Electron-Phonon Coupling

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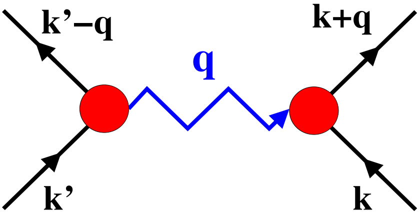

Outline

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   - Green functions and perturbation
   - Electron self-energy
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Electron-phonon Hamiltonian

Electron-ion Hamiltonian

Basic constituents: electrons and ions (nucleus + core electrons)

$$\mathcal{H} = T_e + V_{ee} + T_i + V_{ii} + H_{e-i}$$

- T_e and T_i: kinetic energies of electrons and ions
- V_{ee}: Coulomb interaction among electrons
- V_{ii}: interaction energy among ions
- H_{e-i}: interaction between electrons and ions

- Approximate decoupling of dynamics possible due to very different masses of electron and ions
  - Idea goes back to: M. Born and W. Heisenberg: Ann. d. Phys. **74**, 1 (1926)
  - Correct expansion: M. Born and R. Oppenheimer: Ann. d. Phys, **84**, 457 (1927)
  - Application to solids: G.V. Chester and A. Houghton: Proc. Phys. Soc. **73**, 609 (1959)

Born-Oppenheimer expansion

Task: solve

$$\mathcal{H}\Psi(\underline{\mathbf{r}}, \underline{\mathbf{R}}) = \mathcal{E}\Psi(\underline{\mathbf{r}}, \underline{\mathbf{R}})$$

Expansion of ionic coordinates: $\mathbf{R}_i = \mathbf{R}_i^0 + \kappa \mathbf{u}_i$

Small parameter: $\kappa = (m/M)^{1/4} \leq 0.1$ (except H and He)

Lowest order: adiabatic or Born-Oppenheimer approximation

$$\Psi(\underline{\mathbf{r}}, \underline{\mathbf{R}}) = \chi(\underline{\mathbf{R}})\psi(\underline{\mathbf{r}}; \underline{\mathbf{R}})$$

$\rightarrow$ decoupling

$$\begin{aligned}
[T_e + V_{ee} + H_{e-i}(\underline{\mathbf{R}})]\psi_n(\underline{\mathbf{r}}; \underline{\mathbf{R}}) &= E_n(\underline{\mathbf{R}})\psi_n(\underline{\mathbf{r}}; \underline{\mathbf{R}}) \\
[T_i + V_{ii}(\underline{\mathbf{R}}) + E_n(\underline{\mathbf{R}})]\chi(\underline{\mathbf{R}}) &= \mathcal{E}\chi(\underline{\mathbf{R}})
\end{aligned}$$

Electronic wavefunction depends parametrically on $\underline{\mathbf{R}}$

Electron-phonon vertex

1st order beyond the adiabatic approximation:

$$\langle n|\delta_{\mathbf{R}} V|n'\rangle$$

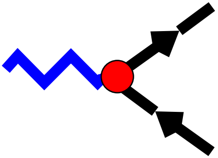
$\delta_{\mathbf{R}} V$: change of potential felt by the electrons under an atom displacement $\mathbf{R} = \mathbf{R}_0 + \mathbf{u}$.

Bare vertex: $\delta_{\mathbf{R}} V = \mathbf{u} \cdot \nabla V^0|_{\mathbf{R}_0}$

Screening is important (metals):

$$\delta_{\mathbf{R}} V = \mathbf{u} \cdot \epsilon^{-1} \nabla V^0|_{\mathbf{R}_0}$$

ϵ^{-1}: inverse dielectric matrix



$\mathbf{u} \propto b + b^\dagger \rightarrow$ phonon creation/annihilation

Fröhlich Hamiltonian

Minimal Hamiltonian (Fröhlich 1952)

$$
\begin{aligned}
H &= H_e + H_{ph} + H_{e-ph} \\
H_e &= \sum_{\mathbf{k}\nu\sigma} \epsilon_{\mathbf{k}\nu} c^\dagger_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma} \\
H_{ph} &= \sum_{\mathbf{q}j} \omega_{\mathbf{q}j} \left(b^\dagger_{\mathbf{q}j} b_{\mathbf{q}j} + \frac{1}{2} \right) \\
H_{e-ph} &= \sum_{\mathbf{k}\nu\nu'\sigma} \sum_{\mathbf{q}j} g^{\mathbf{q}j}_{\mathbf{k}+\mathbf{q}\nu',\mathbf{k}\nu} c^\dagger_{\mathbf{k}+\mathbf{q}\nu'\sigma} c_{\mathbf{k}\nu\sigma} \left(b_{\mathbf{q}j} + b^\dagger_{-\mathbf{q}j} \right)
\end{aligned}
$$

- H_e: band electrons (noninteracting)
- H_{ph}: harmonic phonons
- H_{e-ph}: lowest-order electron-phonon interaction

Normal-state effects

Green functions

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Imaginary-time Green functions (single band)

$$
\begin{aligned}
G(k,\tau) &= -\langle T_\tau c_{k\sigma}(\tau) c^\dagger_{k\sigma}(0)\rangle \\
D(q,\tau) &= -\langle T_\tau (b_q(\tau) + b^\dagger_{-q}(\tau))(b_{-q}(0) + b^\dagger_q(0))\rangle
\end{aligned}
$$

Fourier representation and Matsubara frequencies

$$
\begin{aligned}
G(k,i\omega_n) &= \frac{1}{2}\int_{-\beta}^{\beta} d\tau e^{i\omega_n\tau} G(k,\tau) & \omega_n &= (2n+1)\pi T \\
D(q,i\nu_m) &= \frac{1}{2}\int_{-\beta}^{\beta} d\tau e^{i\nu_m\tau} D(q,\tau) & \nu_m &= 2m\pi T
\end{aligned}
$$

Bare Green functions

$$
\begin{aligned}
G_0(k,i\omega_n) &= \frac{1}{i\omega_n - \epsilon_k} \\
D_0(q,i\nu_m) &= \frac{1}{i\nu_m - \omega_q} - \frac{1}{i\nu_m + \omega_q}
\end{aligned}
$$

