulomb interaction

$$V_{eff}(q, i\nu) = \frac{e^2}{\varepsilon_0 q^2} + |M_q|^2 \mathcal{D}(q, i\nu)$$

2) simplified BCS level

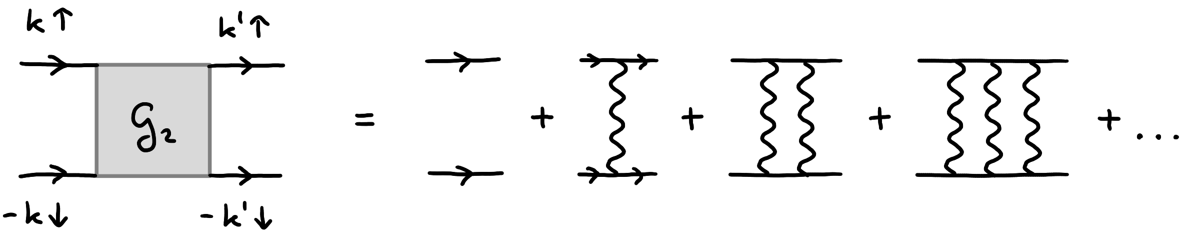


$\rightarrow -V_{kk'}$

Factorized $V_{kk'} = -V w_k w_{k'}$ with $w_k = \begin{cases} 1 & \varepsilon_k \text{ less than } \hbar\omega_D \text{ from Fermi level} \\ 0 & \text{otherwise} \end{cases}$

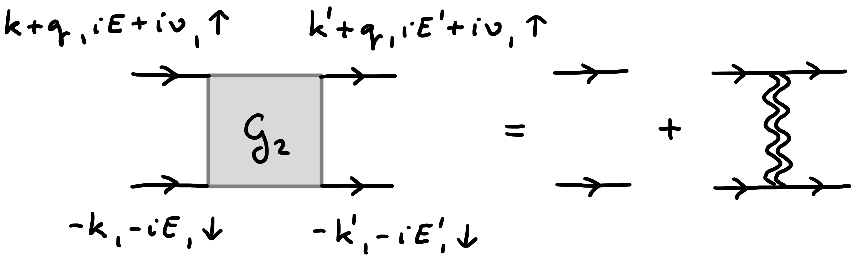
③ Cooper instability

in short: two-particle propagator diverges below T_c → condensation into Cooper pairs

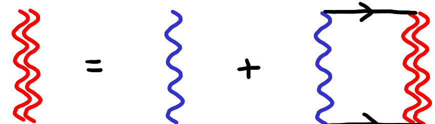


+ other classes

• two-electron propagation (particle-particle channel x particle-hole channel)



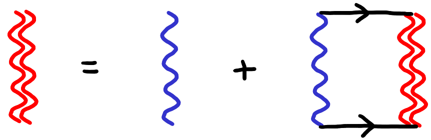
summation of ladder diagrams

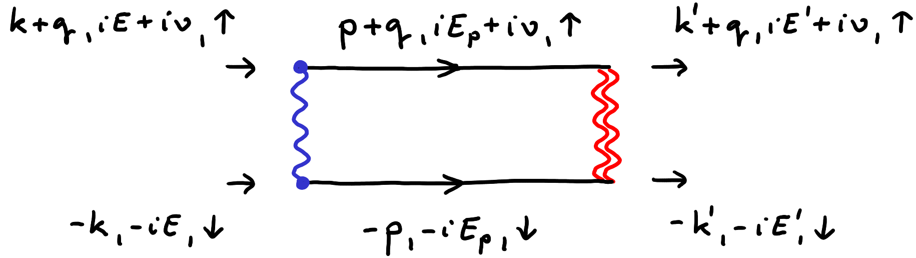


$$-\Lambda = -V_{eff} + (-V_{eff})\,\mathcal{G}_0\mathcal{G}_0(-\Lambda)$$

$$\rightarrow \quad \Lambda = ?$$

- Λ-equation in BCS case





$$-\Lambda = -V_{eff} + (-V_{eff})\, \mathcal{G}_0 \mathcal{G}_0 (-\Lambda)$$

$$-\Lambda(k, iE, k', iE', q, i\nu) = -\underbrace{V_{kk'}}_{V w_k w_{k'}} + \sum_p \frac{1}{\beta} \sum_{iE_p} \underbrace{V_{kp}}_{-V w_k w_p}\, \mathcal{G}_0(p+q, iE_p+i\nu)\, \mathcal{G}_0(-p, -iE_p)\, \Lambda(p, iE_p, k', iE', q, i\nu)$$

