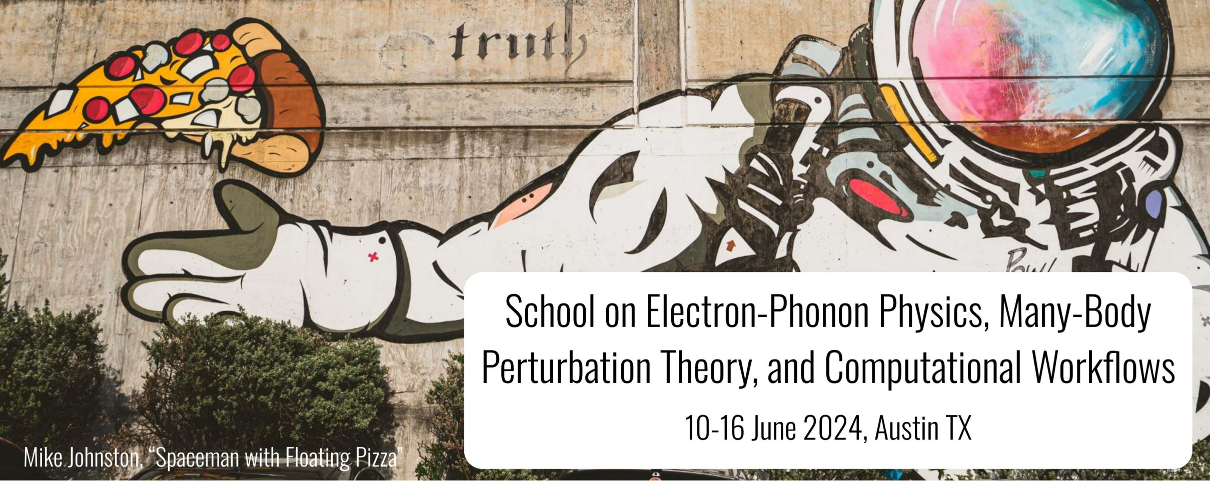

Mike Johnston, “Spaceman with Floating Pizza”

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

U.S. DEPARTMENT OF ENERGY

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Lecture Wed.2

Superconductors and Migdal-Eliashberg theory

Roxana Margine

Department of Physics, Applied Physics, and Astronomy

Binghamton University - State University of New York

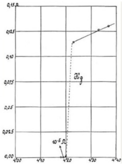
Lecture Summary

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

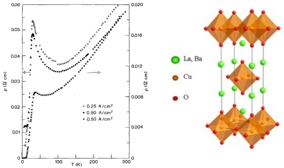
Superconductivity Milestones

1911	1986	2001	2008	2015	2020	2023	2023
Hg	Cuprates	MgB_2	Fe-based	H_3S	CSH_x	Lu-N-H	LK-99
4.2 K	30-170 K	39 K	6-100 K	203 K	288 K	294 K	400 K

Experiment



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



Bednorz and Müller,
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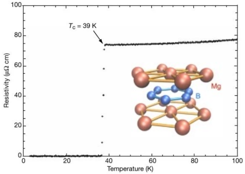
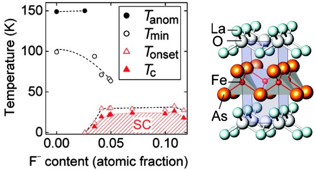
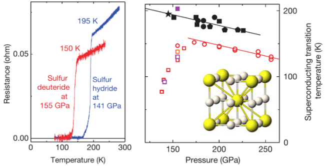


Nagamatsu *et. al.*, Nature 410, 63 (2001)



Kamihara *et. al.*, JACS 130, 3296 (2008)



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

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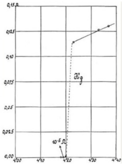
Hg	Cuprates	MgB_2	Fe-based	H_3S
4.2 K	30-170 K	39 K	6-100 K	203 K

Experiment



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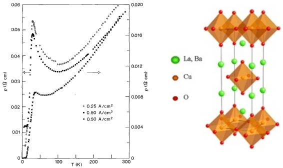

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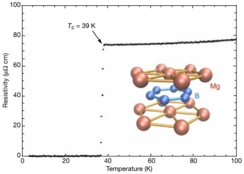

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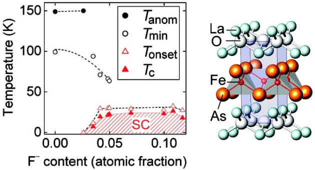

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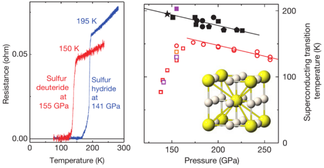

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Superconductivity Milestones

Experiment

- 1911 Hg 4.2 K
- 1986 Cuprates 30-170 K
- 2001 MgB_2 39 K
- 2008 Fe-based 6-100 K
- 2015 H_3S 203 K

