Electron-Phonon Coupling

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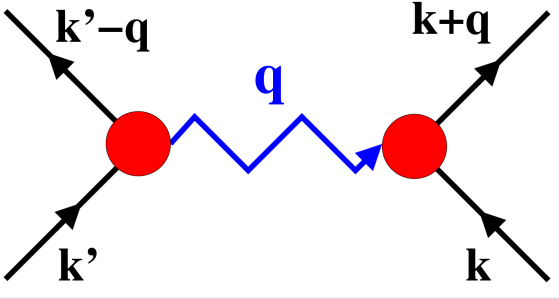
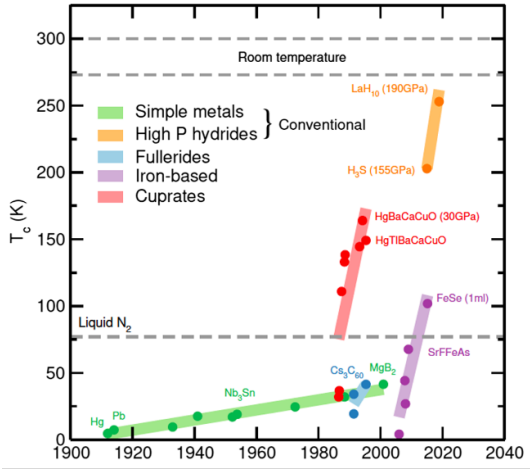
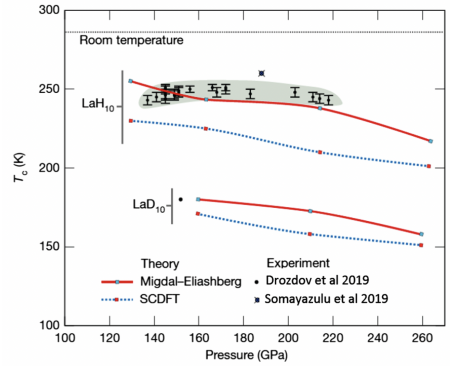


Comeback of phonon-mediated superconductivity





Pickett, Reviews of Modern Physics 95, 021001 (2023)

Outline

Electron-phonon Hamiltonian

Electron-phonon vertex

Fundamental Hamiltonian of 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)

Electron-phonon vertex: 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

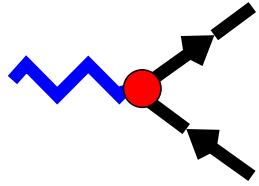
1st order beyond the adiabatic approximation: $\langle n|\delta_{\mathbf{R}} V|n'\rangle$

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

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

Screened vertex: $\delta_{\mathbf{R}} V = \mathbf{u} \cdot \epsilon^{-1} \nabla V^0|_{\mathbf{R}_0}$ ϵ^{-1}: inverse dielectric matrix

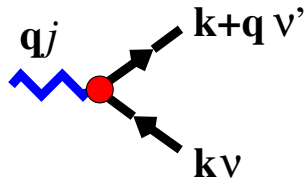
Solid: displacement $\mathbf{u} \propto b + b^\dagger \rightarrow$ phonon creation/annihilation



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

Many-body perturbation: Self-energies

Dyson equations and self-energies

$$
\begin{aligned}
G(k, i\omega_n)^{-1} &= G_0(k, i\omega_n)^{-1} - \Sigma(k, i\omega_n) && \text{electrons} \\
D(q, i\nu_m)^{-1} &= D_0(q, i\nu_m)^{-1} - \Pi(q, i\nu_m) && \text{phonons}
\end{aligned}
$$

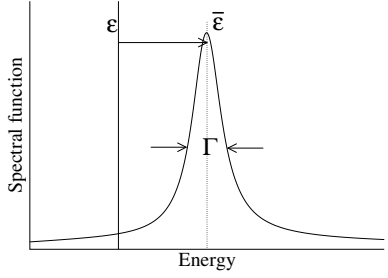
Quasiparticle picture

Spectral function

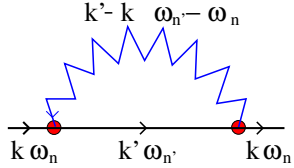
$$
\begin{aligned}
A(k, \epsilon) &= -\mathrm{Im} G(k, i\omega_n \to \epsilon + i\delta) \\
&= -\mathrm{Im} \frac{1}{\epsilon - \epsilon_k - \Sigma(k, \epsilon)}
\end{aligned}
$$