Many-body perturbation: Self-energies

Dyson equations and self-energies

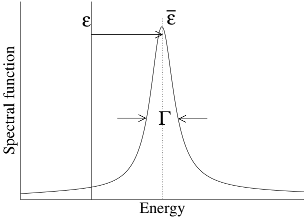
$$G(k, i\omega_n)^{-1} = G_0(k, i\omega_n)^{-1} - \Sigma(k, i\omega_n)$$
$$D(q, i\nu_m)^{-1} = G_0(q, i\nu_m)^{-1} - \Pi(q, i\nu_m)$$

Quasiparticle picture

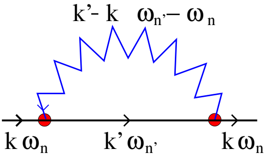
Retarded GF: $G(k, \epsilon) = G(k, i\omega_n \to \epsilon + i\delta) = [\epsilon - \epsilon_k - \Sigma(k, \epsilon)]^{-1}$

Small Σ

- QP-energy shift: $\bar{\epsilon}_k = \epsilon_k + \mathrm{Re}\Sigma(k, \bar{\epsilon}_k)$
- Linewidth ($\propto 1/\tau$): $\Gamma_k = -2\mathrm{Im}\Sigma(k, \bar{\epsilon}_k)$



Electron self-energy



$$\Sigma_{ep}(k, i\omega_n) = -\frac{1}{\beta}\sum_{n'}\frac{1}{N_q}\sum_{k',q} g^q_{k',k} G_0(k', i\omega_{n'})(g^q_{k',k})^* D_0(q, i\omega_{n'} - i\omega_n)$$

Performing Matsubara frequency sum

$$\Sigma_{ep}(k, i\omega_n) = \frac{1}{N_q}\sum_{k',q}|g^q_{k',k}|^2\left[\frac{b(\omega_q) + f(\epsilon_{k'})}{i\omega_n + \omega_q - \epsilon_{k'}} + \frac{b(\omega_q) + 1 - f(\epsilon_{k'})}{i\omega_n - \omega_q - \epsilon_{k'}}\right]$$

Straightforward analytic continuation: $i\omega_n \rightarrow \epsilon + i\delta$

Electron self-energy

$$\mathrm{Im}\Sigma_{ep}(k,\epsilon) = -\pi \frac{1}{N_q} \sum_{k',q} |g^q_{k',k}|^2 \left[\delta(\epsilon - \epsilon_{k'} + \omega_q)(b(\omega_q) + f(\epsilon_{k'})) \right.$$
$$\left. + \delta(\epsilon - \epsilon_{k'} - \omega_q)(b(\omega_q) + 1 - f(\epsilon_{k'}))\right]$$

Collect all q-dependent parts

$$\mathrm{Im}\Sigma_{ep}(k,\epsilon) = -\pi \sum_{k'} \frac{1}{N_q} \sum_{q} |g^q_{k',k}|^2 \int d\omega \delta(\omega - \omega_q)$$
$$\left[\delta(\epsilon - \epsilon_{k'} + \omega)(b(\omega) + f(\epsilon_{k'})) \right.$$
$$\left. + \delta(\epsilon - \epsilon_{k'} - \omega)(b(\omega) + 1 - f(\epsilon_{k'}))\right]$$

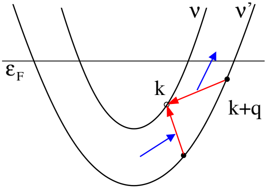
Introduce

$$\alpha^2 F^{\pm}_k(\epsilon,\omega) = \frac{1}{N_q} \sum_q \delta(\omega - \omega_q) \sum_{k'} |g^q_{k',k}|^2 \delta(\epsilon - \epsilon_{k'} \pm \omega)$$

Electron self-energy

$$\mathrm{Im}\Sigma_{ep}(k,\epsilon) = -\pi \int_0^\infty d\omega \Big\{ \alpha^2 F_k^+(\epsilon,\omega)[b(\omega)+f(\omega+\epsilon)]$$
$$+\alpha^2 F_k^-(\epsilon,\omega)[b(\omega)+f(\omega-\epsilon)] \Big\}$$

Scattering processes



"+": phonon emission
"–": phonon absorption

Quasielastic approximation:

$$\alpha^2 F^+ \approx \alpha^2 F^- \approx \alpha^2 F_k(\epsilon,\omega) = \frac{1}{N_q}\sum_q \delta(\omega-\omega_q)\sum_{k'} |g^q_{k',k}|^2 \delta(\epsilon-\epsilon_{k'})$$

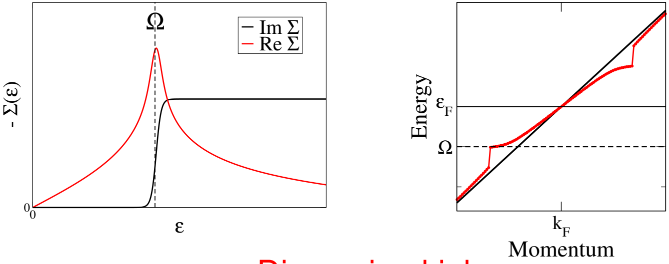
Electron self-energy

Illustration: Einstein model ($T \to 0$)

$$\mathrm{Im}\Sigma_{ep}(k,\epsilon) \to -\pi A(\epsilon)\left[2 - \Theta(\Omega-\epsilon) - \Theta(\Omega+\epsilon)\right]$$

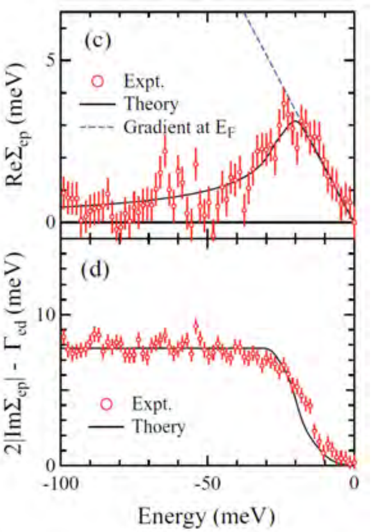
Real part via Kramers-Kronig relation

$$\mathrm{Re}\Sigma_{ep}(k,\epsilon) = \frac{1}{\pi}\int d\epsilon' \frac{\mathrm{Im}\Sigma_{ep}(k,\epsilon')}{\epsilon-\epsilon'}$$



Dispersion kinks

Electron self-energy



Experimental self-energy from Cu(110) surface band

- continuous phonon spectrum
- broadened step in Σ_{ep}

APRES data after Jiang *et al.*, PRB **89**, 085404 (2014)

Electron self-energy

Coupling constant

$$\lambda_k = 2 \int d\omega \frac{\alpha^2 F_k(\bar{\epsilon}_k, \omega)}{\omega}$$

depends on electronic state!