Theory

- 1957 BCS theory
- 1960 Eliashberg theory
- 1964-65 DFT
- 1987 DFPT

Superconductivity Milestones

1911
Hg
4.2 K

1986
Cuprates
30-170 K

2001
MgB_2
39 K

2008
Fe-based
6-100 K

2015
H_3S
203 K

Experiment

Theory

1957
BCS
theory

1960
Eliashberg
theory

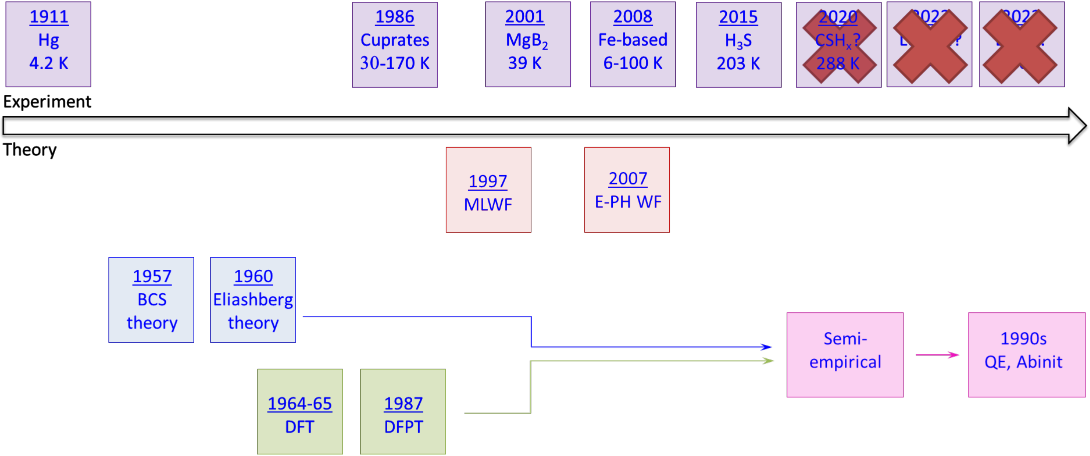
1964-65
DFT

1987
DFPT

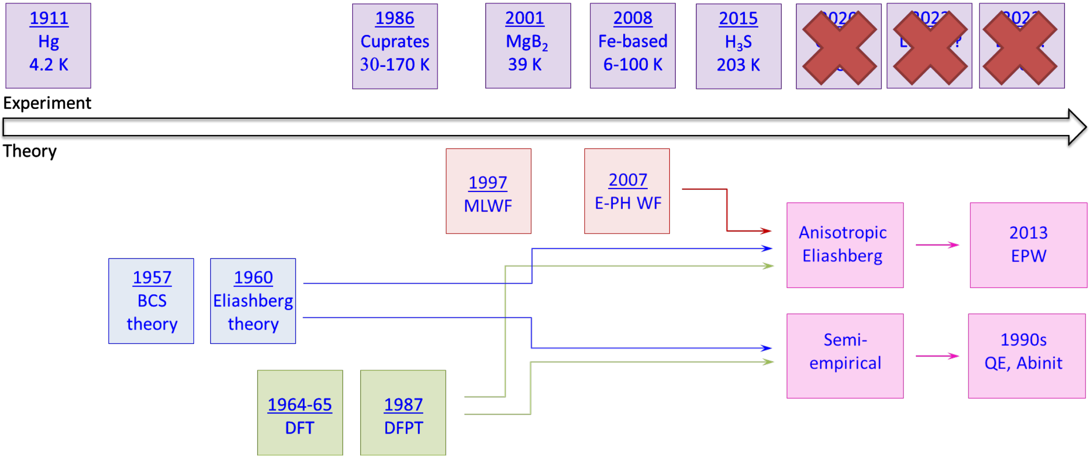
Semi-
empirical

1990s
QE, Abinit

Superconductivity Milestones



Superconductivity Milestones



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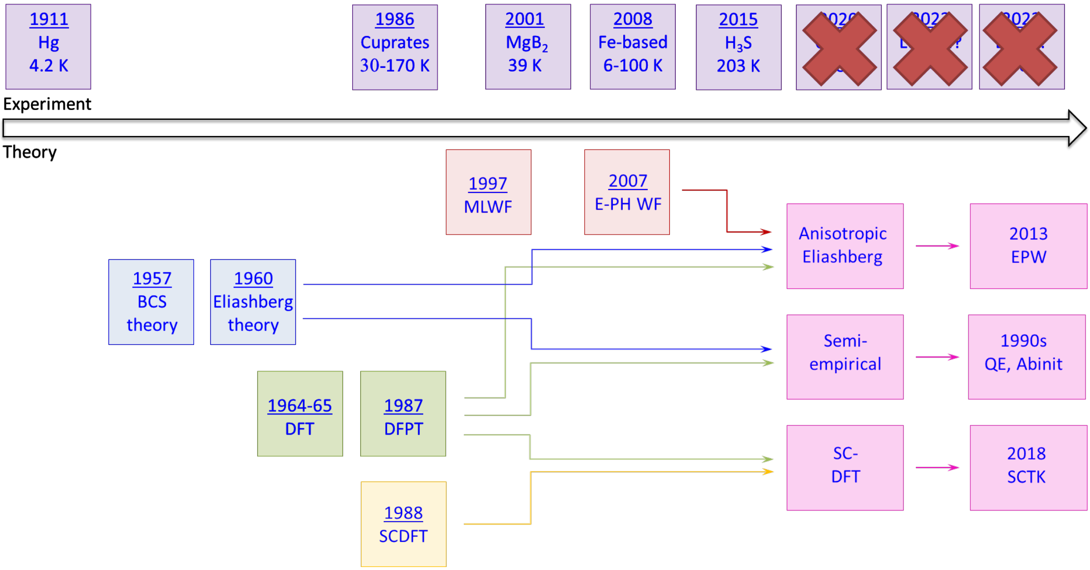
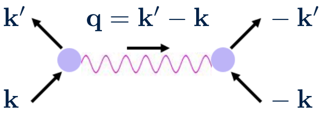
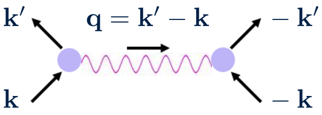
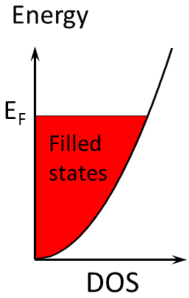




Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)

BCS theory





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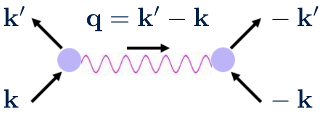

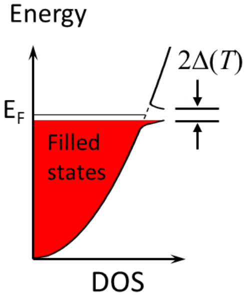

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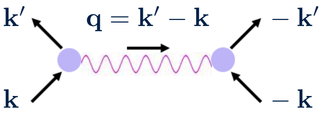
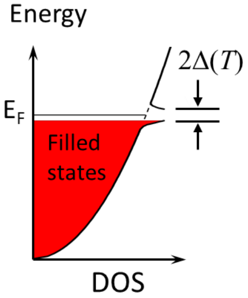