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 summmation

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

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

Electron self-energy

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

Collect all q-dependent parts

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

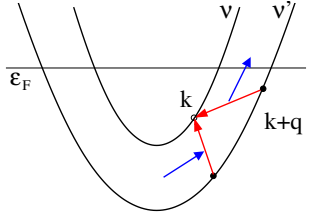
Introduce

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

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

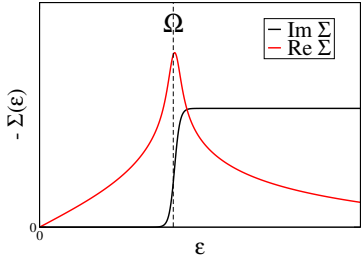
Quasielastic approximation:

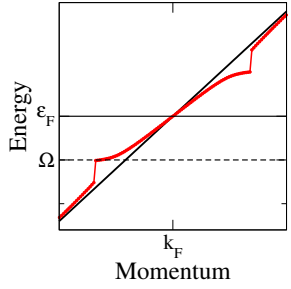
$$\alpha^2 F^+ \approx \alpha^2 F^- \approx \alpha^2 F_k(\epsilon,\omega) = \frac{1}{N_q} \sum_q \delta(\omega - \omega_q) \sum_{k'} |g^q_{k',k}|^2 \delta(\epsilon - \epsilon_{k'} \cancel{\pm \omega})$$

Electron self-energy

Illustration: Einstein model ($T \to 0$) $\quad \mathrm{Im}\Sigma_{ep}(k,\epsilon) \to -\pi A(\epsilon)[2 - \Theta(\Omega - \epsilon) - \Theta(\Omega + \epsilon)]$

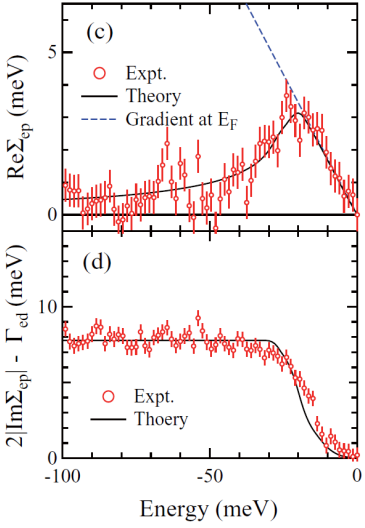
Real part via Kramers-Kronig relation $\quad \mathrm{Re}\Sigma_{ep}(k,\epsilon) = \frac{1}{\pi} \int d\epsilon' \frac{\mathrm{Im}\Sigma_{ep}(k,\epsilon')}{\epsilon - \epsilon'}$





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!

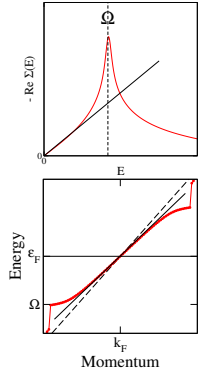
Experimental access

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

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

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

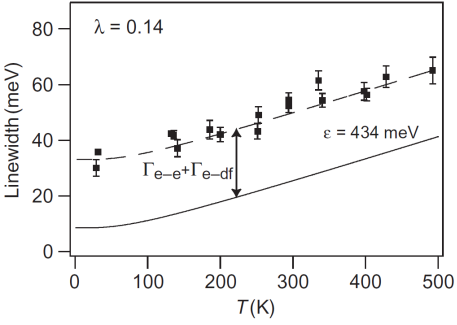
$\rightarrow$ Velocity: $\bar{v}_F = v_F/(1+\lambda_{k_F})$
$\rightarrow$ Mass enhancement: $m_k^* = m_k(1+\lambda_k)$



Electron self-energy

(2) T-dependence of linewidth

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

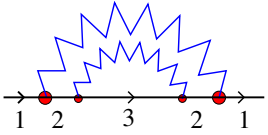


Cu(111) surface state

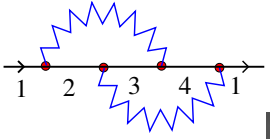
ARPES data after McDougall *et al.*, PRB **51**, 13891 (1995)