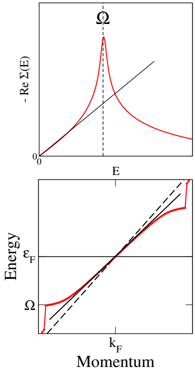
Experimental access

(1) Slope of of $\mathrm{Re}\Sigma_{ep}$ at E_F

$$\lambda_k = -\left.\frac{\partial \mathrm{Re}\Sigma_{ep}(k,\epsilon)}{\partial \epsilon}\right|_{\epsilon=0, T=0}$$

From $\bar{\epsilon}_k = \epsilon_k + \mathrm{Re}\Sigma(k, \bar{\epsilon}_k)$

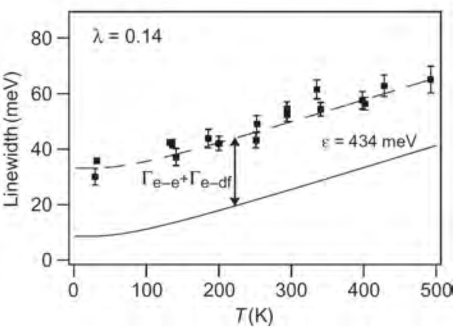
Velocity: $\bar{v}_F = v_F/(1+\lambda_{k_F})$
Mass enhancement: $m_k^* = m_k(1+\lambda_k)$



Electron self-energy

(2) T-dependence of linewidth

$$\begin{aligned}\Gamma_k(T) &= \pi\int_0^\infty d\omega\left\{\alpha^2F_k(\bar{\epsilon}_k,\omega)\left[2b(\omega)+f(\omega+\bar{\epsilon}_k)+f(\omega-\bar{\epsilon}_k)\right]\right\}\\ &\approx 2\pi\lambda_k T \qquad\qquad \text{for } T\gg\omega_{\text{ph}}\end{aligned}$$

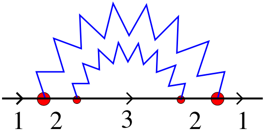


Cu(111) surface state

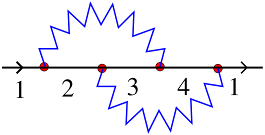
ARPES data after McDougall *et al.*, PRB **51**, 13891 (1995)

Migdal's theorem

Higher-order self energy diagrams



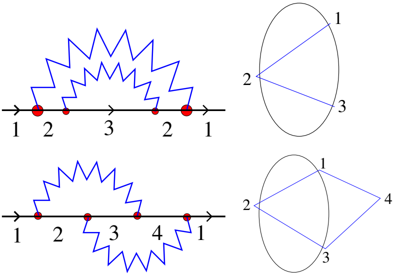
self-energy correction of inner line



vertex correction

Migdal (1958):
Vertex corrections are smaller by a factor $\omega_D/\epsilon_F \approx 0.1$ compared to self-energy corrections (for those parts of Green function most influenced by phonons)

Migdal's theorem



Phase space argument

- large contributions for small energy differences $\epsilon_{12} = \epsilon_1 - \epsilon_2$ and ϵ_{23}
- momentum conservation forces large ϵ_{14}
- one intermediate momentum must be small
  $\rightarrow$ reduced phase space
  $\rightarrow$ suppression $\propto \omega_D/\epsilon_F$

Good approximation:

- take only self-energy diagrams: $G_0 \rightarrow G$ in inner lines
- but: this lead to small corrections only (Holstein, Migdal)

$\Rightarrow$ original diagram sufficient

Migdal's theorem

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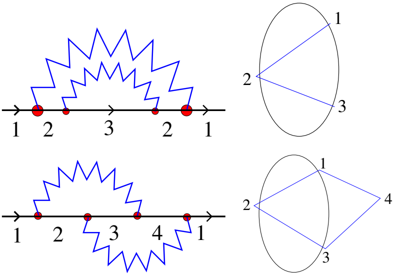

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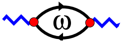
  $\rightarrow$ reduced phase space
  $\rightarrow$ suppression $\propto \omega_D/\epsilon_F$

Theorem fails for

- Very small Fermi surface (both momenta are small)
  Example: doped semiconductors
- Quasi-1D metals ("nesting")
- Small electronic bandwidth ($\omega_D \approx \epsilon_F$)

Phonon self-energy: Linewidth

$\gamma = -2\,\mathrm{Im}$ 

$$\gamma_{\mathbf{q}} = 2\pi \frac{1}{N_k} \sum_{\mathbf{k}} |g^{\mathbf{q}}_{\mathbf{k+q},\mathbf{k}}|^2 [f(\epsilon_{\mathbf{k}\nu}) - f(\epsilon_{\mathbf{k+q}})] \delta[\omega_{\mathbf{q}} + (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}})]$$

Simplifications for $\omega_{\mathbf{q}} \ll$ electronic scale

$$f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{k+q}}) \approx f'(\epsilon_{\mathbf{k}})(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}}) \to -f'(\epsilon_{\mathbf{k}})\omega_{\mathbf{q}}$$

$T \to 0$: $f'(\epsilon_{\mathbf{k}}) \to -\delta(\epsilon_{\mathbf{k}})$ and drop $\omega_{\mathbf{q}}$ in δ-function

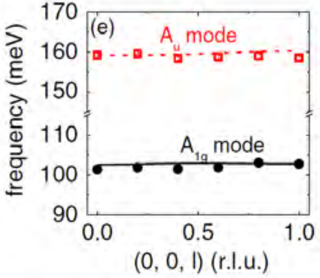
$$\boxed{\gamma_{\mathbf{q}} \approx 2\pi\omega_{\mathbf{q}} \frac{1}{N_k} \sum_{\mathbf{k}} |g^{\mathbf{q}}_{\mathbf{k+q},\mathbf{k}}|^2 \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k+q}})}$$

