2023 Virtual School on Many-Body Calculations using EPW and BerkeleyGW

June 5-9 2023

NSF · U.S. DEPARTMENT OF ENERGY · TACC TEXAS ADVANCED COMPUTING CENTER

Lecture Tue.1

Superconductors and Migdal-Eliashberg theory

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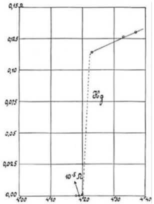
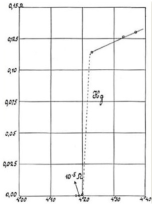
Lecture Summary

- Superconductivity milestones
- BCS theory of superconductivity
- Nambu-Gor'kov formalism and Migdal-Eliashberg theory
- Density functional theory for superconductors
- Examples from calculations
- Outlook

Superconductivity milestones



Onnes, Commun. Phys. Lab.
Univ. Leiden. Suppl. 29 (1911)



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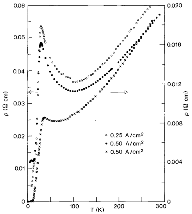
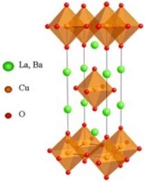
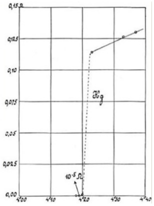




Bednorz and Müller, Z. Phys. B - Cond. Matter 64, 189 (1986)

Superconductivity milestones



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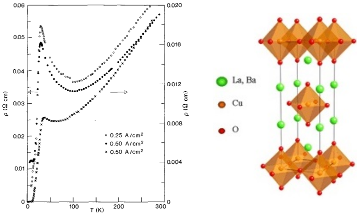

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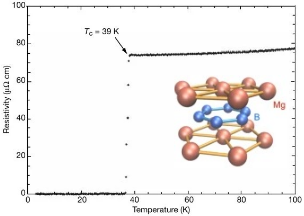
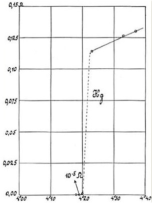


Nagamatsu *et. al.*, Nature 410, 63 (2001)

Superconductivity milestones



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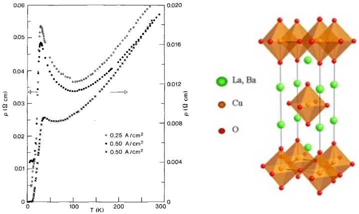

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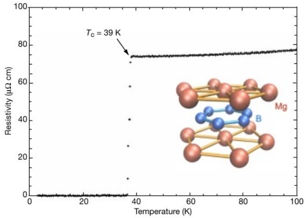

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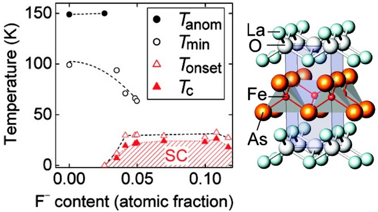

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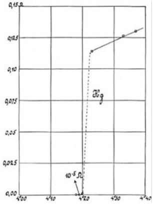
Superconductivity milestones



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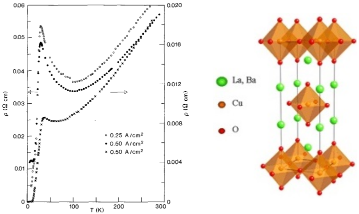

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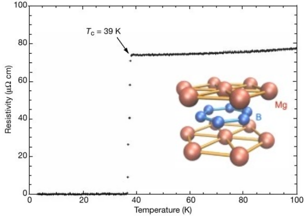

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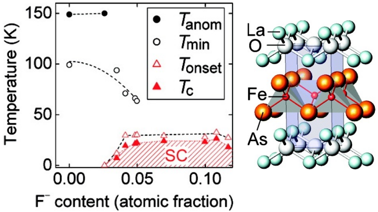

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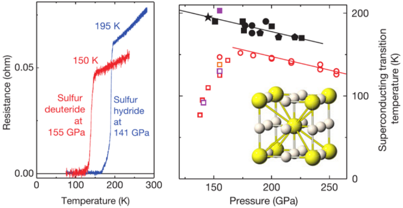
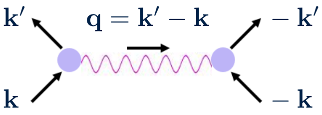


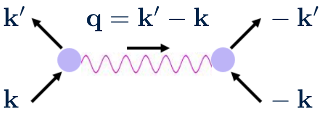
Drozdov *et. al.* Nature 73, 525 (2015)

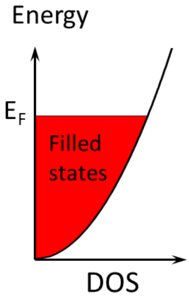
BCS theory



Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)

BCS theory





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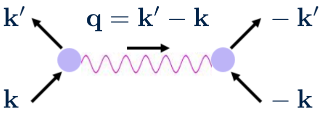

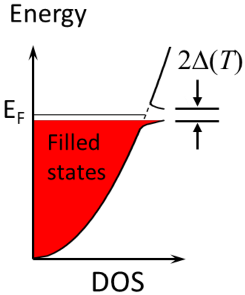

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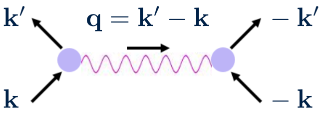
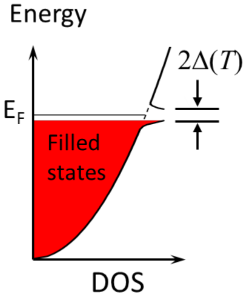