Migdal's theorem

Higher-order self energy diagrams



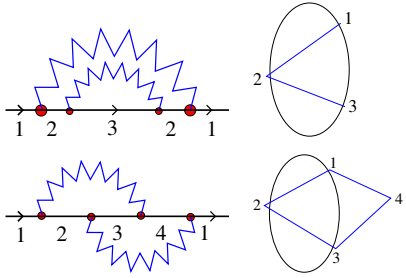
self-energy correction of inner line



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

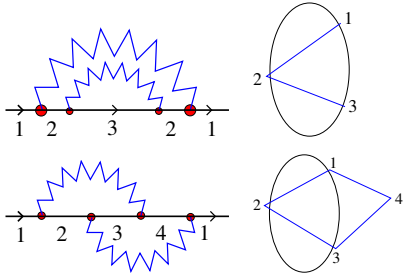
- large contributions for small energy differences $\epsilon_{12} = \epsilon_1 - \epsilon_2$ and ϵ_{23}
- momentum conservation forces large ϵ_{14}
- one intermediate momentum must be small
  $\rightarrow$ reduced phase space
  $\rightarrow$ suppression $\propto \omega_D/\epsilon_F$

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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  $\rightarrow$ reduced phase space
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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

$$\mathrm{Im}\,\Pi(\omega) = \mathrm{Im}$$ 

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

Simplifications ($\omega_{\mathbf{q}} \ll$ electronic scale)

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

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

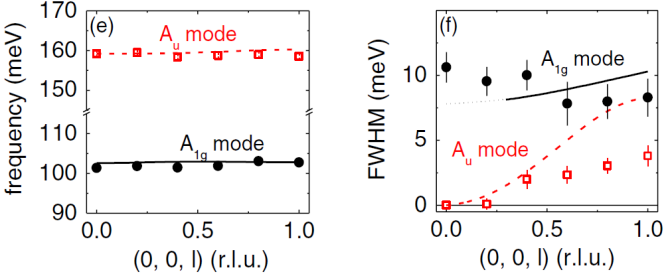
$$\gamma_{\mathbf{q}} \approx 2\pi\omega_{\mathbf{q}} \frac{1}{N_k} \sum_{\mathbf{k}} |g^{\mathbf{q}}_{\mathbf{k}+\mathbf{q},\mathbf{k}}|^2 \delta(\epsilon_{\mathbf{k}})\delta(\epsilon_{\mathbf{k}+\mathbf{q}})$$

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)

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 branch)

$$H_0 = H_e + H_{ph} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \left(b^\dagger_{\mathbf{q}} b_{\mathbf{q}} + \frac{1}{2} \right)$$

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

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

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

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

Effective electron-electron interaction

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

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

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

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

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

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

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

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

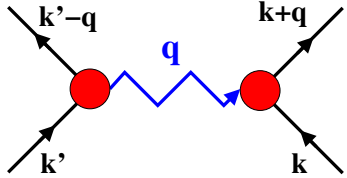
Effective electron-electron interaction

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

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



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 $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}| > \omega_{\mathbf{q}}$

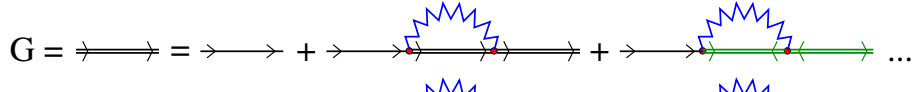
$\Rightarrow$ phonon-mediated interaction is always attractive for small energy differences

Strong-coupling theory: 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)

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



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

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

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

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

Nambu formalism

Dyson equation $\rightarrow$ self-energy $\qquad \underline{G}^{-1}(k, i\omega_n) = \underline{G}_0^{-1}(k, i\omega_n) - \underline{\Sigma}(k, i\omega_n)$

Nice feature

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

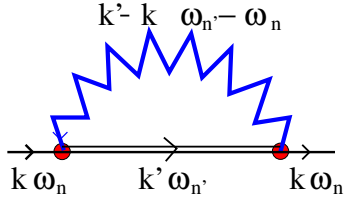
Bare Green function

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

Strong-coupling theory: Eliashberg approach

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 $\underline{G}$

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

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

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

Strong-coupling theory: Isotropic gap equation

Simplifications (1)

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

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

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

Simplifications (2)

- Take momenta k,k' on Fermi surface only
- Take Fermi-surface averages of Z and Φ, e.g.