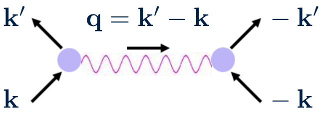
superconducting gap ↓ paring potential ↓

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

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

↑ quasiparticle excitation energy

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



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

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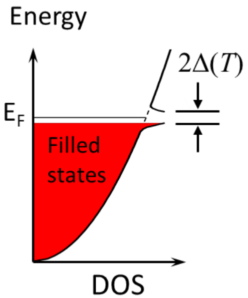

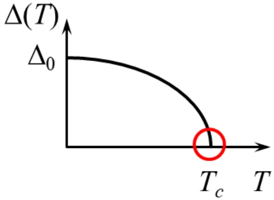

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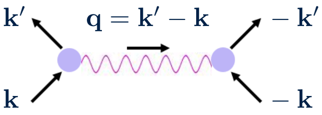

superconducting gap

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

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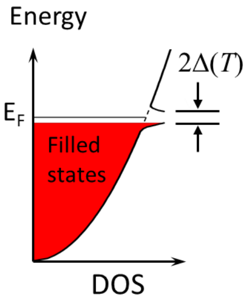
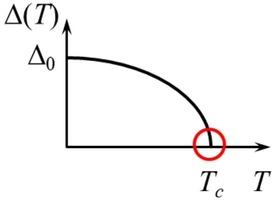
quasiparticle
excitation energy





- 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)

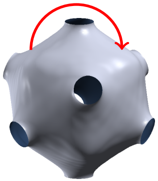
McMillan-Allen-Dynes formula for critical temperature

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

Coulomb pseudopotential

e-ph coupling strength

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



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

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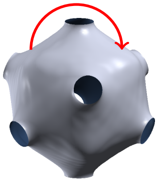

$$T_c{}^{\mathrm{ML}} = f_\omega f_\mu T_c{}^{\mathrm{AD}}$$

Xie *et al.* Npj. Comput. Mater. 8, 1 (2022)

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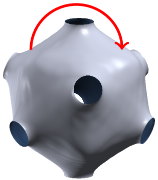

$$T_c^{\mathrm{ML}} = f_\omega f_\mu T_c^{\mathrm{AD}}$$

Xie *et al.* Npj. Comput. Mater. 8, 1 (2022)

- can be easily calculated (e.g., QE, Abinit)
- works reasonably well for isotropic superconductors
- fails for multi-band 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

Wick's time-ordering operator

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

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

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

- 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.

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

dressed phonon propagator

screened Coulomb interaction

paring self-energy

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

$V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}$

$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = g_{nm\nu}(\mathbf{q},\mathbf{k})$  $g_{mn\nu}(\mathbf{k},\mathbf{q})$ $+$  (Tue.2.Giustino)

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

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

screened Coulomb interaction: $V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}$

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = g_{nm\nu}(\mathbf{q},\mathbf{k})$$

$$g_{mn\nu}(\mathbf{k},\mathbf{q}) \quad +$$

(Tue.2.Giustino)

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

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

e-ph matrix elements

interacting Green's function

Fan-Migdal self-energy

GW self-energy

Migdal's theorem

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

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

Migdal-Eliashberg approximation

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

bare phonon propagator

$$D^{(0)}_{\mathbf{q}\nu}(i\omega_j) = \frac{2\omega_{\mathbf{q}\nu}}{(i\omega_j)^2 - \omega^2_{\mathbf{q}\nu}}$$

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

bare phonon propagator

$$D^{(0)}_{\mathbf{q}\nu}(i\omega_j) = \frac{2\omega_{\mathbf{q}\nu}}{(i\omega_j)^2 - \omega^2_{\mathbf{q}\nu}}$$

anisotropic e-ph coupling strength

e-ph interaction

$$V^{\rm e-ph}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j) = \sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D^{(0)}_{\mathbf{q}\nu}(i\omega_j) = -\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j)}{N_{\rm F}}$$

Migdal-Eliashberg approximation

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

bare phonon propagator

$$D^{(0)}_{\mathbf{q}\nu}(i\omega_j) = \frac{2\omega_{\mathbf{q}\nu}}{(i\omega_j)^2 - \omega^2_{\mathbf{q}\nu}}$$

anisotropic e-ph coupling strength

e-ph interaction

$$V^{\rm e-ph}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j) = \sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D^{(0)}_{\mathbf{q}\nu}(i\omega_j) = -\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j)}{N_{\rm F}}$$

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

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

bare phonon propagator

$$D^{(0)}_{\mathbf{q}\nu}(i\omega_j) = \frac{2\omega_{\mathbf{q}\nu}}{(i\omega_j)^2 - \omega^2_{\mathbf{q}\nu}}$$

anisotropic e-ph coupling strength

e-ph interaction

$$V^{\rm e-ph}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j) = \sum_\nu |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D^{(0)}_{\mathbf{q}\nu}(i\omega_j) = -\frac{\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j)}{N_{\rm F}}$$

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

Migdal-Eliashberg theory

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

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

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

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:

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

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

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

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

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

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

Migdal-Eliashberg theory

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

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

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

Migdal-Eliashberg theory

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

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

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

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{1}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) + V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$
$$\times\left\{i\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_0 + [(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})]\,\hat{\tau}_3 - \Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'}) Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_1\right\}$$

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

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

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

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\frac{1}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[V^{\rm e-ph}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) + V^{\rm c}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$
$$\times\left\{i\omega_{j'}Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_0 + \left[(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\rm F}) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\right]\hat{\tau}_3 - \Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_1\right\}$$

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

Migdal-Eliashberg theory

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

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

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

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{BZ}}\frac{1}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[V^{e-ph}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) + V^{c}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$
$$\times \{i\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_0 + [(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) + \chi_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})]\,\hat{\tau}_3 - \Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})\hat{\tau}_1\}$$

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

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

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW

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

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

$$\Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}\frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[V^{\rm e-ph}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) + V^{\rm c}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW

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

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

$$\Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\Delta_{m\mathbf{k+q}}(i\omega_{j'})Z_{m\mathbf{k+q}}(i\omega_{j'})}{\Theta_{m\mathbf{k+q}}(i\omega_{j'})}\left[V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j - i\omega_{j'}) + V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k+q}}\right]$$

$$N_e = \sum_{n}\int\frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}}\left[1 - 2T\sum_{j}\frac{(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)}{\Theta_{n\mathbf{k}}(i\omega_j)}\right]$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW

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

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

$$\Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) + V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

$$N_e = \sum_n\int\frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}}\left[1 - 2T\sum_j\frac{(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}}) + \chi_{n\mathbf{k}}(i\omega_j)}{\Theta_{n\mathbf{k}}(i\omega_j)}\right]$$

- 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

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

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

- 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

Anisotropic Migdal-Eliashberg equations on imaginary axis: FSR

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

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

- 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

e-ph interaction

$$V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j) = \sum_{\nu} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D^{(0)}_{\mathbf{q}\nu}(i\omega_j)$$

EPW

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

Lee *et al.*, npj Comput. Mater. 9, 156 (2023)

Anisotropic Migdal-Eliashberg equations on imaginary axis

e-ph interaction

$$V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j) = \sum_{\nu} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D^{(0)}_{\mathbf{q}\nu}(i\omega_j)$$

EPW

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

Lee *et al.*, npj Comput. Mater. 9, 156 (2023)

static screened Coulomb interaction

$$\mu_{\mathrm{c}} = N_{\mathrm{F}} \langle\langle V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \rangle\rangle_{\mathrm{FS}}$$

STERNHEIMER GW

Schlipf *et al.*, Comput. Phys. Commun. 247, 106856 (2020) e-ph interaction

$$V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j) = \sum_{\nu} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 D^{(0)}_{\mathbf{q}\nu}(i\omega_j)$$

EPW

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

Lee *et al.*, npj Comput. Mater. 9, 156 (2023)

static screened Coulomb interaction

$$\mu_{\mathrm{c}} = N_{\mathrm{F}}\langle\langle V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k+q}}\rangle\rangle_{\mathrm{FS}}$$

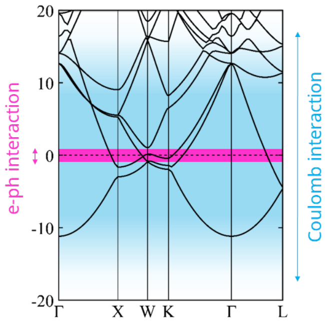
TERNHEIMER SGW

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

Coulomb pseudopotential

$$\mu^*_{\mathrm{c}} = \frac{\mu_{\mathrm{c}}}{1+\mu_{\mathrm{c}}\log(\omega_{\mathrm{el}}/\omega_{\mathrm{ph}})}$$

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



Anisotropic Migdal-Eliashberg equations on imaginary axis: FSR

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

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

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- The coupled nonlinear equations need to be solved self-consistently at each temperature T

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- The equations must be evaluated on dense electron $\mathbf{k}$- and phonon $\mathbf{q}$-meshes to properly describe anisotropic effects

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- The coupled nonlinear equations need to be solved self-consistently at each temperature T
- The equations must be evaluated on dense electron $\mathbf{k}$- and phonon $\mathbf{q}$-meshes to properly describe anisotropic effects
- The sum over Matsubara frequencies must be truncated (a typical cutoff of the order of 1 eV)

Intermediate representation method

Intermediate representation (IR) method enables solving the anisotropic Migdal-Eliashberg equations:

- less than 100 sampled Matsubara frequencies
- inclusion of the Coulomb retardation effect

Shinaoka *et al.*, Comput. Phys. Rev. B 96, 035147 (2017)
Li *et al.*, Phys. Rev. B 101, 035144 (2020)
Wallerberger *et al.*, SoftwareX 21, 101266 (2023)

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Represent Green's functions from IR basis functions:

$$G(i\omega_j) = \sum_l G_l \hat{U}_l(i\omega_j) \quad \text{Matsubara-frequency domain}$$

$$G(\tau_i) = \sum_l G_l U_l(\tau_i) \quad \text{imaginary-time domain}$$

G_l are IR basis coefficients

$\hat{U}_l(i\omega_j)$ and $U_l(\tau_i)$ are IR basis functions (precomputed and material independent)

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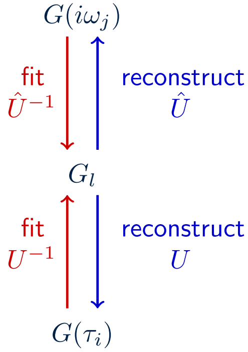

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Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

$$i\omega_j \left[1 - Z_{n\mathbf{k}}(i\omega_j)\right] = T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{i\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})$$

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

$$\Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j) = -T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'}) Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \left[V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) + V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

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$$\Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}\frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}\left[V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) + V^{\mathrm{c}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}\right]$$

normal self-energy

$$\Sigma^{\mathrm{N}}_{n\mathbf{k}}(i\omega_j) = i\omega_j\left[1 - Z_{n\mathbf{k}}(i\omega_j)\right] + \chi_{n\mathbf{k}}(i\omega_j)$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

$$i\omega_j \left[1 - Z_{n\mathbf{k}}(i\omega_j)\right] = T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{i\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})$$

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pairing self-energy

$$\phi_{n\mathbf{k}}(i\omega_j) = \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j)$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

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

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$$G_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j) + \epsilon_{n\mathbf{k}} - \epsilon_F + \chi_{n\mathbf{k}}(i\omega_j)}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

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Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

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$$\Sigma^{\mathrm{N}}_{n\mathbf{k}}(i\omega_j) = i\omega_j\left[1 - Z_{n\mathbf{k}}(i\omega_j)\right] + \chi_{n\mathbf{k}}(i\omega_j)$$

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normal Green's function

$$G_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j) + \epsilon_{n\mathbf{k}} - \epsilon_F + \chi_{n\mathbf{k}}(i\omega_j)}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

annormalus Green's function

$$F_{n\mathbf{k}}(i\omega_j) = -\frac{\Delta_{n\mathbf{k}}(i\omega_j)Z_{n\mathbf{k}}(i\omega_j)}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

$$\Sigma^{\rm N}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\rm BZ}}G_{m\mathbf{k+q}}(i\omega_{j'})V^{\rm e-ph}_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j - i\omega_{j'})$$