$\rightarrow \Lambda(k, iE, \ldots) \sim w_k w_{k'}$ and iE, iE' independent

adapted notation: $\Lambda(k, iE, k', iE', q, i\nu) = \Lambda(q, i\nu)\, w_k w_{k'}$

core function:
$$\phi(q, i\nu) = \sum_p \frac{1}{\beta} \sum_{iE_p} w_p^2\, \mathcal{G}_0(p+q, iE_p+i\nu)\, \mathcal{G}_0(-p, -iE_p)$$
$$= \sum_p w_p^2 \frac{1}{\beta} \sum_{iE_p} \frac{1}{iE_p + i\nu - \varepsilon_{p+q}} \frac{1}{-iE_p - \varepsilon_p}$$

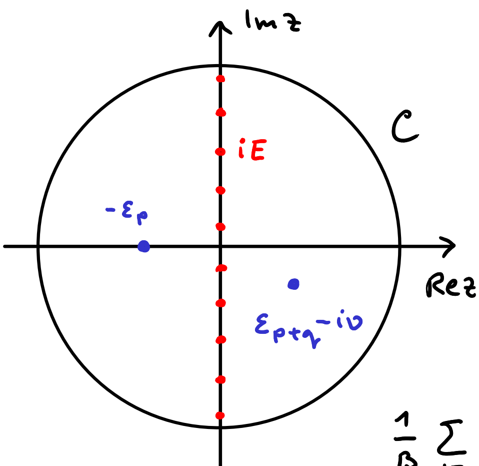
solution: $\Lambda(q, i\nu) = -V + V \phi(q, i\nu)\, \Lambda(q, i\nu) \longrightarrow \Lambda(q, i\nu) = \dfrac{-V}{1 - V\phi(q, i\nu)}$

- evaluation of the Matsubara sum

$$\frac{1}{\beta}\sum_{iE}\frac{1}{iE+i\nu-\varepsilon_{p+q}}\,\frac{1}{-iE-\varepsilon_p} = \frac{1}{\beta}\sum_{iE} f(iE) \quad \text{with} \quad f(z) = \frac{1}{z+i\nu-\varepsilon_{p+q}}\,\frac{-1}{z+\varepsilon_p}$$

observation: $n_F(z) = \dfrac{1}{e^{\beta z}+1}$ has poles at iE $\left(e^{\beta iE} = -1\right)$

expansion around $z = iE$: $n_F(z) = \dfrac{1}{1+e^{\beta iE}e^{\beta(z-iE)}} \approx \dfrac{1}{-\beta(z-iE)}$



$$\oint_C f(z)\,n_F(z)\,dz = 0 \quad \text{due to } f \sim \frac{1}{z^2} \text{ at } |z|\to\infty$$

by residue theorem

$$-\frac{1}{\beta}\sum_{iE} f(iE) - \frac{n_F(\varepsilon_{p+q}-i\nu)}{\varepsilon_{p+q}-i\nu+\varepsilon_p} - \frac{n_F(-\varepsilon_p)}{-\varepsilon_p+i\nu-\varepsilon_{p+q}} = 0$$

$$\frac{1}{\beta}\sum_{iE} f(iE) = \frac{1-n_F(\varepsilon_p)-n_F(\varepsilon_{p+q})}{\varepsilon_p+\varepsilon_{p+q}-i\nu} = \frac{1}{2}\,\frac{\tanh\frac{\beta\varepsilon_p}{2}+\tanh\frac{\beta\varepsilon_{p+q}}{2}}{\varepsilon_p+\varepsilon_{p+q}-i\nu}$$

- pairing instability

$$\Lambda(q, i\nu) = \frac{-V}{1 - V\phi(q, i\nu)} \qquad \phi(q, i\nu) = \sum_p w_p^2 \, \frac{1}{2} \, \frac{\tanh\frac{\beta\varepsilon_p}{2} + \tanh\frac{\beta\varepsilon_{p+q}}{2}}{\varepsilon_p + \varepsilon_{p+q} - i\nu}$$

denominator < 1 enhances the attractive interaction

divergence = instability towards pair formation

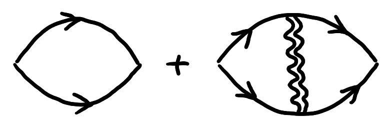
when increasing V – divergence occurs for $V \cdot \max F(q, i\nu)$ reaching 1