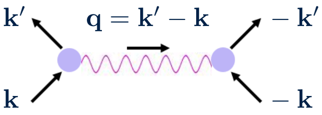
superconducting gap ↓ paring potential ↓

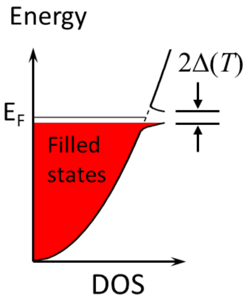
$$\Delta_{n\mathbf{k}} = \sum_m \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \tanh\left(\frac{E_{m\mathbf{k}+\mathbf{q}}}{2k_{\mathrm{B}}T}\right) \frac{V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\Delta_{m\mathbf{k}+\mathbf{q}}}{2E_{m\mathbf{k}+\mathbf{q}}}$$

$$E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})^2 + |\Delta_{n\mathbf{k}}|^2}$$

↑ quasiparticle excitation energy

Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)





superconducting gap

paring potential

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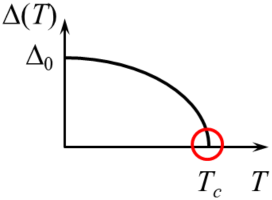
quasiparticle
excitation energy



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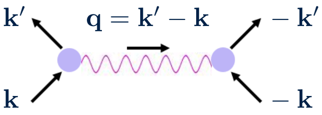

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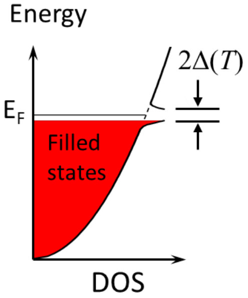
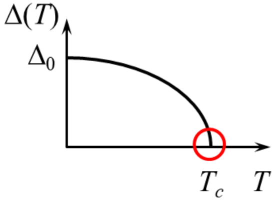




- describes in detail the phenomenology of superconductivity
- is a descriptive theory, material-independent $\rightarrow 2\Delta_0 = 3.53 k_{\mathrm{B}} T_{\mathrm{c}}$
- does not account for the retardation of the e-ph interaction

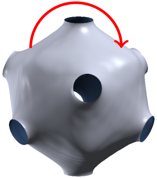
Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)

McMillan-Allen-Dynes formula for critical temperature

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

Coulomb pseudopotential

e-ph coupling strength



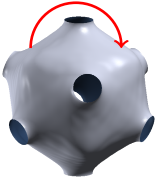
$$\lambda = N_F \left\langle\!\left\langle \sum_\nu \frac{|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2}{\hbar\omega_{\mathbf{q}\nu}} \right\rangle\!\right\rangle_{FS}$$

McMillan Phys. Rev. 167, 331(1968); Allen and Dynes, PRB 12, 905 (1975).

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

Coulomb pseudopotential (μ_c^*)

e-ph coupling strength (λ)



$$\lambda = N_F \left\langle\!\left\langle \sum_\nu \frac{|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2}{\hbar\omega_{\mathbf{q}\nu}} \right\rangle\!\right\rangle_{FS}$$

- can be easily calculated (e.g., QE, Abinit)
- works reasonably well for isotropic superconductors
- fails for multiband and/or anisotropic superconductors
- approximates the Coulomb interaction through μ_c^*

McMillan Phys. Rev. 167, 331(1968); Allen and Dynes, PRB 12, 905 (1975).

Nambu-Gor'kov formalism

A generalized 2×2 matrix Green's function $\hat{G}_{n\mathbf{k}}(\tau)$ is used to describe the propagation of electron quasiparticles and of superconducting Cooper pairs on an equal footing.

imaginary time → τ

Wick's time-ordering operator → T_τ

$$\hat{G}_{n\mathbf{k}}(\tau) = -\langle T_\tau \mathbf{\Psi}_{n\mathbf{k}}(\tau)\mathbf{\Psi}^\dagger_{n\mathbf{k}}(0)\rangle$$

two-component field operator

$$\mathbf{\Psi}_{n\mathbf{k}} = \begin{bmatrix} \hat{c}_{n\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{n-\mathbf{k}\downarrow} \end{bmatrix}$$

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- Diagonal elements are the normal state Green's functions and describe single-particle electronic excitations.

Nambu-Gor'kov formalism

$$\hat{G}_{n\mathbf{k}}(\tau) = -\left[\begin{array}{cc} \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \\ \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \end{array}\right]$$

- Diagonal elements are the normal state Green's functions and describe single-particle electronic excitations.
- Off-diagonal elements are the anomalous Green's functions and describe Cooper pairs amplitudes.

Nambu-Gor'kov formalism

$$\hat{G}_{n\mathbf{k}}(\tau) = -\begin{bmatrix} \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}_{n\mathbf{k}\uparrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \\ \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}^\dagger_{n\mathbf{k}\uparrow}(0)\rangle & \langle T_\tau \hat{c}^\dagger_{n-\mathbf{k}\downarrow}(\tau)\hat{c}_{n-\mathbf{k}\downarrow}(0)\rangle \end{bmatrix}$$

- Diagonal elements are the normal state Green's functions and describe single-particle electronic excitations.
- Off-diagonal elements are the anomalous Green's functions and describe Cooper pairs amplitudes.

$\hat{G}_{n\mathbf{k}}(\tau)$ is periodic in τ and can be expanded in a Fourier series:

$$\hat{G}_{n\mathbf{k}}(\tau) = T\sum_{i\omega_j} e^{-i\omega_j\tau}\hat{G}_{n\mathbf{k}}(i\omega_j)$$

where $i\omega_j = i(2j+1)\pi T$ (j integer) are Matsubara frequencies and T is the temperature.