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$$X^{(1)}_{n\mathbf{k},m\mathbf{k+q}}(\tau_i) = G_{n\mathbf{k}}(\tau_i)\times V_{n\mathbf{k},m\mathbf{k+q}}(\tau_i)$$

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$\phi_{n\mathbf{k}}(i\omega_j) = \Delta_0/[1 + (\omega_j/\omega_{\rm ph})^2]$

↓

$G_{n\mathbf{k}}(i\omega_j), F_{n\mathbf{k}}(i\omega_j), V_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j)$

↓

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

↓

$G_{n\mathbf{k}}(\tau_i), F_{n\mathbf{k}}(\tau_i), V_{n\mathbf{k},m\mathbf{k+q}}(\tau_i)$

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↓

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↓

$X^{(1)}_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j), X^{(2)}_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j)$

↓

$\Sigma^{\rm N}_{n\mathbf{k}}(i\omega_j), \phi_{n\mathbf{k}}(i\omega_j)$

Mori *et al.*, arXiv:2404.11528v1 (2024)

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

$$\Sigma^{\mathrm{N}}_{n\mathbf{k}}(i\omega_j) = -T\sum_{mj'}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}G_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})V^{\mathrm{e-ph}}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})$$

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$$G_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j) + \epsilon_{n\mathbf{k}} - \epsilon_F + \chi_{n\mathbf{k}}(i\omega_j)}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

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↓

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↓

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↓

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↓

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↓

$$X^{(1)}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j),\ X^{(2)}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j)$$

↓

$$\Sigma^{\mathrm{N}}_{n\mathbf{k}}(i\omega_j),\ \phi_{n\mathbf{k}}(i\omega_j)$$

Mori *et al.*, arXiv:2404.11528v1 (2024)

Anisotropic Migdal-Eliashberg equations on imaginary axis: FBW + IR

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$$G_{n\mathbf{k}}(i\omega_j) = -\frac{i\omega_j Z_{n\mathbf{k}}(i\omega_j) + \epsilon_{n\mathbf{k}} - \epsilon_F + \chi_{n\mathbf{k}}(i\omega_j)}{\Theta_{n\mathbf{k}}(i\omega_j)}$$

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$\phi_{n\mathbf{k}}(i\omega_j) = \Delta_0/[1 + (\omega_j/\omega_{\rm ph})^2]$

↓

$G_{n\mathbf{k}}(i\omega_j), F_{n\mathbf{k}}(i\omega_j), V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j)$

$\hat{U}^{-1}$ ↓

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

↓

$G_{n\mathbf{k}}(\tau_i), F_{n\mathbf{k}}(\tau_i), V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\tau_i)$

↓

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↓

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↓

$X^{(1)}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j), X^{(2)}_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j)$

↓

$\Sigma^{\rm N}_{n\mathbf{k}}(i\omega_j), \phi_{n\mathbf{k}}(i\omega_j)$

Mori *et al.*, arXiv:2404.11528v1 (2024)

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↓

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↓

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U ↓

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↓

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↓

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↓

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↓

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↓

$G_{n\mathbf{k}}(i\omega_j),\ F_{n\mathbf{k}}(i\omega_j),\ V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j)$

↓

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↓

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↓

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↓

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↓

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↓

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↓

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U^{-1} ↓

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↓

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↓

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Mori *et al.*, arXiv:2404.11528v1 (2024)

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$\downarrow$

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$\hat{U}\ \downarrow$

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↓

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↓

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↓

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↓

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Mori *et al.*, arXiv:2404.11528v1 (2024)

- The Migdal-Eliashberg 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 $\Delta_{n\mathbf{k}}(i\omega_j)$.

Leavens and Ritchie, Solid State Commun. 53, 137 (1985); Marsiglio, Schossmann, and Carbotte, Phys. Rev. B 37, 4965 (1988)

Anisotropic Migdal-Eliashberg equations on real axis

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- The Migdal-Eliashberg equations need to be solved on the real energy axis to extract information about the spectral properties (e.g., the quasi particle density of states or the single particle excitation spectrum).

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- The Migdal-Eliashberg equations need to be solved on the real energy axis to extract information about the spectral properties (e.g., the quasi particle density of states or the single particle excitation spectrum).
- 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

- The single-particle Green's function on real axis is given by:

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

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$$G^{11}_{n\mathbf{k}}(\omega) = \frac{\omega Z_{n\mathbf{k}}(\omega) + (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})}{\left[\omega Z_{n\mathbf{k}}(\omega)\right]^2 - (\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})^2 - \left[Z_{n\mathbf{k}}(\omega)\Delta_{n\mathbf{k}}(\omega)\right]^2}$$

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$\mathrm{Re}E_{n\mathbf{k}}$ quasiparticle energy renormalized by the superconducting pairing

$\mathrm{Im}E_{n\mathbf{k}}$ quasiparticle inverse lifetime due to the superconducting pairing

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$$E^2_{n\mathbf{k}} = \frac{(\epsilon_{n\mathbf{k}} - \epsilon_{\rm F})^2}{Z^2_{n\mathbf{k}}(E_{n\mathbf{k}})} + \Delta^2_{n\mathbf{k}}(E_{n\mathbf{k}})$$

${\rm Re}E_{n\mathbf{k}}$ quasiparticle energy renormalized by the superconducting pairing

${\rm Im}E_{n\mathbf{k}}$ quasiparticle inverse lifetime due to the superconducting pairing

At Fermi level: $E_{n\mathbf{k}} = {\rm Re}\Delta_{n\mathbf{k}}(E_{n\mathbf{k}})$

This identity defines the leading edge $\Delta_{n\mathbf{k}}$ of the superconducting gap:

$$\Delta_{n\mathbf{k}} = {\rm Re}\Delta_{n\mathbf{k}}(\Delta_{n\mathbf{k}})$$

binding energy of electrons in a Cooper pair

Excitation spectrum of a superconductor

- The single-particle Green's function on real axis is given by:

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

- The poles of the diagonal components of $\hat{G}_{n\mathbf{k}}(\omega)$ give the elemental excitations of the superconductor

$$G^{11}_{n\mathbf{k}}(\omega) = \frac{\omega Z_{n\mathbf{k}}(\omega) + (\epsilon_{n\mathbf{k}} - \epsilon_{\rm F})}{[\omega Z_{n\mathbf{k}}(\omega)]^2 - (\epsilon_{n\mathbf{k}} - \epsilon_{\rm F})^2 - [Z_{n\mathbf{k}}(\omega)\Delta_{n\mathbf{k}}(\omega)]^2}$$

- The pole positions are:

$$E^2_{n\mathbf{k}} = \frac{(\epsilon_{n\mathbf{k}} - \epsilon_{\rm F})^2}{Z^2_{n\mathbf{k}}(E_{n\mathbf{k}})} + \Delta^2_{n\mathbf{k}}(E_{n\mathbf{k}})$$

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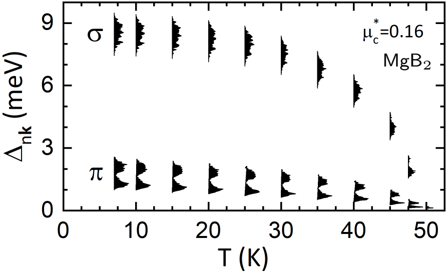

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Superconducting quasiparticle density of states and spectral function

- Superconducting quasiparticle density of states:

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

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

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$$\frac{N_S(\omega)}{N_{\mathrm{F}}} = \sum_n \int \frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}} \frac{\delta(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})}{N_{\mathrm{F}}} \mathrm{Re}\left[\omega/\sqrt{\omega^2 - \Delta^2_{n\mathbf{k}}(\omega)}\right]$$

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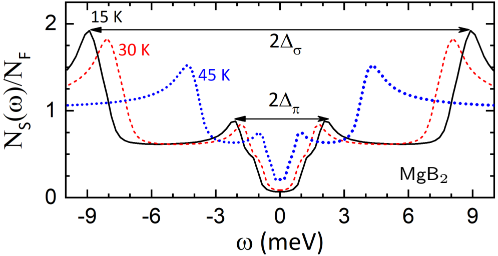

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

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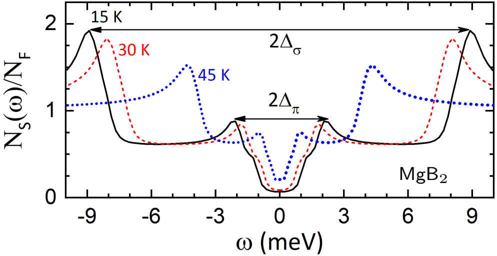

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

- Spectral function:

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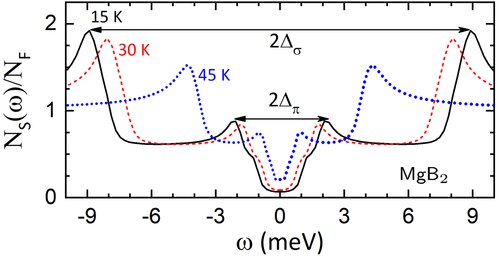

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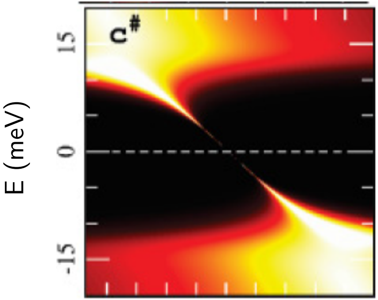

CaC_6 normal state

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

- Superconducting quasiparticle density of states:

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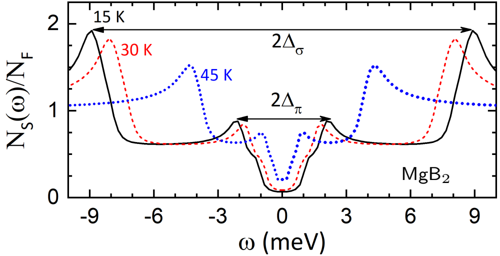

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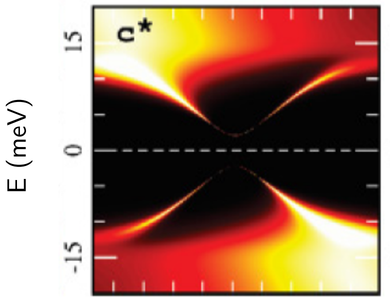


CaC_6 superconducting state

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 $\longrightarrow$

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

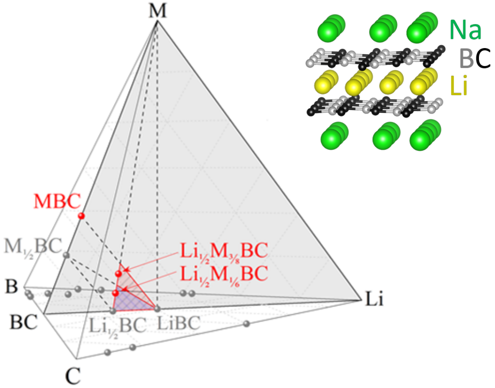
quasiparticle excitation energy $\longrightarrow$

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

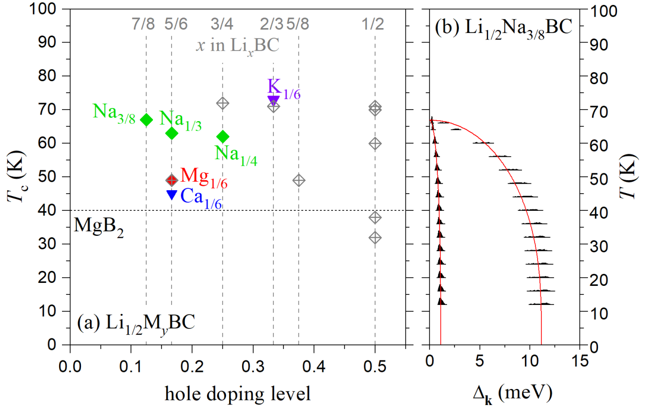
Lüders *et al.*, Phys. Rev. B 72, 024545 (2005); Marques *et al.*, Phys. Rev. B 72, 024546 (2005); Sanna, Pellegrini and Gross, Phys. Rev. Lett. 125, 057001 (2020)