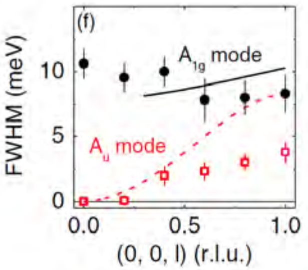
Formula often used in context of superconductivity (Allen, PRB **6**, 2577 (1972))

Phonon self-energy: Linewidth (2)

- $\gamma_{\mathbf{q}}$ measurable quantity (e.g., via inelastic neutron or x-ray scattering)
- but need to separate from other contributions: anharmonicity, defects

Example: YNi_2B_2C





Weber *et al.*, PRL **109**, 057001 (2012)

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Phonon-mediated superconductivity

Effective electron-electron interaction

Hamiltonian: $$H = H_0 + \eta H_1$$

Canonical transformation: $$H' = e^{-\eta S} H e^{\eta S}$$

$$\begin{aligned} \Rightarrow H' &= H + \eta[H,S] + \frac{\eta^2}{2}[[H,S],S] + O(\eta^3) \\ &= H_0 + \eta(H_1 + [H_0,S]) + \eta^2[H_1,S] + \frac{\eta^2}{2}[[H_0,S],S] + O(\eta^3) \end{aligned}$$

Condition to eliminate linear term: $$H_1 + [H_0,S] = 0$$

$$\begin{aligned} \Rightarrow H' &= H_0 + H_{\text{eff}} + O(\eta^3) \\ H_{\text{eff}} &= \frac{\eta^2}{2}[H_1,S] \end{aligned}$$

Effective electron-electron interaction

Application to Fröhlich Hamiltonian (single band, single phonon)

$$\begin{aligned} H_0 &= H_e + H_{ph} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \left(b^\dagger_{\mathbf{q}} b_{\mathbf{q}} + \frac{1}{2} \right) \\ H_1 &= \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}} \right) \end{aligned}$$

Ansatz: $$S = \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(x_{\mathbf{k},\mathbf{q}} b_{\mathbf{q}} + y_{\mathbf{k},\mathbf{q}} b^\dagger_{-\mathbf{q}} \right)$$

Evaluating the commutators

$$\begin{aligned} [H_e, S] &= \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(x_{\mathbf{k},\mathbf{q}} b_{\mathbf{q}} + y_{\mathbf{k},\mathbf{q}} b^\dagger_{-\mathbf{q}} \right) \\ [H_{ph}, S] &= \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(-x_{\mathbf{k},\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}} + y_{\mathbf{k},\mathbf{q}} \omega_{-\mathbf{q}} b^\dagger_{-\mathbf{q}} \right) \end{aligned}$$

Effective electron-electron interaction

Combining ($\omega_{\mathbf{q}} = \omega_{-\mathbf{q}}$)

$$H_1 + [H_0, S] = \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \Big\{ \big(1 + (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} - \omega_{\mathbf{q}}) x_{\mathbf{k},\mathbf{q}}\big) b_{\mathbf{q}} + \big(1 + (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} + \omega_{\mathbf{q}}) y_{\mathbf{k},\mathbf{q}}\big) b^\dagger_{-\mathbf{q}} \Big\}$$

vanishes for

$$x_{\mathbf{k},\mathbf{q}} = (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} + \omega_{\mathbf{q}})^{-1} \quad \text{and} \quad y_{\mathbf{k},\mathbf{q}} = (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{q}})^{-1}\,.$$

Effective interaction: $H_{\text{eff}} = \frac{\eta^2}{2}[H_1, S]$

Recall

$$H_1 = \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}}\right)$$

$$S = \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(x_{\mathbf{k},\mathbf{q}} b_{\mathbf{q}} + y_{\mathbf{k},\mathbf{q}} b^\dagger_{-\mathbf{q}}\right)$$

Effective electron-electron interaction

$$
\begin{aligned}
H_1 &= \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}} \right) \\
S &= \sum_{\mathbf{kq}} g_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \left(x_{\mathbf{k},\mathbf{q}} b_{\mathbf{q}} + y_{\mathbf{k},\mathbf{q}} b^\dagger_{-\mathbf{q}} \right)
\end{aligned}
$$

$[H_1, S] \rightarrow [Aa, Bb]$ with $A, B \propto c^\dagger c$ and $a, b \propto xb + yb^\dagger$

Use $[Aa, Bb] = AB[a, b] + [A, B]ab - [A, B][a, b]$

- $[A, B][a, b] \rightarrow$ one-electron term, actually vanishes
- $[A, B]ab \rightarrow$ electron-two phonon interaction
- $AB[a, b] \propto c^\dagger c c^\dagger c \rightarrow$ effective el.-el. interaction

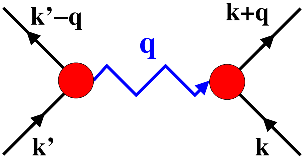
Effective electron-electron interaction

3rd term

$$\begin{aligned} H_{\text{eff}} &= \frac{\eta^2}{2} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} g_{\mathbf{k},\mathbf{q}} g_{\mathbf{k}',-\mathbf{q}} \left(y_{\mathbf{k}',-\mathbf{q}} - x_{\mathbf{k}',-\mathbf{q}} \right) c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} c^\dagger_{\mathbf{k}'-\mathbf{q}} c_{\mathbf{k}'} \\ &= \eta^2 \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} V_{\text{eff}}(\mathbf{k},\mathbf{k}',\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} c^\dagger_{\mathbf{k}'-\mathbf{q}} c_{\mathbf{k}'} \end{aligned}$$

with

$$V_{\text{eff}}(\mathbf{k},\mathbf{k}',\mathbf{q}) = g_{\mathbf{k},\mathbf{q}} g_{\mathbf{k}',-\mathbf{q}} \frac{\omega_{\mathbf{q}}}{(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}'-\mathbf{q}})^2 - \omega^2_{\mathbf{q}}}$$