$\max F(q, i\nu)$ for $q = 0$, $i\nu = 0$

→ instability condition $1 = V \sum_p w_p \frac{1}{2\varepsilon_p} \tanh \frac{\varepsilon_p}{2k_B T_c}$ (identical to T_c equation by BCS)

- alternative use of Λ – pairing susceptibility

$$\chi(k, k', \tau) = \frac{1}{\hbar} \langle [(c_{-k\downarrow} c_{k\uparrow})_\tau, (c^+_{k'\uparrow} c^+_{-k'\downarrow})_0] \rangle \vartheta(\tau)$$

$\chi =$ 

$c^+_{k\uparrow} c^+_{-k\downarrow}$ response to pairing field Δ_k coupled via $H_{int} = \sum_k c^+_{k\uparrow} c^+_{-k\downarrow} \Delta_k$

(4) Propagators in superconducting state

- divergent pair susceptibility below T_c $\rightarrow$ $\langle c^+_{k\uparrow} c^+_{-k\downarrow}\rangle$ spontaneously appearing

  $\rightarrow$ need for anomalous propagators of the type $\mathcal{F} = -\frac{1}{\hbar}\langle T\{c^+_{-k\downarrow}(\tau)\, c^+_{k\uparrow}(0)\}\rangle$

- propagators obtained within mean-field approximation

MF decoupling

$$H_{BCS} = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{kk'} V_{kk'} c^+_{k\uparrow} c^+_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$\langle c^+c^+\rangle cc + c^+c^+\langle cc\rangle$$

$$\rightarrow H_{MF} = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} - \sum_k \left(\Delta_k c^+_{k\uparrow} c^+_{-k\downarrow} + \Delta^*_k c_{-k\downarrow} c_{k\uparrow}\right) \quad \text{with} \quad \Delta_k = -\sum_{k'} V_{kk'} \langle c_{-k\downarrow} c_{k\uparrow}\rangle$$

EOM for the relevant operators

$$\hbar \frac{d}{d\tau} c_{k\uparrow}(\tau) = [H_{MF}, c_{k\uparrow}]_\tau$$

$$= -\varepsilon_k c_{k\uparrow}(\tau) + \Delta_k c^+_{-k\downarrow}(\tau)$$

$$\hbar \frac{d}{d\tau} c^+_{-k\downarrow}(\tau) = \varepsilon_k c^+_{-k\downarrow}(\tau) + \Delta^*_k c_{k\uparrow}(\tau)$$

$$[c^+_{k\uparrow} c_{k\uparrow}, c_{k\uparrow}] = c^+_{k\uparrow} \overbrace{c_{k\uparrow} c_{k\uparrow}}^{0} - \overbrace{c_{k\uparrow} c^+_{k\uparrow} c_{k\uparrow}}^{c_{k\uparrow}}$$

$$[c^+_{k\uparrow} c^+_{-k\downarrow}, c_{k\uparrow}] = c^+_{k\uparrow} c^+_{-k\downarrow} c_{k\uparrow} - c_{k\uparrow} c^+_{k\uparrow} c^+_{-k\downarrow}$$

$$= -\underbrace{\{c_{k\uparrow}, c^+_{k\uparrow}\}}_{1} c^+_{-k\downarrow}$$

EOM for the propagators

normal propagator:

$$\mathcal{G}(k,\tau) = -\frac{1}{\hbar}\langle T\{c_{k\uparrow}(\tau)\,c^{+}_{k\uparrow}(0)\}\rangle = -\frac{1}{\hbar}\langle c_{k\uparrow}(\tau)\,c^{+}_{k\uparrow}(0)\rangle\,\vartheta(\tau) + \frac{1}{\hbar}\langle c^{+}_{k\uparrow}(0)\,c_{k\uparrow}(\tau)\rangle\,\vartheta(-\tau)$$

$$\hbar\frac{d}{d\tau}\mathcal{G}(k,\tau) = -\langle\{c_{k\uparrow}, c^{+}_{k\uparrow}\}\rangle\,\delta(\tau) - \frac{1}{\hbar}\langle T\{\hbar\frac{dc_{k\uparrow}(\tau)}{d\tau}\,c^{+}_{k\uparrow}(0)\}\rangle$$

$$= -\delta(\tau) - \varepsilon_k\,\mathcal{G}(k,\tau) + \Delta_k\,\mathcal{F}(k,\tau)$$

$$-\varepsilon_k c_{k\uparrow}(\tau) + \Delta_k c^{+}_{-k\downarrow}(\tau)$$

anomalous propagator:

$$\varepsilon_k c^{+}_{-k\downarrow}(\tau) + \Delta^{*}_k c_{k\uparrow}(\tau)$$

$$\mathcal{F}(k,\tau) = -\frac{1}{\hbar}\langle T\{c^{+}_{-k\downarrow}(\tau)\,c^{+}_{k\uparrow}(0)\}\rangle$$

$$\hbar\frac{d}{d\tau}\mathcal{F}(k,\tau) = -\langle\{c^{+}_{-k\downarrow}, c^{+}_{k\uparrow}\}\rangle\,\delta(\tau) - \frac{1}{\hbar}\langle T\{\hbar\frac{dc^{+}_{-k\downarrow}(\tau)}{d\tau}\,c^{+}_{k\uparrow}(0)\}\rangle$$

$$= \varepsilon_k\,\mathcal{F}(k,\tau) + \Delta^{*}_k\,\mathcal{G}(k,\tau)$$

Fourier transform $\quad \hbar\frac{d}{d\tau} \to -iE \qquad \delta(\tau) \to 1$

$$\hbar \frac{d}{d\tau} \mathcal{G}(k,\tau) = -\delta(\tau) - \varepsilon_k \mathcal{G}(k,\tau) + \Delta_k \mathcal{F}(k,\tau) \rightarrow 1 = (iE - \varepsilon_k)\mathcal{G}(k,iE) + \Delta_k \mathcal{F}(k,iE)$$

$$\hbar \frac{d}{d\tau} \mathcal{F}(k,\tau) = \varepsilon_k \mathcal{F}(k,\tau) + \Delta_k^* \mathcal{G}(k,\tau) \rightarrow 0 = (iE + \varepsilon_k)\mathcal{F}(k,iE) + \Delta_k^* \mathcal{G}(k,iE)$$

$$\left.\begin{aligned} (iE-\varepsilon_k)\mathcal{G} + \Delta_k \mathcal{F} &= 1 \\ \Delta_k^* \mathcal{G} + (iE+\varepsilon_k)\mathcal{F} &= 0 \end{aligned}\right\}$$

$$\det = (iE)^2 - \varepsilon_k^2 - |\Delta_k|^2$$

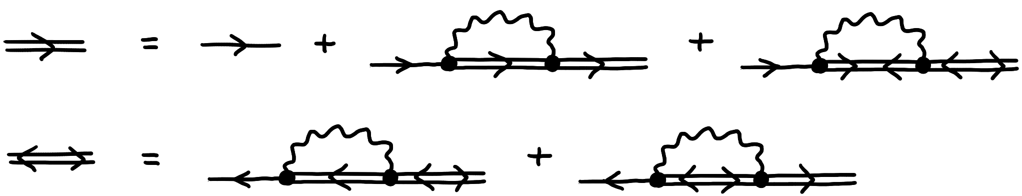
$$\mathcal{G}(k,iE) = \frac{iE + \varepsilon_k}{(iE)^2 - \varepsilon_k^2 - |\Delta_k|^2}$$

$$\mathcal{F}(k,iE) = \frac{-\Delta_k^*}{(iE)^2 - \varepsilon_k^2 - |\Delta_k|^2}$$

$\mathcal{G}$ and $\mathcal{F}$ have poles at $\pm E_k = \pm\sqrt{\varepsilon_k^2 + |\Delta_k|^2}$ $\rightarrow$ quasiparticle dispersion

anomalous $\mathcal{F}$ only appears in SC state with $\Delta_k^* \neq 0$

Gorkov scheme



Лев Петрович Горькóв
(14.6.1929 Moscow
- 28.12.2016 Tallahassee, FL)

- matrix formulation by Nambu (assuming $\Delta_k = \Delta_k^*$)

Yoichiro Nambu
南部 陽一郎
(18.1.1921-5.7.2015)

Nambu spinor $\bar{\Psi}_k = \begin{pmatrix} c_{k\uparrow} \\ c^+_{-k\downarrow} \end{pmatrix}$