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = \begin{bmatrix} G_{n\mathbf{k}}(i\omega_j) & F_{n\mathbf{k}}(i\omega_j) \\ F^*_{n\mathbf{k}}(i\omega_j) & -G_{-n\mathbf{k}}(-i\omega_j) \end{bmatrix}$$

Migdal-Eliashberg theory

paring self-energy

dressed phonon propagator

screened Coulomb interaction

$D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'})$

$V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}$

$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = g_{nm\nu}(\mathbf{q},\mathbf{k})$  $g_{mn\nu}(\mathbf{k},\mathbf{q})$ $+$  (Lecture Mon.1)

$\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})$

$\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})$

e-ph matrix elements

interacting Green's function

$i\omega_j = i(2j+1)\pi T$

Matsubara frequencies

Fan-Migdal self energy

GW self-energy

Migdal-Eliashberg theory

paring self-energy

dressed phonon propagator

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$D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'})$

$V_{n\mathbf{k},m\mathbf{k+q}}$

$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = g_{nm\nu}(\mathbf{q},\mathbf{k})$  $g_{mn\nu}(\mathbf{k},\mathbf{q}) \;+$  (Lecture Mon.1)

$\hat{G}_{m\mathbf{k+q}}(i\omega_{j'})$

$\hat{G}_{m\mathbf{k+q}}(i\omega_{j'})$

e-ph matrix elements

interacting Green's function

$i\omega_j = i(2j+1)\pi T$
Matsubara frequencies

Fan-Migdal self energy

GW self-energy

<u>Migdal's theorem</u>

E-ph vertex corrections are neglected assuming that the neglected terms are of the order of $(m_{\mathrm{e}}/M)^{1/2} \propto \omega_{\mathrm{D}}/\epsilon_{\mathrm{F}}$.

Migdal-Eliashberg approximation

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times \left[\sum_{\nu}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

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bare phonon propagator

$$D_{0,\mathbf{q}\nu}(i\omega_j) = \int_0^\infty d\omega\,\frac{2\omega}{(i\omega_j)^2-\omega^2}\delta(\omega-\omega_{\mathbf{q}\nu})$$

Migdal-Eliashberg approximation

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3$$
$$\times\left[\sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

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anisotropic e-ph coupling strength

$$\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j) = N_{\rm F}\sum_\nu\int_0^\infty d\omega\frac{2\omega}{\omega_j^2+\omega^2}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\delta(\omega-\omega_{\mathbf{q}\nu})$$

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$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\hat{\tau}_3\hat{G}_{m\mathbf{k+q}}(i\omega_{j'})\hat{\tau}_3 \times \left[\lambda_{n\mathbf{k},m\mathbf{k+q}}(\omega_j-\omega_{j'}) + V_{n\mathbf{k},m\mathbf{k+q}}\right]$$

Migdal-Eliashberg approximation

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times \left[\sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

bare phonon propagator

$$D_{0,\mathbf{q}\nu}(i\omega_j) = \int_0^\infty d\omega\frac{2\omega}{(i\omega_j)^2-\omega^2}\delta(\omega-\omega_{\mathbf{q}\nu})$$

anisotropic e-ph coupling strength

$$\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j) = N_{\rm F}\sum_\nu\int_0^\infty d\omega\frac{2\omega}{\omega_j^2+\omega^2}|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2\delta(\omega-\omega_{\mathbf{q}\nu})$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}]$$

Migdal-Eliashberg theory

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ obeys the Dyson's equation in Matsubara space:

$$\hat{G}^{-1}_{n\mathbf{k}}(i\omega_j) \quad = \quad \hat{G}^{-1}_{0,n\mathbf{k}}(i\omega_j) \quad - \quad \hat{\Sigma}_{n\mathbf{k}}(i\omega_j)$$

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non-interacting Green's function

$$\hat{G}^{-1}_{0,n\mathbf{k}}(i\omega_j) = i\omega_j\hat{\tau}_0 - (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})\hat{\tau}_3$$

Pauli matrices

$$\hat{\tau}_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \hat{\tau}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\tau}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Migdal-Eliashberg theory

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ obeys the Dyson's equation in Matsubara space:

$$\hat{G}^{-1}_{n\mathbf{k}}(i\omega_j) \quad = \quad \hat{G}^{-1}_{0,n\mathbf{k}}(i\omega_j) \quad - \quad \hat{\Sigma}_{n\mathbf{k}}(i\omega_j)$$

non-interacting Green's function

$$\hat{G}^{-1}_{0,n\mathbf{k}}(i\omega_j) = i\omega_j\hat{\tau}_0 - (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})\hat{\tau}_3$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = i\omega_j\left[1 - Z_{n\mathbf{k}}(i\omega_j)\right]\hat{\tau}_0 + \chi_{n\mathbf{k}}(i\omega_j)\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1$$

mass renormalization function — energy shift — superconducting gap function

Pauli matrices

$$\hat{\tau}_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \hat{\tau}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{\tau}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Migdal-Eliashberg theory

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = \frac{-1}{\Theta_{n\mathbf{k}}(i\omega_j)} \begin{bmatrix} i\omega_j Z_{n\mathbf{k}}(i\omega_j) + (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j) & \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j) \\ \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j) & i\omega_j Z_{n\mathbf{k}}(i\omega_j) - (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) - \chi_{n\mathbf{k}}(i\omega_j) \end{bmatrix}$$

$$\Theta_{n\mathbf{k}}(i\omega_j) = [\omega_j Z_{n\mathbf{k}}(i\omega_j)]^2 + [(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)]^2 + [Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j)]^2$$

- Diagonal elements are the normal state Green's functions $G_{n\mathbf{k}}(i\omega_j)$ and describe single-particle electronic excitations in the normal state.