Effective electron-electron interaction

Cooper pairs: electrons with opposite momenta ($\mathbf{k}' = -\mathbf{k}$)

$$V_{\text{eff}}(\mathbf{k}, -\mathbf{k}, \mathbf{q}) = |g_{\mathbf{k},\mathbf{q}}|^2 \frac{\omega_{\mathbf{q}}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}})^2 - \omega_{\mathbf{q}}^2}$$

- attractive (< 0) for $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}| < \omega_{\mathbf{q}}$
- repulsive (> 0) for $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}| > \omega_{\mathbf{q}}$

$\Rightarrow$ phonon-mediated interaction is always attractive for small energy differences

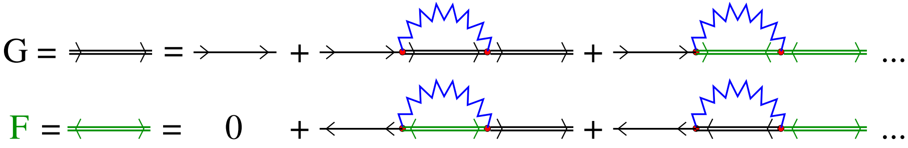
Nambu formalism

Superconducting state

- Macroscopic quantum state, coherent superposition of electron pairs
- Cooper pairs (singlet): $(k\uparrow, -k\downarrow)$
- Anomalous Green functions (Gor'kov 1958) (vanish in normal state)

$$F(k,\tau) = -\langle T_\tau c_{k\uparrow}(\tau) c_{-k\downarrow}(0)\rangle \quad F^*(k,\tau) = -\langle T_\tau c^\dagger_{-k\downarrow}(\tau) c^\dagger_{k\uparrow}(0)\rangle$$

Perturbation



Nambu (1960): clever way to organize diagrammatic expansion

Nambu formalism

Two-component operators

$$\Psi_k = \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} \qquad \Psi^\dagger_k = \begin{pmatrix} c^\dagger_{k\uparrow}\,, & c_{-k\downarrow} \end{pmatrix}$$

Green function

$$\begin{aligned} \underline{G}(k,\tau) &= -\langle T_\tau \Psi_k(\tau)\Psi^\dagger_k(0)\rangle \\ &= \begin{pmatrix} -\langle T_\tau c_{k\uparrow}(\tau)c^\dagger_{k\uparrow}(0)\rangle & -\langle T_\tau c_{k\uparrow}(\tau)c_{-k\downarrow}(0)\rangle \\ -\langle T_\tau c^\dagger_{-k\downarrow}(\tau)c^\dagger_{k\uparrow}(0)\rangle & -\langle T_\tau c^\dagger_{-k\downarrow}(\tau)c_{-k\downarrow}(0)\rangle \end{pmatrix} \\ &= \begin{pmatrix} G(k,\tau) & F(k,\tau) \\ F^*(k,\tau) & -G(-k,-\tau) \end{pmatrix} \end{aligned}$$

Nambu formalism

Fourier transform

$$\underline{G}(k,i\omega_n)=\frac{1}{2}\int_{-\beta}^{\beta}d\tau e^{i\omega_n\tau}\underline{G}(k,\tau)=\begin{pmatrix} G(k,i\omega_n) & F(k,i\omega_n) \\ F^*(k,i\omega_n) & -G(-k,-i\omega_n)\end{pmatrix}$$

Rewriting Fröhlich Hamiltonian

$$H_e=\sum_{k\sigma}\epsilon_k c^\dagger_{k\sigma}c_{k\sigma}\to\sum_k \epsilon_k \Psi^\dagger_k\underline{\tau}_3\Psi_k \qquad \underline{\tau}_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$H_{e-ph}=\sum_{k\sigma}\sum_q g^q_{k'k}c^\dagger_{k'\sigma}c_{k\sigma}\left(b_q+b^\dagger_{-q}\right)\to\sum_{kq}g^q_{k'k}\Psi^\dagger_{k'}\underline{\tau}_3\Psi_k\left(b_q+b^\dagger_{-q}\right)$$

assuming $g^q_{k'k}=g^q_{-k-k'}$ (time-reversal symmetry)

Nambu formalism

Dyson equation $\rightarrow$ self-energy

$$\underline{G}^{-1}(k, i\omega_n) = \underline{G}_0^{-1}(k, i\omega_n) - \underline{\Sigma}(k, i\omega_n)$$

Nice feature

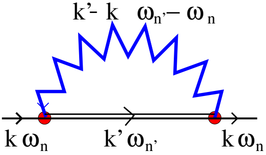
- same diagrammatic expansion
- propagators, vertices 2×2 matrices: $g^q_{k'k} \rightarrow g^q_{k'k}\underline{\tau}_3$

Bare Green function

$$\begin{aligned}
\underline{G}_0(k, i\omega_n) &= \begin{pmatrix} G_0(k, i\omega_n) & 0 \\ 0 & -G_0(-k, -i\omega_n) \end{pmatrix} \\
&= \begin{pmatrix} (i\omega_n - \epsilon_k)^{-1} & 0 \\ 0 & (i\omega_n + \epsilon_k)^{-1} \end{pmatrix} \\
&= (i\omega_n \underline{\tau}_0 - \epsilon_k \underline{\tau}_3)^{-1}
\end{aligned}$$

Eliashberg theory

Eliashberg theory: extension of Migdal's theory to superconducting state



Self-energy in Nambu formalism

$$\underline{\Sigma}(k, i\omega_n) = -\frac{1}{\beta}\sum_{n'}\frac{1}{N_q}\sum_{k',q} g^q_{k'k}\underline{\tau}_3\underline{G}(k', i\omega_{n'})\underline{\tau}_3 g^{-q}_{kk'} D(q, i\omega_{n'} - i\omega_n)$$

General form of $\underline{\Sigma}$

$$\underline{\Sigma}(k, i\omega_n) = i\omega_n[1 - Z(k, i\omega_n)]\underline{\tau}_0 + \chi(k, i\omega_n)\underline{\tau}_3 + \Phi(k, i\omega_n)\underline{\tau}_1 + \overline{\Phi}(k, i\omega_n)\underline{\tau}_2$$

$$\underline{\tau}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \underline{\tau}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \underline{\tau}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \underline{\tau}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Eliashberg theory