Pauli matrices

$$\tau_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

mean-field Hamiltonian

$$H_{MF} = \sum_k \bar{\Psi}_k^+ (\varepsilon_k \tau_3 - \Delta_k \tau_1) \bar{\Psi}_k = \sum_k (c^+_{k\uparrow} \;\; c_{-k\downarrow}) \begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta_k & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^+_{-k\downarrow} \end{pmatrix}$$

matrix propagator

$$\mathcal{G}_{\alpha\beta}(k,\tau) = -\frac{1}{\hbar} \langle T \{ \bar{\Psi}_{k\alpha}(\tau) \, \bar{\Psi}^+_{k\beta}(0) \} \rangle \qquad \mathcal{G} = -\frac{1}{\hbar} \begin{pmatrix} \langle T c_{k\uparrow} c^+_{k\uparrow} \rangle & \langle T c_{k\uparrow} c_{-k\downarrow} \rangle \\ \langle T c^+_{-k\downarrow} c^+_{k\uparrow} \rangle & \langle T c^+_{-k\downarrow} c_{-k\downarrow} \rangle \end{pmatrix}$$

EOM $\hbar \frac{d}{d\tau} \bar{\Psi}_k(\tau) = (-\varepsilon_k \tau_3 + \Delta_k \tau_1) \bar{\Psi}_k(\tau) \rightarrow \mathcal{G}(k, iE) = [iE\tau_0 - \varepsilon_k \tau_3 + \Delta_k \tau_1]^{-1}$

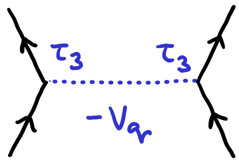
using properties of Pauli matrices: $\mathcal{G}(k, iE) = \dfrac{iE\tau_0 + \varepsilon_k \tau_3 - \Delta_k \tau_1}{(iE)^2 - \varepsilon_k^2 - \Delta_k^2}$

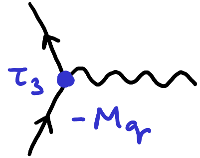
charge operator $\rho_q = -e \sum_k \left(c^+_{k\uparrow} c_{k+q\uparrow} + c^+_{-k-q\downarrow} c_{-k\downarrow} \right) = -e \sum_k \overline{\Psi}^+_k \tau_3 \overline{\Psi}_{k+q}$

diagramatic rules

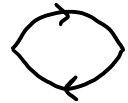
 $\rightarrow -\mathcal{G}$ matrix

 $\rightarrow -\mathcal{D}$ scalar





loop $\rightarrow$ trace



$\Pi \sim \mathrm{Tr}\, \mathcal{G}\mathcal{G}$

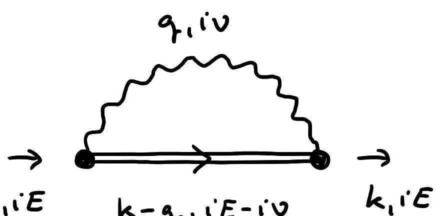
5 Eliashberg theory, gap equations

- renormalized propagator

$$\mathcal{G}(k, iE) = \left[iE\tau_0 - \varepsilon_k \tau_3 - \Sigma(k, iE) \right]^{-1} = \frac{(iE - \Sigma_0)\tau_0 + (\varepsilon_k + \Sigma_3)\tau_3 + \Sigma_1 \tau_1}{(iE-\Sigma_0)^2 - (\varepsilon_k + \Sigma_3)^2 - \Sigma_1^2}$$

- matrix selfenergy

Σ =



$$\Sigma(k, iE) = -\sum_q \frac{1}{\beta} \sum_{i\nu} |M_q|^2 \mathcal{D}(q, i\nu) \times$$
$$\times \tau_3 \mathcal{G}(k-q, iE - i\nu) \tau_3$$

$$= \underbrace{\Sigma_0 \tau_0 + \Sigma_3 \tau_3}_{\text{normal}} + \underbrace{\Sigma_1 \tau_1}_{\text{anomalous}}$$

- BCS case for illustration

replace $|M|^2 \mathcal{D}$ by non-retarded BCS interaction $V_{k,k-q} = -V w_k w_{k-q}$