- Off-diagonal elements are the anomalous Green's functions $F_{n\mathbf{k}}(i\omega_j)$ and describe Cooper pairs amplitudes is the superconducting state.

Migdal-Eliashberg theory

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_0 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

$$\Theta_{n\mathbf{k}}(i\omega_j) = \left[\omega_j Z_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j)\right]^2$$

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_0 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

$$\Theta_{n\mathbf{k}}(i\omega_j) = \left[\omega_j Z_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j)\right]^2$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\hat{\tau}_3 \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

Migdal-Eliashberg theory

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_0 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

$$\Theta_{n\mathbf{k}}(i\omega_j) = \left[\omega_j Z_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j)\right]^2$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - N_{\mathrm{F}}V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}$$
$$\times\left\{i\omega_{j'}Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_0 + \left[(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\right]\hat{\tau}_3 - \Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_1\right\}$$

Migdal-Eliashberg theory

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_0 + [(\epsilon_{n\mathbf{k}} - \epsilon_\mathrm{F}) + \chi_{n\mathbf{k}}(i\omega_j)]\,\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

$$\Theta_{n\mathbf{k}}(i\omega_j) = [\omega_j Z_{n\mathbf{k}}(i\omega_j)]^2 + [(\epsilon_{n\mathbf{k}} - \epsilon_\mathrm{F}) + \chi_{n\mathbf{k}}(i\omega_j)]^2 + [Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j)]^2$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_\mathrm{BZ}}\hat{\tau}_3\hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}]$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_\mathrm{BZ}}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'}) - N_\mathrm{F}V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \times \{i\omega_{j'}Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_0 + [(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})]\,\hat{\tau}_3 - \Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_1\}$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = i\omega_j\,[1 - Z_{n\mathbf{k}}(i\omega_j)]\,\hat{\tau}_0 + \chi_{n\mathbf{k}}(i\omega_j)\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1$$

Migdal-Eliashberg theory

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_0 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

$$\Theta_{n\mathbf{k}}(i\omega_j) = \left[\omega_j Z_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)\right]^2 + \left[Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j)\right]^2$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\hat{\tau}_3 \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_3 \times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - N_{\mathrm{F}} V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}$$
$$\times \left\{i\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_0 + \left[(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\right]\hat{\tau}_3 - \Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'}) Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_1\right\}$$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = i\omega_j\left[1 - Z_{n\mathbf{k}}(i\omega_j)\right]\hat{\tau}_0 + \chi_{n\mathbf{k}}(i\omega_j)\hat{\tau}_3 + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j)\hat{\tau}_1$$

Equating the scalar coefficients of the Pauli matrices leads to the anisotropic Migdal-Eliashberg equations.

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{T}{\omega_j}\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\frac{\omega_{j'}Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\rm F}}$$

$$\chi_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\frac{(\epsilon_{m\mathbf{k}+\mathbf{q}}-\epsilon_{\rm F})+\chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\rm F}}$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\frac{Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\rm F}} - V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{T}{\omega_j}\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\omega_{j'}Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\mathrm{F}}}$$

$$\chi_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{(\epsilon_{m\mathbf{k}+\mathbf{q}}-\epsilon_{\mathrm{F}})+\chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\mathrm{F}}}$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\mathrm{F}}}-V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

$$n_e = 1 - 2T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{(\epsilon_{m\mathbf{k}+\mathbf{q}}-\epsilon_{\mathrm{F}})+\chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{T}{\omega_j} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\rm F}}$$

$$\chi_{n\mathbf{k}}(i\omega_j) = -T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\rm F}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\rm F}}$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \left[\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\rm F}} - V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \right]$$

$$n_e = 1 - 2T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\rm F}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}$$

- only the off-diagonal contributions of the Coulomb self-energy are retained in order to avoid double counting of Coulomb effects

Anisotropic Migdal-Eliashberg equations on imaginary axis: FSR

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\mathrm{F}}} \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}})$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{\omega_j} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \left[\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})}{N_{\mathrm{F}}} - V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \right] \times \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}})$$

- all quantities are evaluated around the Fermi surface $\rightarrow \chi_{n\mathbf{k}}(i\omega_j)$ vanishes when integrated on the Fermi surface because it is an odd function of ω_j
- the electron density of states in the vicinity of the Fermi level is assumed to be constant

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k+q}}(i\omega_{j'})}} \frac{\lambda_{n\mathbf{k},m\mathbf{k+q}}(\omega_j - \omega_{j'})}{N_{\rm F}} \delta(\epsilon_{m\mathbf{k+q}} - \epsilon_{\rm F})$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{\omega_j} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{\Delta_{m\mathbf{k+q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k+q}}(i\omega_{j'})}} \left[\frac{\lambda_{n\mathbf{k},m\mathbf{k+q}}(\omega_j - \omega_{j'})}{N_{\rm F}} - V_{n\mathbf{k},m\mathbf{k+q}} \right] \times \delta(\epsilon_{m\mathbf{k+q}} - \epsilon_{\rm F})$$

anisotropic e-ph coupling strength

$$\lambda_{n\mathbf{k},m\mathbf{k+q}}(\omega_j) = N_{\rm F} \sum_{\nu} \int_0^{\infty} d\omega \frac{2\omega}{\omega_j^2 + \omega^2} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\omega - \omega_{\mathbf{q}\nu})$$

EPW

Poncé *et al.*, Comput. Phys. Commun. 209, 116 (2016)

Anisotropic Migdal-Eliashberg equations on imaginary axis: FSR

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j}\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\omega_{j'}}{\sqrt{\omega_{j'}^2+\Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}}\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\mathrm{F}}}\delta(\epsilon_{m\mathbf{k}+\mathbf{q}}-\epsilon_{\mathrm{F}})$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{\omega_j}\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2+\Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}}\left[\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j-\omega_{j'})}{N_{\mathrm{F}}} - V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right] \times \delta(\epsilon_{m\mathbf{k}+\mathbf{q}}-\epsilon_{\mathrm{F}})$$