Using Dyson equation

$$\begin{aligned}\underline{G}^{-1}(k,i\omega_n) &= \underline{G}_0^{-1}(k,i\omega_n) - \underline{\Sigma}(k,i\omega_n)\\ &= (i\omega_n\underline{\tau}_0 - \epsilon_k\underline{\tau}_3) - \underline{\Sigma}(k,i\omega_n)\\ &= i\omega_n Z(k,i\omega_n)\underline{\tau}_0 - (\epsilon_k + \chi(k,i\omega_n))\underline{\tau}_3 - \Phi(k,i\omega_n)\underline{\tau}_1 - \overline{\Phi}(k,i\omega_n)\underline{\tau}_2\end{aligned}$$

For self-energy we need $\underline{G}$

$$\begin{aligned}\underline{G}(k,i\omega_n) &= \big[i\omega_n Z(k,i\omega_n)\underline{\tau}_0 + (\epsilon_k + \chi(k,i\omega_n))\underline{\tau}_3\\ &\quad + \Phi(k,i\omega_n)\underline{\tau}_1 + \overline{\Phi}(k,i\omega_n)\underline{\tau}_2\big]/\mathcal{D}\end{aligned}$$

with

$$\mathcal{D} := \det \underline{G}^{-1} = (i\omega_n Z)^2 - (\epsilon_k + \chi)^2 - \Phi^2 - \overline{\Phi}^2$$

Eliashberg theory

Plug into expression for $\underline{\Sigma}$ and separate τ-components

$$
\begin{aligned}
i\omega_n(1 - Z(k, i\omega_n)) &= -\frac{1}{\beta}\sum_{n'}\frac{1}{N_q}\sum_{k',q}|g^q_{k'k}|^2 D(q, i\omega_{n'} - i\omega_n)\frac{i\omega_{n'} Z(k', i\omega_{n'})}{\mathcal{D}(k', i\omega_{n'})}\\
\chi(k, i\omega_n) &= -\frac{1}{\beta}\sum_{n'}\frac{1}{N_q}\sum_{k',q}|g^q_{k'k}|^2 D(q, i\omega_{n'} - i\omega_n)\frac{\epsilon_{k'} + \chi(k', i\omega_{n'})}{\mathcal{D}(k', i\omega_{n'})}\\
\Phi(k, i\omega_n) &= \frac{1}{\beta}\sum_{n'}\frac{1}{N_q}\sum_{k',q}|g^q_{k'k}|^2 D(q, i\omega_{n'} - i\omega_n)\frac{\Phi(k', i\omega_{n'})}{\mathcal{D}(k', i\omega_{n'})}\\
\overline{\Phi}(k, i\omega_n) &= \frac{1}{\beta}\sum_{n'}\frac{1}{N_q}\sum_{k',q}|g^q_{k'k}|^2 D(q, i\omega_{n'} - i\omega_n)\frac{\overline{\Phi}(k', i\omega_{n'})}{\mathcal{D}(k', i\omega_{n'})}
\end{aligned}
$$

Eliashberg equations

Eliashberg theory

Quasiparticles: solutions of

$$\mathcal{D}(k, i\omega_n \to \epsilon + i\delta) = 0$$

or

$$\mathcal{D}(k, \epsilon + i\delta) = (\epsilon Z)^2 - (\epsilon_k + \chi)^2 - \Phi^2 - \overline{\Phi}^2 = 0$$

$$\Rightarrow \qquad E_k = \sqrt{\frac{(\epsilon_k + \chi)^2}{Z^2} + \frac{\Phi^2 + \overline{\Phi}^2}{Z^2}}$$

- Z: QP renormalization factor
- χ: energy shift
- Φ,$\overline{\Phi}$: gap function

$$\Delta(k, i\omega_n) = \frac{\Phi(k, i\omega_n) - i\overline{\Phi}(k, i\omega_n)}{Z(k, i\omega_n)}$$

Isotropic gap equation

Simplifications (1)

- $\overline{\Phi} = 0$: gauge choice (homogeneous superconductor)
- $\chi = 0$: particle-hole symmetry
- Ignore changes in phonon propagator:

$$D(q, i\nu_m) \to D_0(q, i\nu_m) = \int d\omega \delta(\omega - \omega_q) \frac{2\omega}{(i\nu_m)^2 - \omega^2}$$

$$\begin{aligned}
\Phi(k, i\omega_n) &= \frac{1}{\beta} \sum_{n'} \frac{1}{N_k} \sum_{k',q} |g^q_{k'k}|^2 D(q, i\omega_{n'} - i\omega_n) \frac{\Phi(k', i\omega_{n'})}{\mathcal{D}(k', i\omega_{n'})} \\
&\approx \frac{1}{\beta} \int d\omega \frac{1}{N_k} \sum_{k'} \sum_{q} |g^q_{k'k}|^2 \delta(\omega - \omega_q) \sum_{n'} \frac{-2\omega}{(\omega_{n'} - \omega_n)^2 + \omega^2} \frac{\Phi(k', i\omega_{n'})}{\mathcal{D}(k', i\omega_{n'})}
\end{aligned}$$

Coupling function

$$\alpha^2 F(k, k', \omega) = N(0) \sum_q |g^q_{k'k}|^2 \delta(\omega - \omega_q)$$

Isotropic gap equation

$$\Phi(k,i\omega_n) \quad \approx \quad \frac{1}{\beta}\int d\omega \frac{1}{N(0)N_k}\sum_{k'}\alpha^2F(k,k',\omega)\sum_{n'}\frac{-2\omega}{(\omega_{n'}-\omega_n)^2+\omega^2}\frac{\Phi(k',i\omega_{n'})}{\mathcal{D}(k',i\omega_{n'})}$$

Main k-dependence from ϵ_k in $\mathcal{D} = -(\omega_n Z)^2 - \epsilon_k^2 - \Phi^2$

Simplifications (2)

- Take momenta k,k' on Fermi surface only
- Take Fermi-surface averages, e.g.

$$\Phi(i\omega_n) = \frac{1}{N_k}\sum_k w_k\Phi(k,i\omega_n) \qquad w_k = \frac{\delta(\epsilon_k)}{N(0)}$$