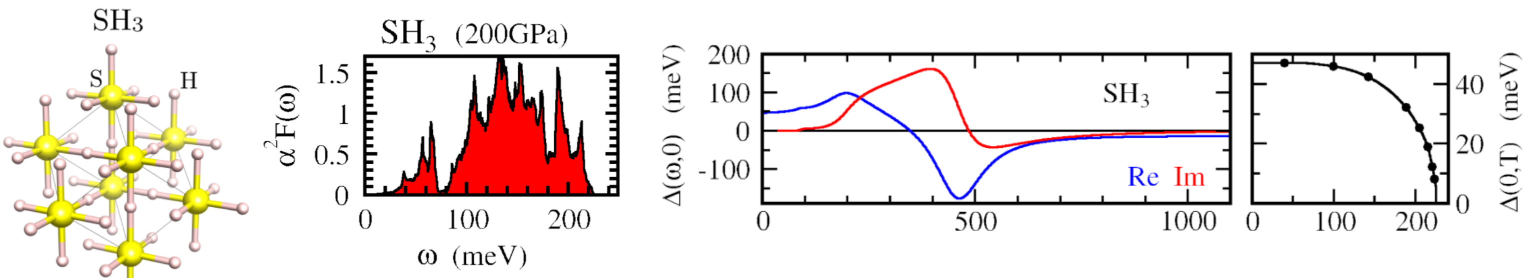
$$\Sigma(k, iE) = V w_k \sum_{k'} w_{k'} \frac{1}{\beta} \sum_{iE'} \tau_3 \frac{(iE' - \Sigma_0)\tau_0 + (\varepsilon_k + \Sigma_3) + \Sigma_1 \tau_1}{(iE' - \Sigma_0)^2 - (\varepsilon_k + \Sigma_3)^2 - \Sigma_1^2} \tau_3 \quad \sim w_k$$

iE independent

τ_1 component $\Sigma_1(k) = -\Delta_k$, $\Sigma_0 = 0$, Σ_3 ignored , $\tau_3 \tau_1 \tau_3 = -\tau_1$:

$$\Delta_k = \sum_{k'} V_{kk'} \frac{1}{\beta} \sum_{iE} \frac{\Delta_{k'}}{(iE)^2 - \varepsilon_{k'}^2 - \Delta_{k'}^2} = -\sum_{k'} V_{kk'} \frac{1}{2E_{k'}} \tanh \frac{\beta E_{k'}}{2} \qquad E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2}$$

- real Eliashberg example - retardation effects included



Sanna et al., J. Phys. Soc. Jpn. 87, 041012 (2018)

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Efficient anisotropic Migdal-Eliashberg calculations with an intermediate representation basis and Wannier interpolation

Hitoshi Mori,[1,2] Takuya Nomoto,[3,4] Ryotaro Arita,[2,3] and Elena R. Margine[1]

[1] *Department of Physics, Applied Physics, and Astronomy, Binghamton University–SUNY, Binghamton, New York 13902, USA*

[2] *RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wako 351-0198, Japan*

[3] *Research Center for Advanced Science and Technology, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8904, Japan*

[4] *Department of Physics, Tokyo Metropolitan University, Hachioji, Tokyo 192-0397, Japan*

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In this study, we combine the *ab initio* Migdal-Eliashberg approach with the intermediate representation of the Green's function, enabling accurate and efficient calculations of the momentum-dependent superconducting gap function while fully considering the effect of the Coulomb retardation. Unlike the conventional scheme that relies on a uniform sampling across Matsubara frequencies, demanding hundreds to thousands of points, the intermediate representation works with fewer than 100 sampled Matsubara Green's functions. The developed methodology is applied to investigate the superconducting properties of three representative low-temperature elemental metals: aluminum, lead, and niobium. The results demonstrate the power and reliability of our computational technique to accurately solve the *ab initio* anisotropic Migdal-Eliashberg equations even at extremely low temperatures below 1 K.