- the static screened Coulomb interaction $N_{\mathrm{F}}V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}$ is embedded into the semi-empirical pseudopotential μ_c^*

Anisotropic Migdal-Eliashberg equations on imaginary axis: FSR

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}} \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}} [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_\mathrm{c}^*] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})$$

- the static screened Coulomb interaction $N_\mathrm{F} V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}$ is embedded into the semi-empirical pseudopotential μ_c^*

Coulomb pseudopotential $\mu_\mathrm{c}^* = \dfrac{\mu_\mathrm{c}}{1 + \mu_\mathrm{c} \log(\omega_\mathrm{el}/\omega_\mathrm{ph})}$ $\qquad \mu_\mathrm{c} = N_\mathrm{F} \langle\langle V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \rangle\rangle_\mathrm{FS}$

Morel and Anderson, Phys. Rev. 125, 1263 (1962)

Schlipf *et al.*, Comput. Phys. Commun. 247, 106856 (2020)

Anisotropic Migdal-Eliashberg equations on imaginary axis: FSR

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j N_{\mathrm{F}}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}})$$

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- $Z_{n\mathbf{k}}$ and $\Delta_{n\mathbf{k}}$ are only meaningful for $n\mathbf{k}$ at or near the Fermi surface

Anisotropic Migdal-Eliashberg equations on real axis

- The Migdal-Eliasberg equations on the imaginary frequency axis are computationally efficient (sums over a finite number of Matsubara frequencies) and they are adequate for calculating the T_{c} and $\Delta_{n\mathbf{k}}(i\omega_j)$.

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- Solutions on the real energy axis can be obtained by analytic continuation of the solutions along the imaginary frequency axis using Padé approximants (very light computationally) or an iterative procedure (very heavy computationally).

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Excitation spectrum of a superconductor

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$$\hat{G}_{n\mathbf{k}}(\omega) = \frac{\omega Z_{n\mathbf{k}}(\omega)\hat{\tau}_0 + (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})\hat{\tau}_3 + \Delta_{n\mathbf{k}}(\omega) Z_{n\mathbf{k}}(\omega)\hat{\tau}_1}{\left[\omega Z_{n\mathbf{k}}(\omega)\right]^2 - (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})^2 - \left[Z_{n\mathbf{k}}(\omega)\Delta_{n\mathbf{k}}(\omega)\right]^2}$$

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binding energy of electrons in a Cooper pair

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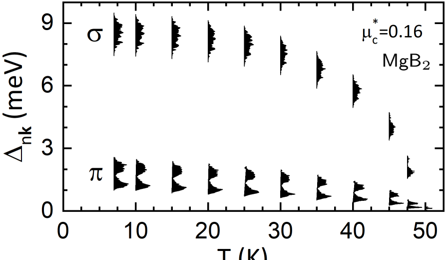

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Superconducting quasiparticle density of states and spectral function

- Superconducting quasiparticle density of states:

$$\frac{N_{n\mathbf{k},S}(\omega)}{N_{\mathrm{F}}} = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\epsilon_{n\mathbf{k}} \mathrm{Im} G_{n\mathbf{k}}^{11}(\omega)$$

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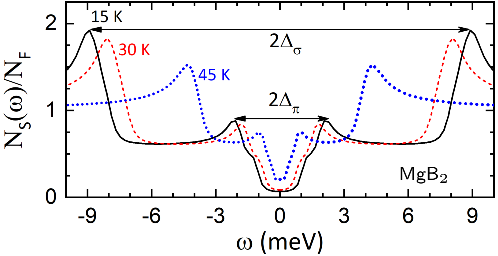

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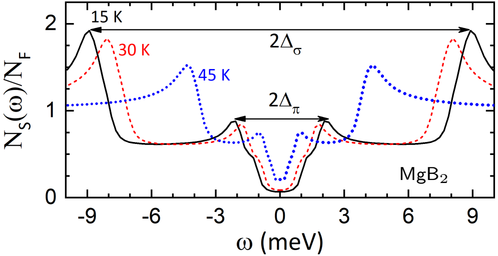

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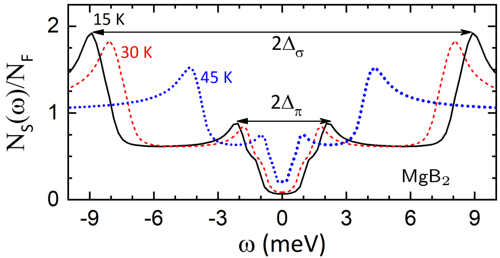

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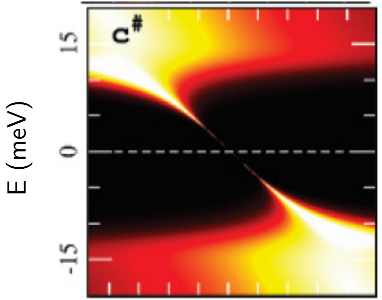

CaC_6 normal state

Sanna *et al.*, Phys. Rev. B 85, 184514 (2012)

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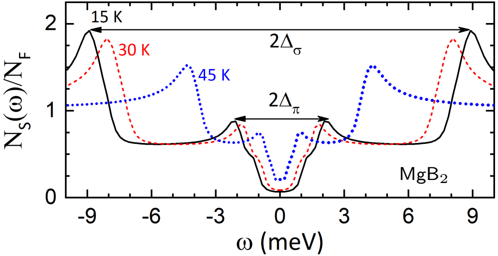