Eliashberg function

$$\begin{aligned}\alpha^2F(\omega) \quad &= \quad \frac{1}{N_k^2}\sum_{kk'}w_k w_{k'}\alpha^2F(k,k',\omega)\\ &= \quad \frac{1}{N(0)}\frac{1}{N_k^2}\sum_{kk'}|g^q_{k'k}|^2\delta(\epsilon_k)\delta(\epsilon_{k'})\delta(\omega-\omega_q)\end{aligned}$$

Isotropic gap equation

$$\Phi(i\omega_n) = -\frac{1}{\beta}\sum_{n'}\int d\omega \frac{2\omega\alpha^2 F(\omega)}{(\omega_n - \omega_{n'})^2 + \omega^2}\Phi(i\omega_{n'})\frac{1}{N_q}\sum_{k'}\frac{1}{\mathcal{D}(\epsilon_{k'}, i\omega_{n'})}$$

The final k sum is converted into an integral ($N(\epsilon) \to N(0)$)

$$\frac{1}{N_q}\sum_{k'}\frac{1}{\mathcal{D}(\epsilon_{k'}, i\omega_{n'})} = \int d\epsilon N(\epsilon)\frac{1}{\mathcal{D}(\epsilon, i\omega_{n'}))} \approx \frac{\pi N(0)}{\sqrt{[(\omega_{n'} Z(i\omega_{n'})]^2 + \Phi(i\omega_{n'})^2}}$$

Isotropic gap equation

Using $\Delta(i\omega_n) = \Phi(i\omega_n)/Z(i\omega_n)$

$$
\begin{aligned}
i\omega_n(1 - Z(i\omega_n)) &= -\pi \frac{1}{\beta} \sum_{n'} \Lambda(\omega_n - \omega_{n'}) \frac{\omega_{n'}}{\sqrt{\omega_{n'}^2 + \Delta(i\omega_{n'})^2}} \\
\Delta(i\omega_n) Z(i\omega_n) &= \pi \frac{1}{\beta} \sum_{n'} \Lambda(\omega_n - \omega_{n'}) \frac{\Delta(i\omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta(i\omega_{n'})^2}}
\end{aligned}
$$

Kernel

$$
\Lambda(\nu_m) = \int d\omega \frac{2\omega\alpha^2 F(\omega)}{(\nu_m)^2 + \omega^2}
$$

- represents phonon-mediated pairing interaction
- solely depends on $\alpha^2 F(\omega) \rightarrow$ normal-state property
- positive $\rightarrow$ always attractive
- frequency dependence $\rightarrow$ retardation

Isotropic gap equation

Eliashberg function: relation to previous normal-state quantities

$$\alpha^2 F(\omega) = \frac{1}{N(0)} \frac{1}{N_k^2} \sum_{kk'} |g^q_{k'k}|^2 \delta(\epsilon_k)\delta(\epsilon_{k'})\delta(\omega - \omega_q)$$

State-dependent spectral function

$$\alpha^2 F_k(\epsilon, \omega) = \frac{1}{N_q} \sum_q \delta(\omega - \omega_q) \sum_{k'} |g^q_{k',k}|^2 \delta(\epsilon - \epsilon_{k'})$$

$$\Rightarrow \quad \alpha^2 F(\omega) = \sum_k \frac{\delta(\epsilon_k)}{N(0)} \alpha^2 F_k(\epsilon = 0, \omega)$$

Phonon linewidth

$$\gamma_q \approx 2\pi\omega_q \frac{1}{N_k} \sum_{kk'} |g^q_{k',k}|^2 \delta(\epsilon_k)\delta(\epsilon_{k'})$$

$$\Rightarrow \quad \alpha^2 F(\omega) = \frac{1}{2\pi N(0)} \frac{1}{N_q} \sum_q \frac{\gamma_q}{\omega_q} \delta(\omega - \omega_q)$$

Isotropic gap equation

Kernel

$$\Lambda(\nu_m) = \int d\omega \frac{2\omega\alpha^2 F(\omega)}{(\nu_m)^2 + \omega^2}$$

Maximum at $\nu_m = 0$: coupling constant

$$\boxed{\lambda = 2 \int d\omega \frac{\alpha^2 F(\omega)}{\omega}}$$

State-dependent coupling constant

$$\lambda = \sum_k \frac{\delta(\epsilon_k)}{N(0)} \lambda_k$$

Phonon coupling-constant

$$\lambda = \frac{1}{N_q} \sum_q \frac{1}{\pi N(0)} \frac{\gamma_q}{\omega_q^2} =: \frac{1}{N_q} \sum_q \lambda_q$$

Isotropic gap equation

Coulomb effects

$$\mu = N(0)\langle\langle V_C(k,k')\rangle\rangle_{FS}$$

Scaling down (Morel and Anderson, 1962)

$$\mu^*(\omega_c) = \frac{\mu}{1+\mu\ln(\epsilon_0/\omega_c)}$$

Modification of kernel in eq. for Δ

$$\Lambda(i\omega_n - i\omega_{n'}) \to [\Lambda(i\omega_n - i\omega_{n'}) - \mu^*(\omega_c)]\Theta(\omega_c - |\omega_{n'}|)$$

- Reduction of T_c
- Scaling down: fails if low-energy excitations are important

First principles approach: Superconducting DFT

$\to$ following talk by Antonio Sanna

Isotropic gap equation

Transition temperature T_c

- largest T with non-trivial solution
- depends on input $\alpha^2 F$ and μ^*: normal state properties

Approximate solution (McMillan 1968, Allen and Dynes 1975) valid for $\lambda < 2$ and $\mu^* < 0.15$

$$T_c = \frac{\omega_{\log}}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right]$$

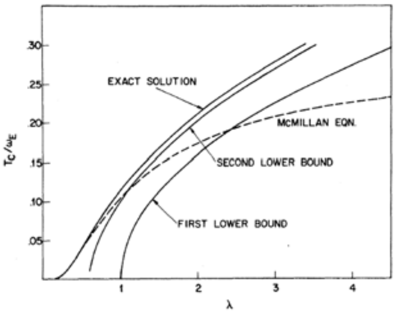
Prefactor

$$\omega_{\log} = \exp\left[\int d\omega \log(\omega) W(\omega)\right] \qquad W(\omega) = \frac{2}{\lambda} \frac{\alpha^2 F(\omega)}{\omega}$$