Supeconductivity in Li-M-BC phases: FSR

Prediction of ambient-pressure $Li_{1/2}Na_{3/8}BC$

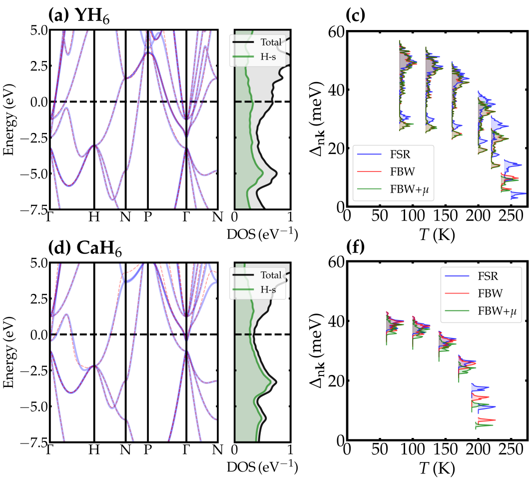


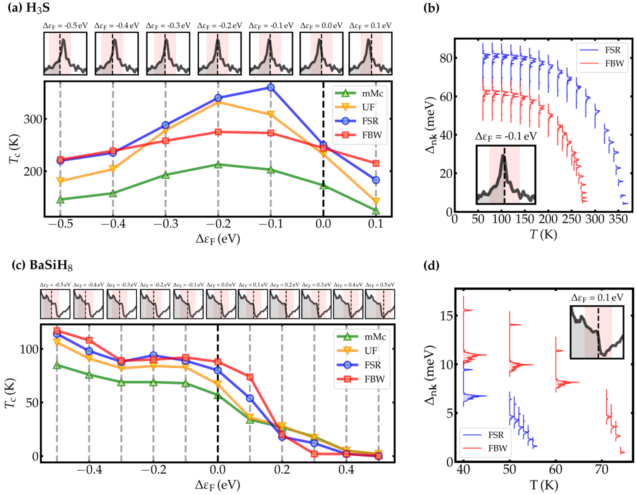
Prospect of high-T_c superconductivity



Tomassetti, Kafle, Marcial, Margine, and Kolmogorov, J. Mater. Chem. C 12, 4870 (2024)

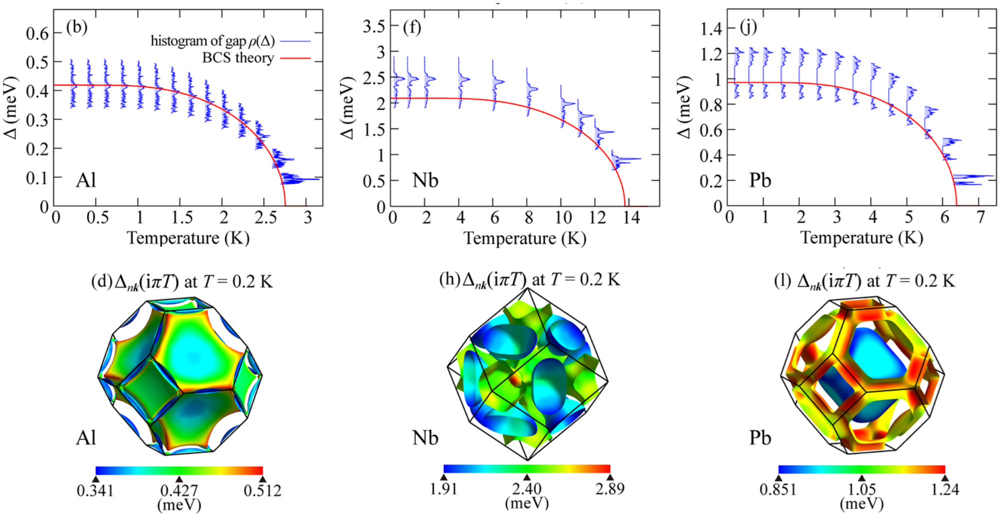
Superconductivity in hydrides: FBW vs. FSR





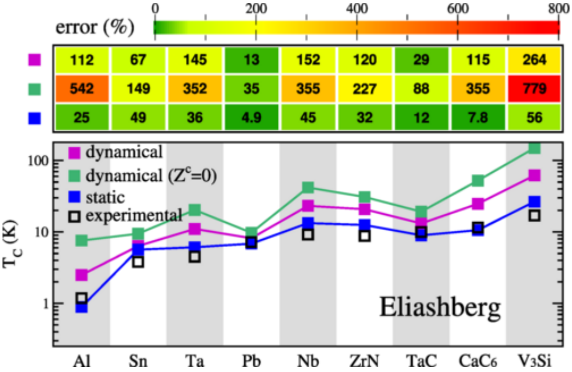
Lucrezi, Ferreira, Hajinazar, Mori, Paudyal, Margine, and Heil, Commun. Phys. 7:33 (2024)

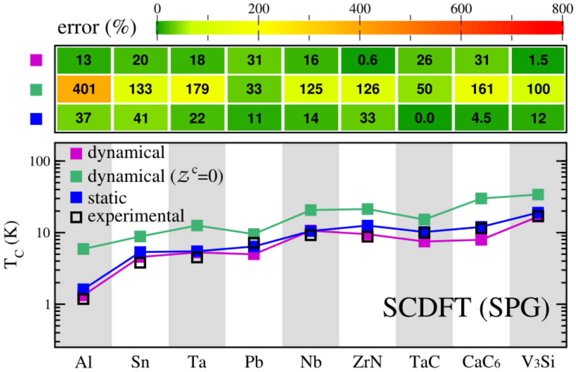
Superconductivity in elemental metals: FBW + IR



Mori *et al.*, arXiv:2404.11528v1 (2024)