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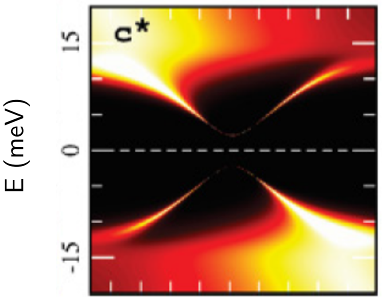


CaC_6 superconducting state

Sanna *et al.*, Phys. Rev. B 85, 184514 (2012)

Density functional theory for superconductors (SCDFT)

$\mathcal{Z}$ accounts for e-ph interactions

kernel $\mathcal{K}$ accounts for e-ph and e-e interactions

superconducting gap function $\longrightarrow$

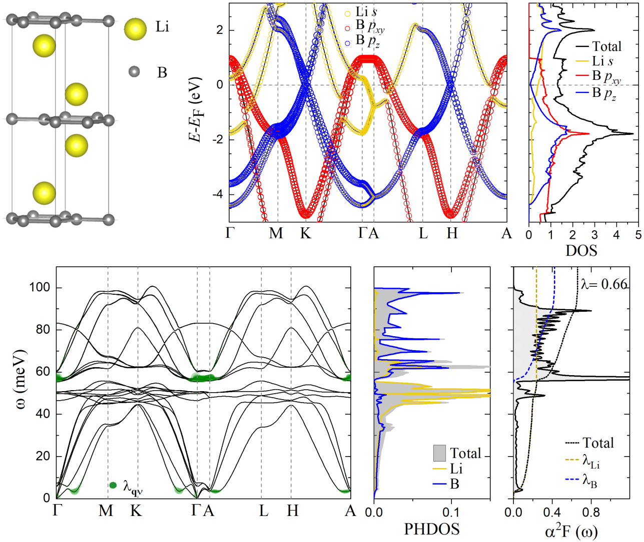
$$\Delta_{n\mathbf{k}} = -\mathcal{Z}_{n\mathbf{k}}\Delta_{n\mathbf{k}} - \sum_m \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\mathcal{K}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\Delta_{m\mathbf{k}+\mathbf{q}}}{2E_{m\mathbf{k}+\mathbf{q}}} \tanh\left(\frac{E_{m\mathbf{k}+\mathbf{q}}}{2k_{\mathrm{B}}T}\right)$$

quasiparticle excitation energy $\longrightarrow$

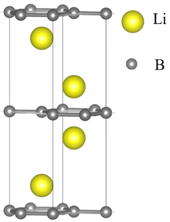
$$E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})^2 + |\Delta_{n\mathbf{k}}|^2}$$

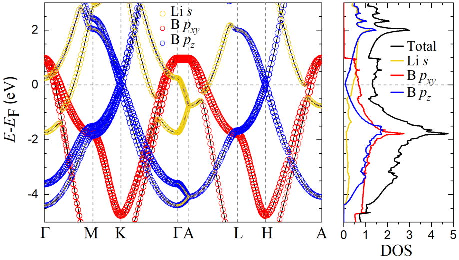
Lüders *et al.*, Phys. Rev. B 72, 024545 (2005); Marques *et al.*, Phys. Rev. B 72, 024546 (2005); Sanna, Pellegrini and Gross, Phys. Rev. Lett. 125, 057001 (2020).

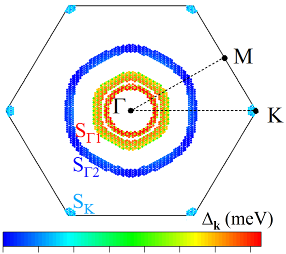
Supeconductivity in LiB: FSR

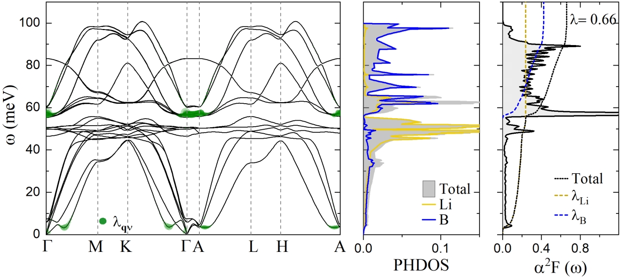


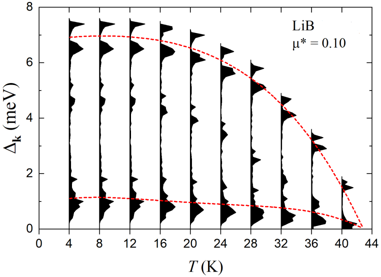
Kolmogorov and Curtarolo, Phys. Rev. B 73, 180501(R) (2006); Kafle *et al.*, Phys. Rev. Materials 6, 084801 (2022).





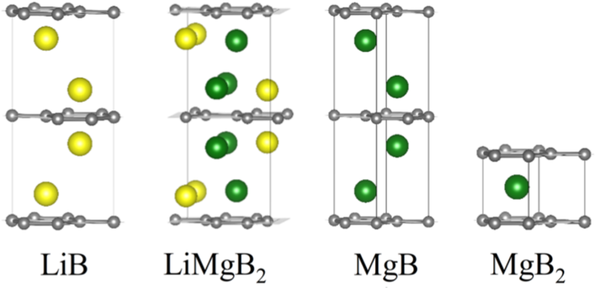


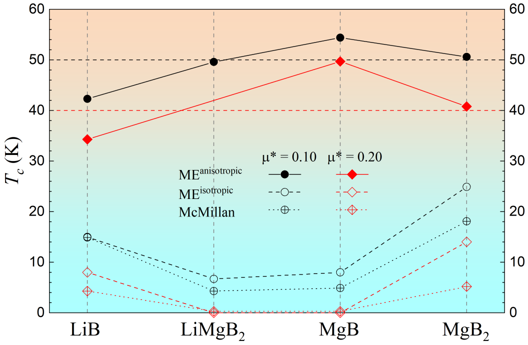




Kolmogorov and Curtarolo, Phys. Rev. B 73, 180501(R) (2006); Kafle *et al.*, Phys. Rev. Materials 6, 084801 (2022).