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

Isotropic gap equation

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

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

Gap function: $\Delta(i\omega_n) = \Phi(i\omega_n)/Z(i\omega_n)$

Eliashberg function: $\alpha^2F(\omega) = N(0)\sum_{kk'}|g^q_{k'k}|^2 w_k w_{k'}\delta(\omega - \omega_q)$

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

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

Isotropic gap equation

$$\omega_n(1-Z(i\omega_n)) = -\pi\frac{1}{\beta}\sum_{n'}[\Lambda(\omega_n-\omega_{n'})-\mu^*(\omega_c)]\Theta(\omega_c-|\omega_{n'}|)\frac{\omega_{n'}}{\sqrt{\omega_{n'}^2+\Delta(i\omega_{n'})^2}}$$

$$\Delta(i\omega_n)Z(i\omega_n) = \pi\frac{1}{\beta}\sum_{n'}[\Lambda(\omega_n-\omega_{n'})-\mu^*(\omega_c)]\Theta(\omega_c-|\omega_{n'}|)\frac{\Delta(i\omega_{n'})}{\sqrt{\omega_{n'}^2+\Delta(i\omega_{n'})^2}}$$

Gap function: $\Delta(i\omega_n)=\Phi(i\omega_n)/Z(i\omega_n)$

Eliashberg function: $\alpha^2F(\omega)=N(0)\sum_{kk'}|g^q_{k'k}|^2 w_k w_{k'}\delta(\omega-\omega_q)$

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

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

Coulomb effects

- Scaling down (Morel and Anderson, 1962)

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

- Reduction of T_c

Isotropic gap equation: relation to normal-state quantities

Eliashberg function

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

State-dependent spectral function

$$\begin{aligned}\alpha^2F_k(\epsilon,\omega) &= \frac{1}{N_q}\sum_q\delta(\omega-\omega_q)\sum_{k'}|g^q_{k',k}|^2\delta(\epsilon-\epsilon_{k'})\\ \Rightarrow\qquad \alpha^2F(\omega) &= \frac{1}{N_k}\sum_k\frac{\delta(\epsilon_k)}{N(0)}\alpha^2F_k(\epsilon=0,\omega)\end{aligned}$$

Phonon linewidth

$$\begin{aligned}\gamma_q &\approx 2\pi\omega_q\frac{1}{N_k}\sum_{kk'}|g^q_{k',k}|^2\delta(\epsilon_k)\delta(\epsilon_{k'})\\ \Rightarrow\qquad \alpha^2F(\omega) &= \frac{1}{2\pi N(0)}\frac{1}{N_q}\sum_q\frac{\gamma_q}{\omega_q}\delta(\omega-\omega_q)\end{aligned}$$

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

$$\lambda = \frac{1}{N_k} \sum_k \frac{\delta(\epsilon_k)}{N(0)} \lambda_k$$

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: Transition temperature T_c

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

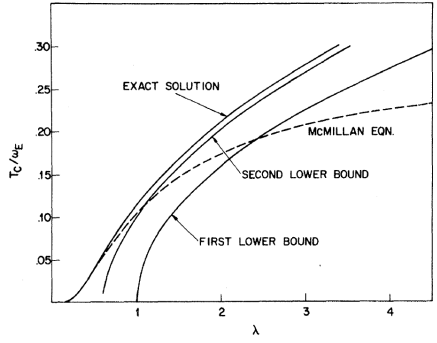
Approximate solution valid for $\lambda < 2$ and $\mu^* < 0.15$
(McMillan 1968, Allen and Dynes 1975)

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

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

Asymptotic behavior: no intrinsic upper bound

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



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

Density functional theory approach

Density functional perturbation theory: Basics

Single-particle (Kohn-Sham) equations

$$\left\{ -\nabla^2 + v_{\text{eff}}(\mathbf{r}) \right\} \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

Effective potential

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

with

$$v_H(\mathbf{r})[n] = \frac{\delta E_H}{\delta n(\mathbf{r})} \qquad v_{XC}(\mathbf{r})[n] = \frac{\delta E_{XC}}{\delta n(\mathbf{r})}$$

Density

$$n(\mathbf{r}) = \sum_i f_i |\psi_i(\mathbf{r})|^2 \qquad f_i\text{: occupation numbers}$$

$E_{XC}[n]$: exchange-correlation; approximated (LDA, GGA, ...)