Migdal-Eliashberg with ab initio Coulomb interactions vs. SCDFT





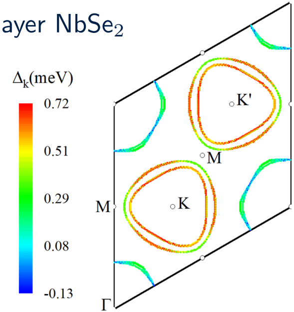
Davydov, Sanna, Pellegrini, Dewhurst, Sharma, and Gross, Phys. Rev. B 102, 214508 (2020)

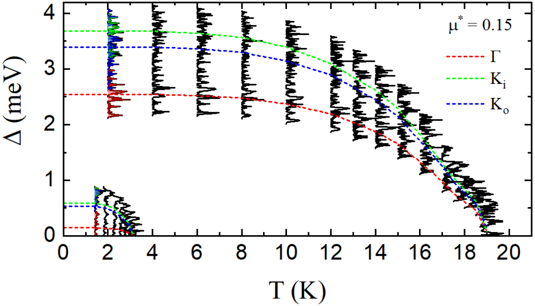
Migdal-Eliashberg theory with spin fluctuations

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

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

monolayer $NbSe_2$

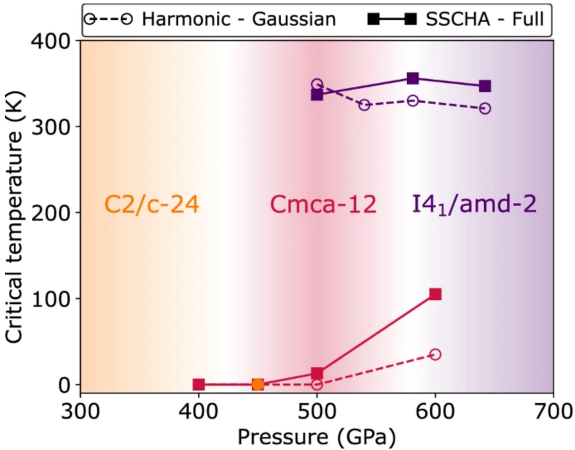


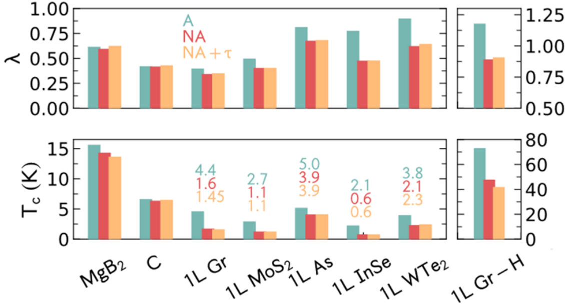


Das, Paudyal, Margine, Agterberg, and Mazin, npj Comput Mater 9, 66 (2023)

Anharmonic and non-adiabatic phononic effects

solid hydrogen



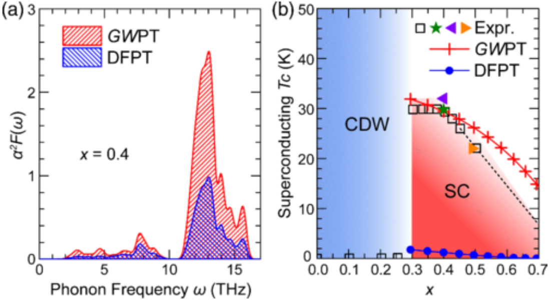


Dangić *et al.*, Commun. Phys. 7:150 (2024)

Girotto and Novko, Phys. Rev. B 107, 064310 (2023)

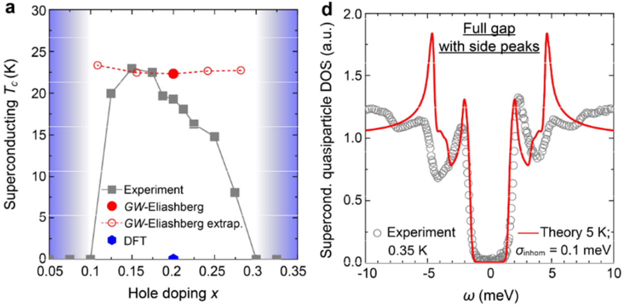
Migdal-Eliashberg theory with GW and GWPT

$Ba_{1-x}K_xBiO_3$



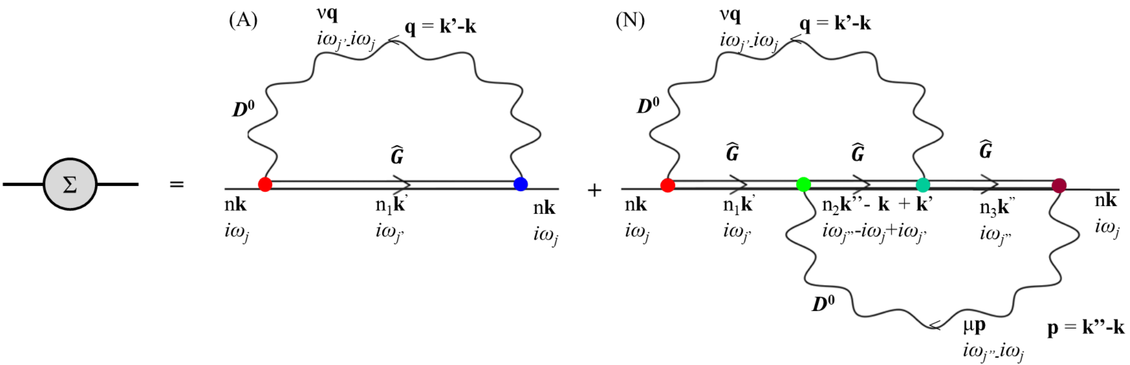
Li *et al.*, Phys. Rev. Lett. 122, 186402 (2019)

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



(Fri.3.Li)

Li and Louie, arXiv:2210.12819 (2023).



Kostur and Mitrović, Phys. Rev. B 50, 12774 (1994); Grimaldi, Pietronero and Strässler, Phys. Rev. B 52, 10530 (1995)

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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