Supeconductivity in Li-Mg-B phases





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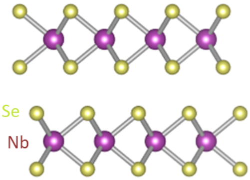
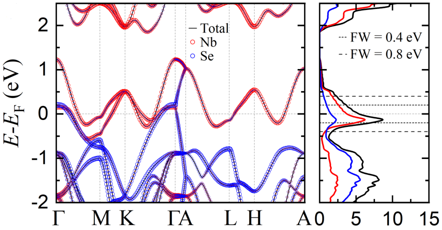
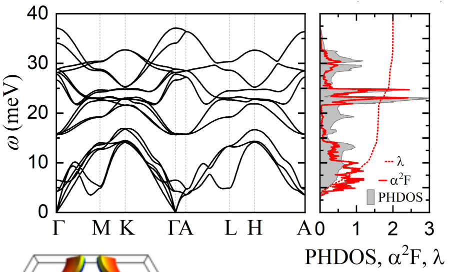
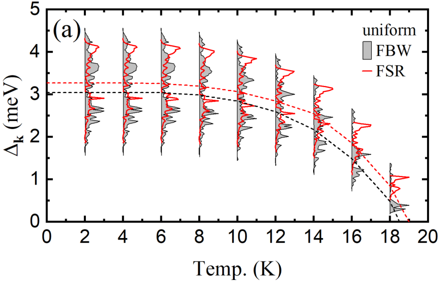
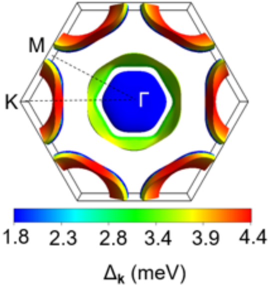
Superconductivity in 2H-$NbSe_2$: FBW vs. FSR





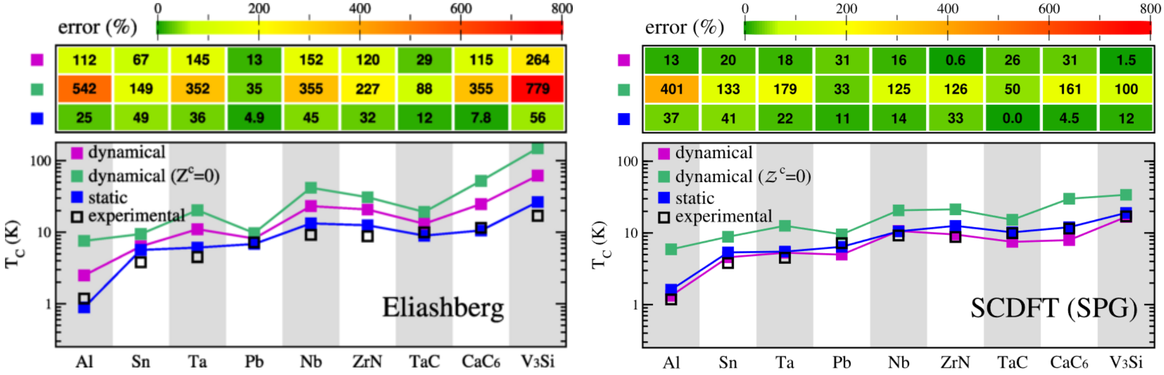






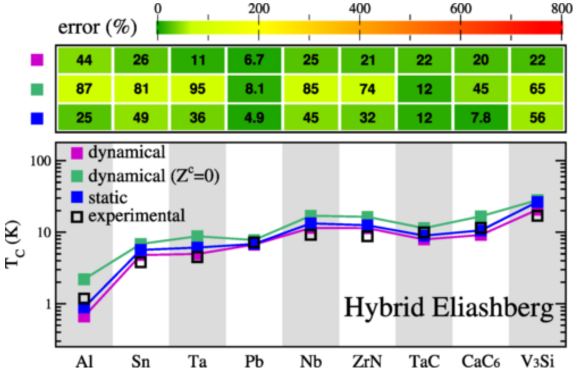
Lee *et al.* arXiv:2302.08085 (2023).

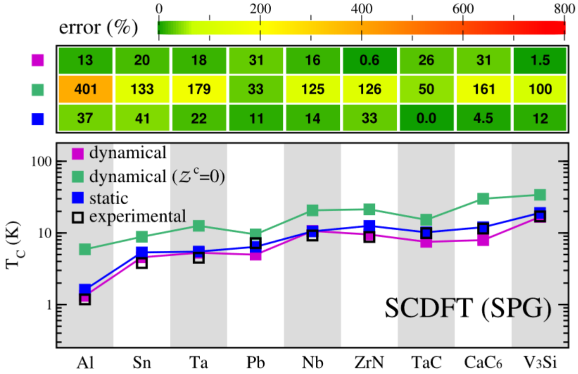
Migdal-Eliashberg with ab initio Coulomb interactions vs. SCDFT



Davydov, Sanna, Pellegrini, Dewhurst, Sharma, and Gross, Phys. Rev. B 102, 214508 (2020).