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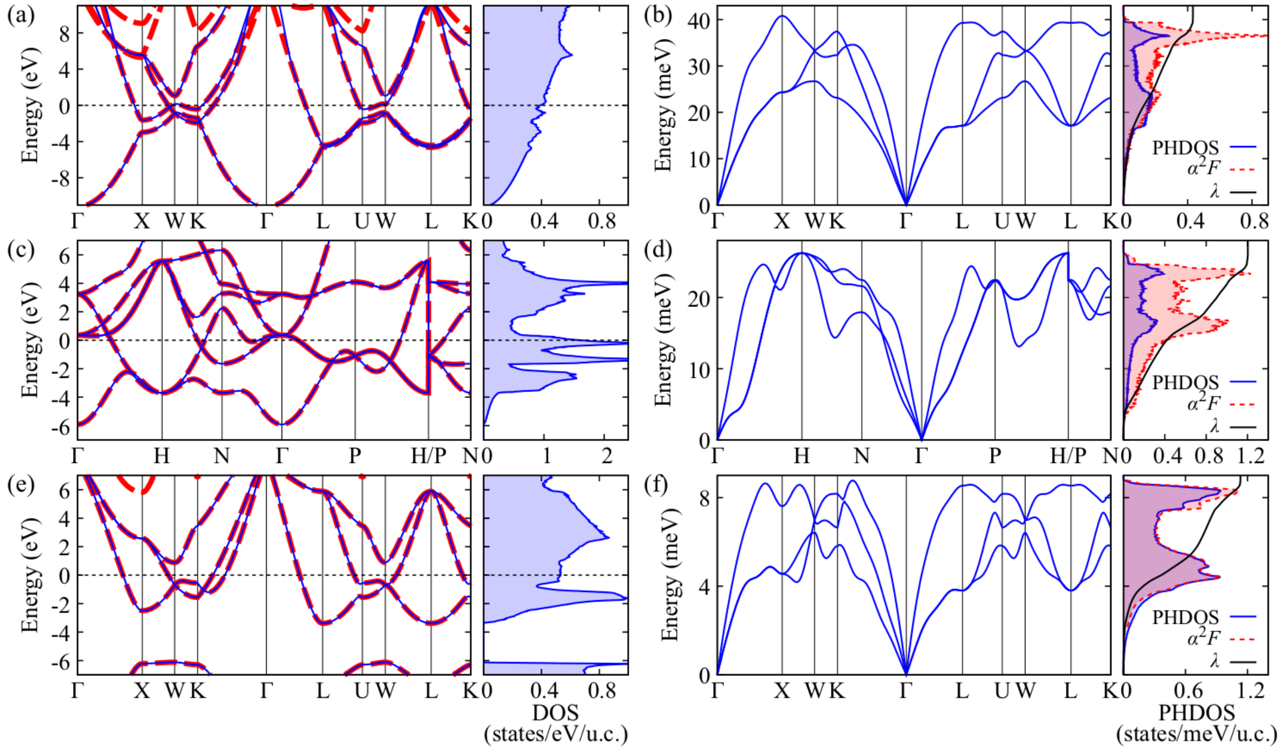

FIG. 2. (a) The calculated electronic band structure and the density of states (DOS) with respect to the Fermi energy for Al. The dashed red lines represent the DFT bands, and the solid blue lines represent the Wannier bands. (b) The phonon dispersion and the phonon density of states (PHDOS), the isotropic Eliashberg spectral function $\alpha^2F(\omega)$, and the cumulative electron-phonon coupling strength $\lambda(\omega)$ for Al. The corresponding results for Nb and Pb are shown in (c)–(f), respectively.