Density functional perturbation theory: Linear response

Perturbation δv_{eff}: $\delta\psi_i(\mathbf{r}) = \sum_{j(\neq i)} \frac{\langle j|\delta v_{\text{eff}}|i\rangle}{\epsilon_i - \epsilon_j}\psi_j(\mathbf{r})$

Linear density response

$$\begin{aligned}\delta n(\mathbf{r}) &= \sum_i f_i[\psi_i^*(\mathbf{r})\delta\psi_i(\mathbf{r}) + \delta\psi_i^*(\mathbf{r})\psi_i(\mathbf{r})] \\ &= \sum_{i\neq j} \frac{f_i - f_j}{\epsilon_i - \epsilon_j}\langle j|\delta v_{\text{eff}}|i\rangle\psi_i^*(\mathbf{r})\psi_j(\mathbf{r}) = \int d^3r'\chi_0(\mathbf{r},\mathbf{r}')\delta v_{\text{eff}}(\mathbf{r}')\end{aligned}$$

with charge susceptibility $\chi_0(\mathbf{r},\mathbf{r}') = \sum_{i\neq j} \frac{f_i - f_j}{\epsilon_i - \epsilon_j}\psi_i^*(\mathbf{r})\psi_j(\mathbf{r})\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')$

Density functional perturbation theory: Linear response

Variation of effective potential $v_{\text{eff}}[n] = v_{\text{ext}} + v_H[n] + v_{XC}[n]$

$$\delta v_{\text{eff}}(\mathbf{r}) = \delta v_{\text{ext}}(\mathbf{r}) + \delta v_{\text{scr}}(\mathbf{r}) = \delta v_{\text{ext}}(\mathbf{r}) + \int d^3r' I(\mathbf{r},\mathbf{r}')\delta n(\mathbf{r}')$$

with kernel

$$I(\mathbf{r},\mathbf{r}') \equiv \frac{\delta v_{\text{H}}(\mathbf{r})}{\delta n(\mathbf{r}')} + \frac{\delta v_{\text{XC}}(\mathbf{r})}{\delta n(\mathbf{r}')} = \frac{2}{|\mathbf{r}-\mathbf{r}'|} + \frac{\delta^2 E_{XC}}{\delta n(\mathbf{r})\delta n(\mathbf{r}')}$$

Dielectric screening

$$\delta n = \chi_0 \delta v_{\text{eff}}\,, \quad \delta v_{\text{eff}} = \delta v_{\text{ext}} + I\delta n \quad \Rightarrow \delta v_{\text{eff}} = \delta v_{\text{ext}} + I\chi_0 \delta v_{\text{eff}}$$

$$\Rightarrow \delta v_{\text{eff}} = [1 - I\chi_0]^{-1}\delta v_{\text{ext}} = \epsilon^{-1}\delta v_{\text{ext}} \quad \text{and} \quad \delta n = \chi_0 \epsilon^{-1}\delta v_{\text{ext}}$$

$\epsilon(\mathbf{r},\mathbf{r}')$: (static) dielectric matrix

- historically first route persued (Pick *et al.*1970, Resta 1985)

DFPT: Modern formulation

Simple case: non-metal, gap between conduction and valence states

Starting from

$$\begin{aligned} \delta n(\mathbf{r}) &= \sum_{i \neq j} \frac{f_i - f_j}{\epsilon_i - \epsilon_j} \langle j | \delta v_{\text{eff}} | i \rangle \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) \\ &\Rightarrow \quad 2 \sum_{cv} \frac{1}{\epsilon_v - \epsilon_c} \langle c | \delta v_{\text{eff}} | v \rangle \psi_v^*(\mathbf{r}) \psi_c(\mathbf{r}) \end{aligned}$$

Rewriting

$$\delta n(\mathbf{r}) = 2 \sum_v \psi_v^*(\mathbf{r}) \Delta_v(\mathbf{r})$$

with definition

$$|\Delta_v\rangle = \sum_c \frac{1}{\epsilon_v - \epsilon_c} |c\rangle \langle c | \delta v_{\text{eff}} | v \rangle$$

DFPT: Modern formulation

How to calculate $|\Delta_v\rangle = \sum_c \frac{1}{\epsilon_v - \epsilon_c} |c\rangle\langle c|\delta v_{\text{eff}}|v\rangle$?

Not directly, but use a linear equation!

$$(H - \epsilon_v)|\Delta_v\rangle \quad = \quad -\sum_c |c\rangle\langle c|\delta v_{\text{eff}}|v\rangle = -P_c \delta v_{\text{eff}}|v\rangle = (P_v - 1)\delta v_{\text{eff}}|v\rangle$$

- $P_v (P_c)$ projection onto valence (conduction) space
- advantage: final form contains only valence space quantities

"Sternheimer" - equation

atomic physics: Sternheimer, 1954, Phys. Rev. 951, **96** (1954)