Migdal-Eliashberg with ab initio Coulomb interactions vs. SCDFT



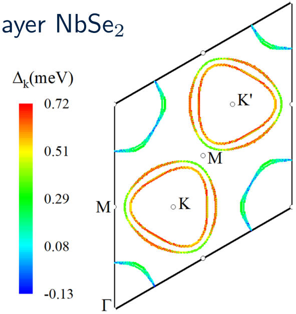


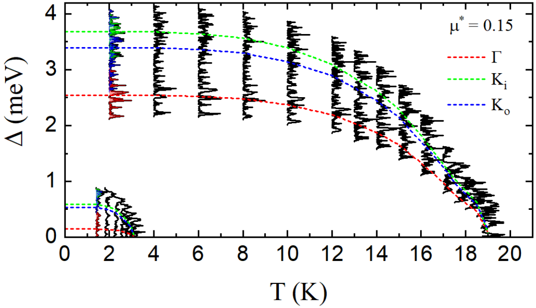
Davydov, Sanna, Pellegrini, Dewhurst, Sharma, and Gross, Phys. Rev. B 102, 214508 (2020).

$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\omega_{j'} \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}} \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) + \lambda^\mathrm{sf}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'})\right]$$

$$Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_\mathrm{F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})}{\sqrt{\omega_{j'}^2 + \Delta^2_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}} \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \lambda^\mathrm{sf}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_c^*\right]$$

monolayer $NbSe_2$





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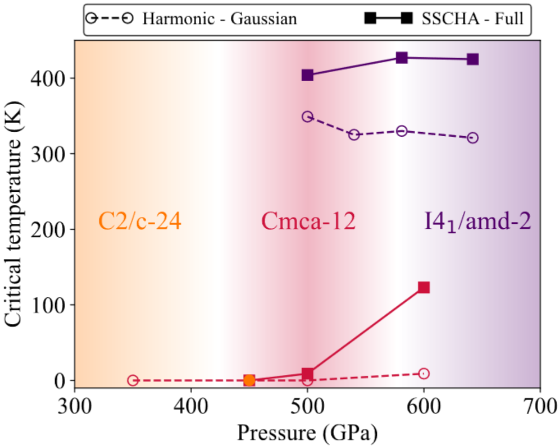
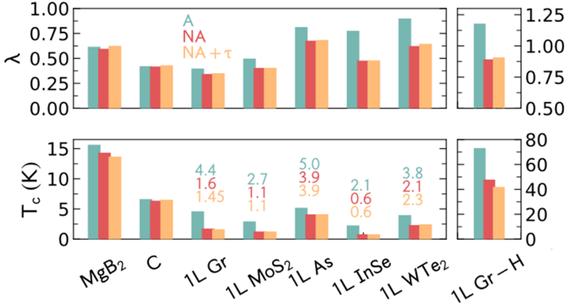
Anharmonic and non-adiabatic phononic effects

solid hydrogen





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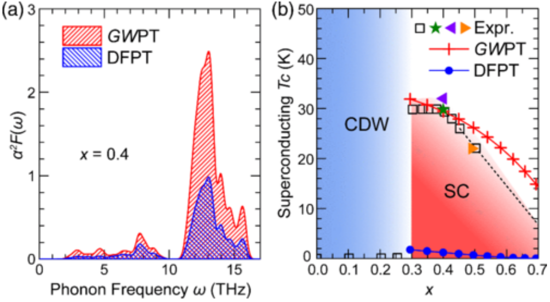
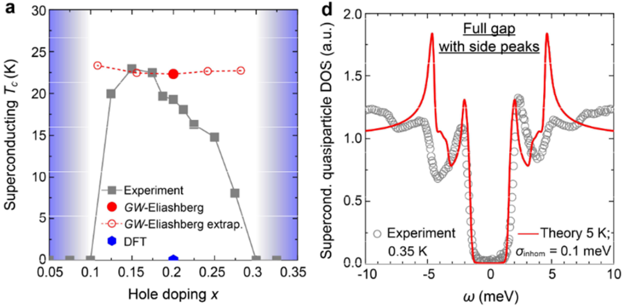
Migdal-Eliashberg theory with GW and GWPT

$Ba_{1-x}K_xBiO_3$

infinite-layer $Nd_{0.8}Sr_{0.2}NiO_2$





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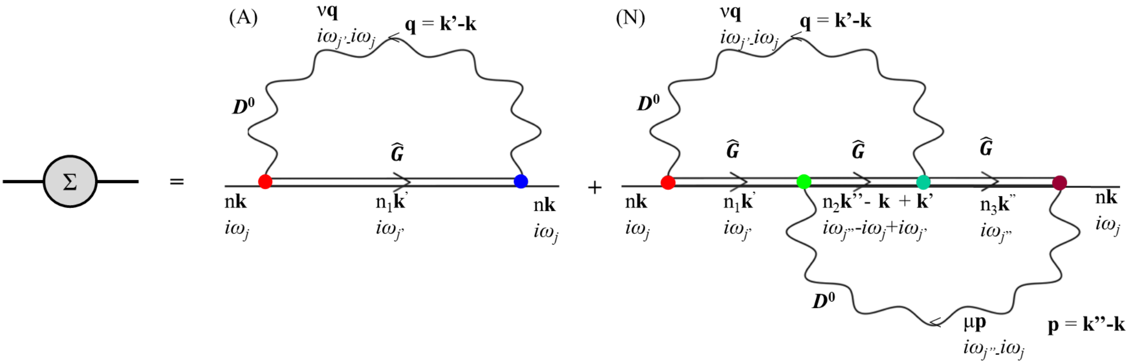

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Take-home messages

- The Migdal-Eliashberg equations can be obtained from a rigorous many-body framework
- The Eliashberg theory provides a well-defined scheme for modeling superconducting properties from first-principles
- The standard implementation of the Eliashberg formalism can be expanded to include additional effects

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