Isotropic gap equation

Asymptotic behavior: no intrinsic upper bound

$$T_c \propto c(\mu^*)\sqrt{\lambda < \omega^2 >} \qquad c(\mu^*) \approx 0.15...0.2$$



Allen and Dynes, PRB **12**, 905 (1975)

Density functional theory approach

Density functional theory approach

DFT: mapping of many-body problem onto effective single particle system

$$\Big\{-\nabla^2 + v_{\mathrm{eff}}(\mathbf{r})\Big\}\psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

$$v_{\mathrm{eff}}[n] = v_{\mathrm{ext}} + v_{\mathrm{scr}}[n] = v_{\mathrm{ext}} + v_H[n] + v_{XC}[n]$$

$$n(\mathbf{r}) = \sum_i f_i |\psi_i(\mathbf{r})|^2 \qquad \text{electron density}$$

Electron-phonon vertex via linear response

$$\begin{aligned}
\delta v_{\mathrm{eff}}(\mathbf{r}) &= \delta v_{\mathrm{ext}}(\mathbf{r}) + \delta v_{\mathrm{scr}}(\mathbf{r}) = \delta v_{\mathrm{ext}}(\mathbf{r}) + \int d^3r' \, I(\mathbf{r},\mathbf{r}')\delta n(\mathbf{r}') \\
I(\mathbf{r},\mathbf{r}') &\equiv \frac{\delta v_{\mathrm{scr}}(\mathbf{r})}{\delta n(\mathbf{r}')} = \frac{\delta v_{\mathrm{H}}(\mathbf{r})}{\delta n(\mathbf{r}')} + \frac{\delta v_{\mathrm{XC}}(\mathbf{r})}{\delta n(\mathbf{r}')} = \frac{2}{|\mathbf{r}-\mathbf{r}'|} + \frac{\delta^2 E_{XC}}{\delta n(\mathbf{r})\delta n(\mathbf{r}')}
\end{aligned}$$

Density functional theory approach

1st-order perturbation
$$\delta\psi_i(\mathbf{r}) = \sum_{j(\neq i)} \frac{\langle j|\delta v_{\text{eff}}|i\rangle}{\epsilon_i - \epsilon_j}\psi_j(\mathbf{r})$$

$$\Rightarrow \delta n(\mathbf{r}) = \sum_{i\neq j} \frac{f_i - f_j}{\epsilon_i - \epsilon_j}\langle j|\delta v_{\text{eff}}|i\rangle \psi_i^*(\mathbf{r})\psi_j(\mathbf{r})$$

$\Rightarrow$ screened variation of effective potential $\delta v_{\text{eff}}(\mathbf{r})$

Periodic displacement

$$u_{ls} = U_s^{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}_{ls}^0} + (U_s^{\mathbf{q}})^* e^{-i\mathbf{q}\mathbf{R}_{ls}^0}$$

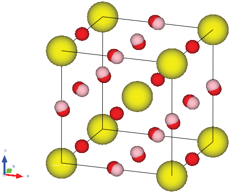
Electron-phonon vertex

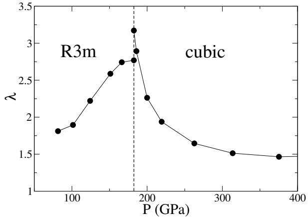
$$g_{\mathbf{k}+\mathbf{q}\nu',\mathbf{k}\nu}^{\mathbf{q}j} = \sum_s \frac{\eta_s(\mathbf{q}j)}{\sqrt{2M_s\omega_{\mathbf{q}j}}}\langle \mathbf{k}+\mathbf{q}\nu'|\frac{\partial v_{\text{eff}}}{\partial U_s^{\mathbf{q}}}|\mathbf{k}\nu\rangle$$

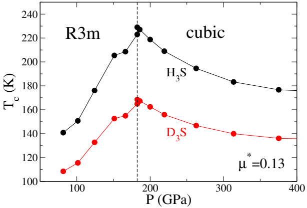
Density functional theory approach

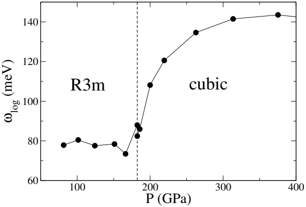
Example 1: high-pressure high-T_c material: H_3S

$T_c = 203$ K at 200 GPa (Dozdov 2015)







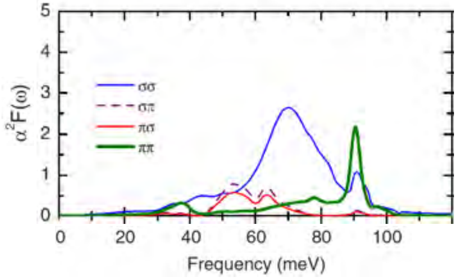


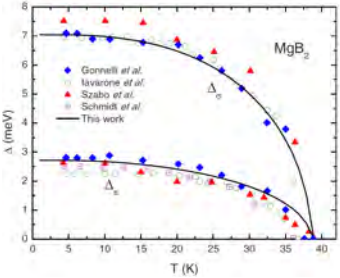
Density functional theory approach

Example 2: multiband superconductor MgB_2 ($T_c = 39$ K)

Extension: multiband gap equation

$$\alpha^2 F_{\nu\nu'}(\omega) = \frac{1}{N_{\nu'}(0)} \frac{1}{N_q} \sum_{\mathbf{q}j,\mathbf{k}} |g^{\mathbf{q}j}_{\mathbf{k}+\mathbf{q}\nu',\mathbf{k}\nu}|^2 \delta(\omega - \omega_{\mathbf{q}j}) \delta(\epsilon_{\mathbf{k}\nu}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}\nu'})$$





O. de la Peña Seaman *et al.*, PRB **82**, 224508 (2010)

Summary

- Introduction to electron-phonon coupling in metals
- Focus of quasiparticle renormalization
- Normal state: information about coupling strength from renormalized electronic dispersion and electron or phonon linewidths
- Discussions of Migdal's theorem and its limitations
- Eliashberg theory and derivation of isotropic gap equations
- DFT approach: provides insight into the microscopic form of coupling, on the basis of realistic atomic and electronic structures
- Current challenges: extend Eliashberg framework to
  - anharmonicity
  - materials with small electronic energy scales
  - strongly correlated systems