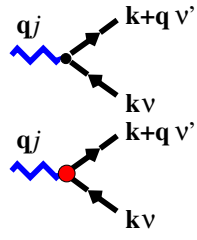
solid state: Baroni *et al.*, PRL **59**, 1861 (1987); Zein, Sov. Phys. Solid State **26**, 1825 (1984)

Iterative solution: $\rightarrow \delta n$ and δv_{eff}

Electron-phonon vertex from DFPT

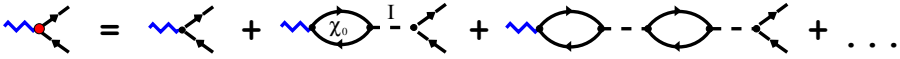
Bare vertex $g^{(0)\mathbf{q}j}_{\mathbf{k}+\mathbf{q}\nu',\mathbf{k}\nu} = \langle \mathbf{k}+\mathbf{q}\nu' | \delta^{\mathbf{q}j} v_{\text{ext}} | \mathbf{k}\nu \rangle$

Screened vertex $g^{\mathbf{q}j}_{\mathbf{k}+\mathbf{q}\nu',\mathbf{k}\nu} = \langle \mathbf{k}+\mathbf{q}\nu' | \delta^{\mathbf{q}j} v_{\text{eff}} | \mathbf{k}\nu \rangle$



easily accessible in DFPT

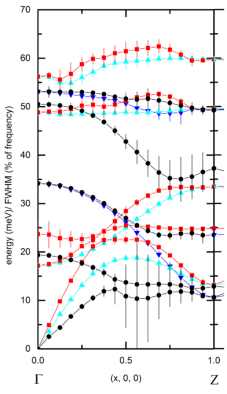
Relationship to bare vertex: $\delta v_{\text{eff}} = \delta v_{\text{ext}} + I\chi_0 \delta v_{\text{eff}}$

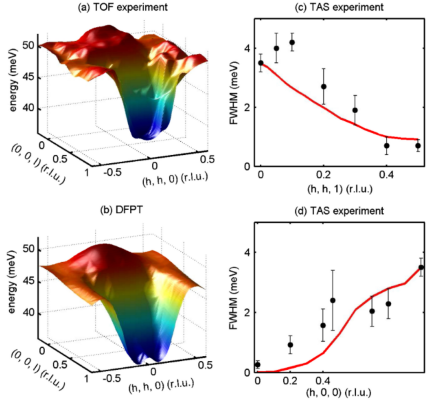


- screening via static Kohn-Sham (non-interacting) susceptibility χ_0
- electron-electron interaction represented by $I = I_H + I_{XC} \rightarrow$ includes exchange-correlation

Example 1: Phonon renormalization

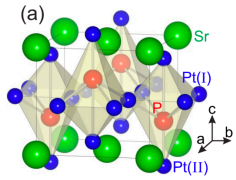
YNi_2B_2C





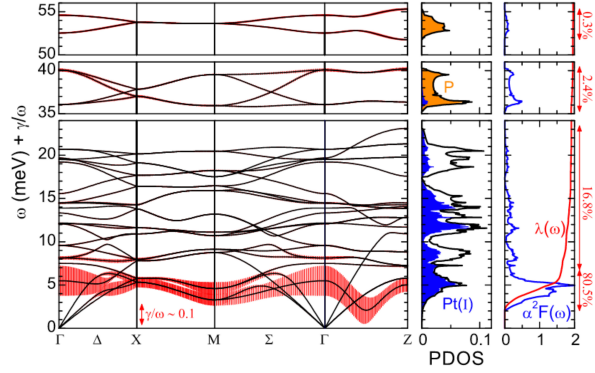
Weber *et al.*, PRL **109**, 057001 (2012), PRB **89**, 104503 (2014)

Example 2: Superconductivity of $SrPt_3P$



$T_C = 8.4$ K

Zocco *et al.*, PRB **92**, 220504 (2015)



- Predicts soft-mode (Pt(1)) with strong coupling, confirmed by IXS measurements
- Contributes 80% to total $\lambda \approx 2$

Summary

- Effect of electron-phonon interaction on quasiparticle renormalization
- Normal state: renormalized electronic dispersion and electron or phonon linewidths provide information about coupling strength, which is experimentally accessible
- Discussions of Migdal's theorem and its limitations
- Eliashberg theory and isotropic gap equations establish link between electron-phonon coupling and superconducting properties
- DFT approach: provides insight into the microscopic form of coupling based on realistic atomic and electronic structures

Current challenges: extend Eliashberg framework to

- anharmonicity
- materials with small electronic energy scales
- strongly correlated systems