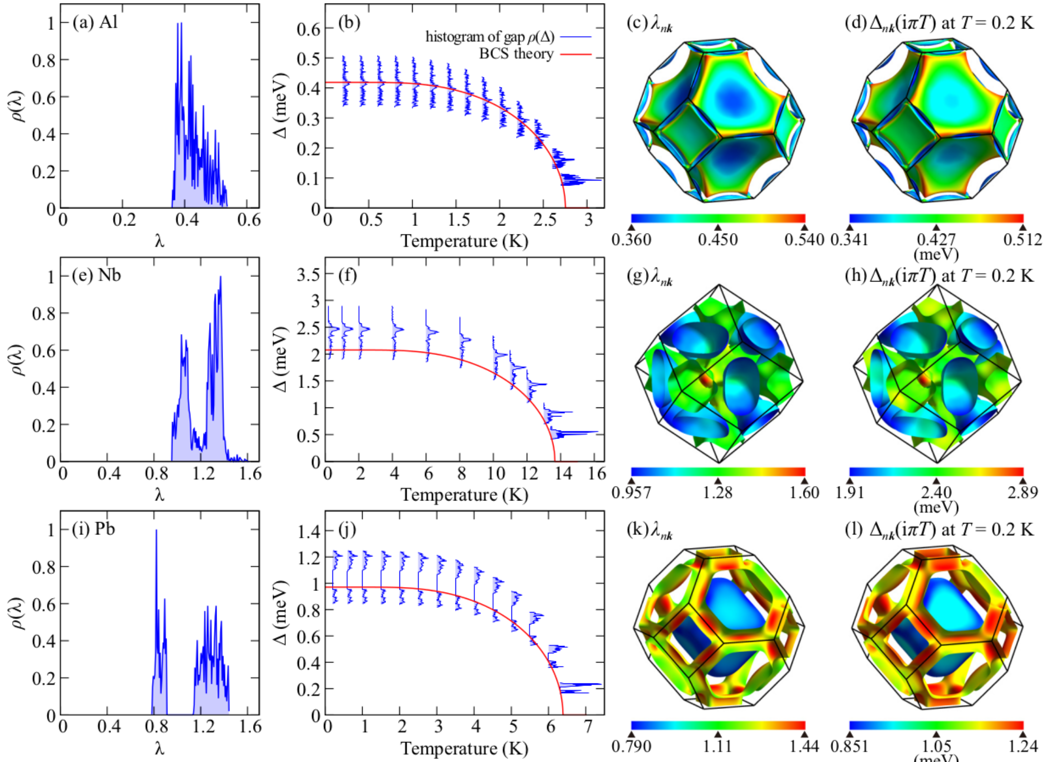

FIG. 3. The histogram of (a) the state-dependent electron-phonon coupling strength $\rho(\lambda)$ and (b) the superconducting gap function $\rho(\Delta)$ at the lowest Matsubara frequency for different temperatures for Al. Solid red line in (b) represents the temperature dependence of the superconducting gap expected from the BCS theory in the weak coupling limit. The state-dependent (c) electron-phonon coupling strength and (d) superconducting gap function on the Fermi surface for Al. The corresponding results for Nb and Pb are shown in (e)–(l), respectively. The calculations were performed with 96^3 $\boldsymbol{k}$ and $\boldsymbol{q}$ grids, a 48^3 $\boldsymbol{k}_{\mathrm{C}}$ grid, and an inner window of 0.5 eV. The images on the Fermi surface were rendered using the FERMISURFER software [48].

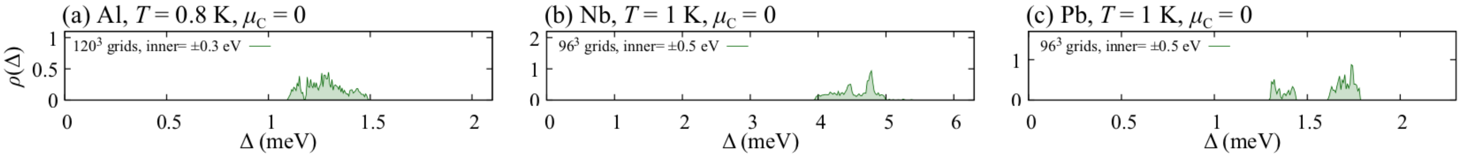

FIG. 6. Convergence of the superconducting gap function with respect to the $\boldsymbol{k}$- and $\boldsymbol{q}$-grid sampling and the inner window. The temperature is set to $T = 0.8$ K for Al and $T = 1$ K for Nb and Pb. The calculations were performed without the Coulomb interaction ($\mu_C = 0$).

TABLE I. Comparison between the transition temperatures (in kelvin) obtained in this work and in previous theoretical studies [21,22,61]. We use the following abbreviations: w SF, with spin fluctuation; w/o SF, without spin fluctuation; w SO, with spin-orbit interaction; and w/o SO, without spin-orbit interaction. In this work, we employ the anisotropic Eliashberg formalism with a constant Coulomb parameter μ_C. In the isotropic Eliashberg formalism employed in Refs. [21,22], as well as in the isotropic SCDFT formalism employed in Ref. [21], the Coulomb interaction was treated as an energy-dependent function. In Ref. [21], the dynamical approach was employed for the screened Coulomb interaction, in addition to the static approach. The anisotropic SCDFT formalism in Ref. [61] considered the momentum dependence of the dynamical Coulomb interaction. SPG denotes the parametrization proposed by Sanna, Pellegrini, and Gross [72] for the SCDFT formalism.

	A. Davydov *et al.* [21]				C. Pellegrini *et al.* [22]	M. Kawamura *et al.* [61]				This work	
	Isotropic Δ				Isotropic Δ	Anisotropic $\Delta(\boldsymbol{k})$				Anisotropic $\Delta(\boldsymbol{k})$	
	Eliashberg		SCDFT (SPG)		Eliashberg	SCDFT				Eliashberg	Expt.
	Static	Dynamical	Static	Dynamical	Static	Dynamical				Static	
	w/o SF, w/o SO				w/o SF, w/o SO	w/o SF, w/o SO	w SF, w/o SO	w/o SF, w SO	w SF, w SO	w/o SF, w/o SO	
Al	0.9	2.5	1.6	1.3	1.03	1.9	0.89	1.9	0.88	2.75 (~2.2)[a]	1.14
Nb	13.3	23.2	7.3	7.8	12.4	14	7.6	13	7.5	13.7	9.20
Pb	6.9	8.2	5.4	3.8	6.85	4.4	3.7	6.9	6.0	6.39	7.19

[a] The value in parentheses is a transition temperature roughly estimated from the histogram with the 96^3 $\boldsymbol{k}_C$ grid at 0.2 K as described in Appendix C.