



U.S. DEPARTMENT OF
ENERGY

TACC
TEXAS ADVANCED COMPUTING CENTER



Lecture Wed.2

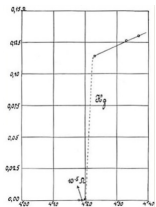
Superconductors and Migdal-Eliashberg theory

Roxana Margine

Department of Physics, Applied Physics, and Astronomy
Binghamton University - State University of New York

- Superconductivity milestones
- BCS theory of superconductivity
- McMillan-Allen-Dynes formula for critical temperature
- Nambu-Gor'kov formalism and Migdal-Eliashberg theory
- Density functional theory for superconductors
- Examples from calculations

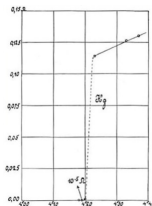
Superconductivity Milestones



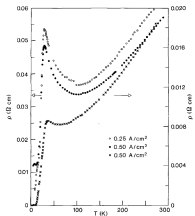
Onnes, Commun. Phys. Lab.

Univ. Leiden. Suppl. 29 (1911)

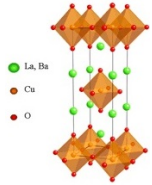
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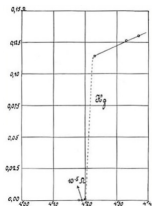
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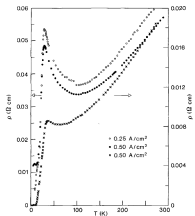
Bednorz and Müller, Z. Phys. B - Cond. Matter
64, 189 (1986)



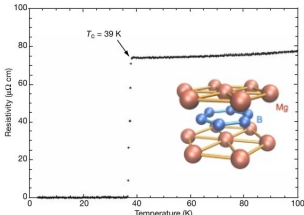
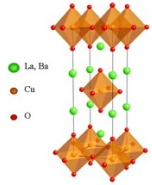
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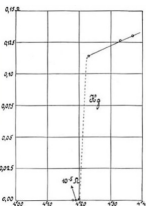


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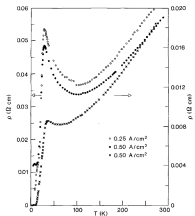


Nagamatsu et. al., Nature 410, 63 (2001)

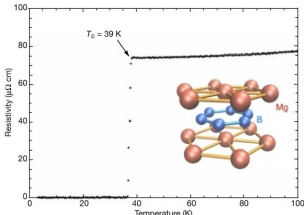
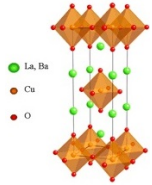
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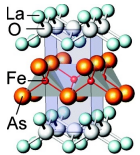
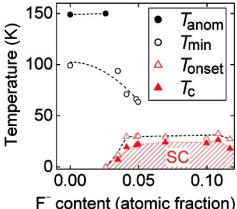
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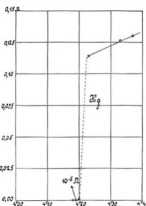


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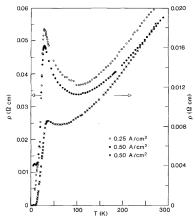


Kamihara et. al., JACS 130, 3296 (2008)

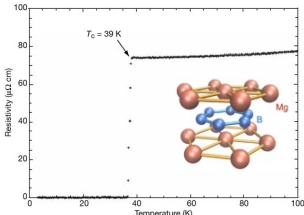
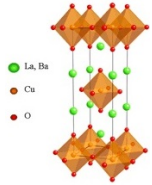
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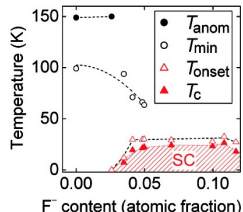
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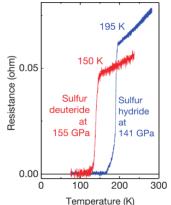
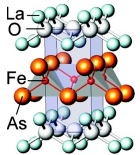
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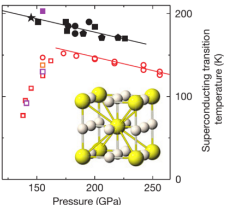
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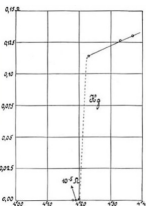
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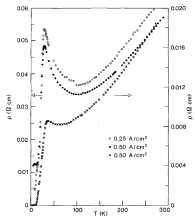
Drozdov et. al. Nature 73, 525 (2015)



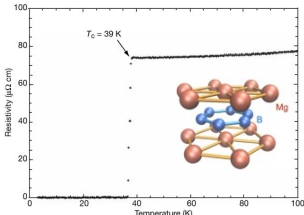
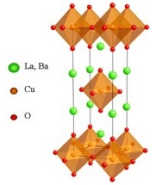
Superconductivity Milestones



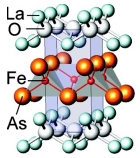
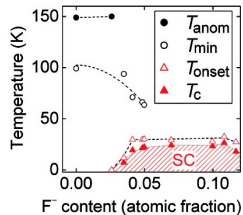
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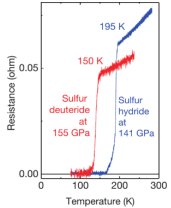
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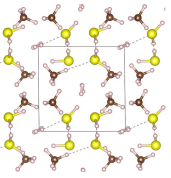
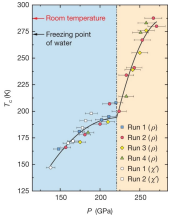
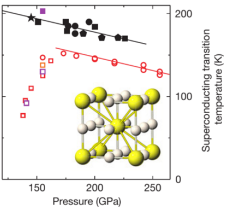
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Drozdov et. al. Nature 73, 525 (2015)



Snider et. al. Nature 583, 373 (2020)

Superconductivity Milestones

E
X
P

1911
Hg

1986
cuprates

2001
MgB₂

2008
Fe-based

2015
H₃S

2020
CSH_x



T
H
E
O
R
Y

Superconductivity Milestones

E
X
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1911
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T
H
E
O
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1957
BCS
theory

1960
Eliashberg
theory

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T
H
E
O
R
Y

1957
BCS
theory

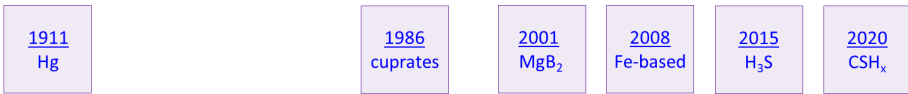
1960
Eliashberg
theory

1964-65
DFT

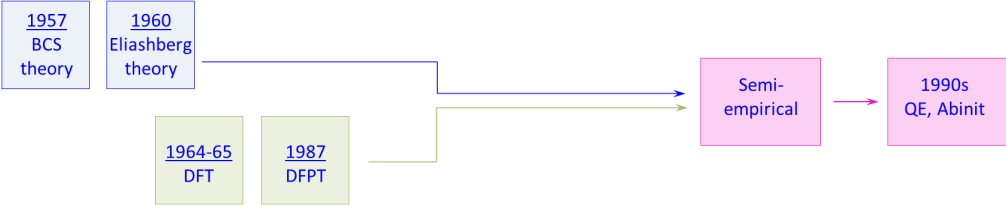
1987
DFPT

Superconductivity Milestones

E
X
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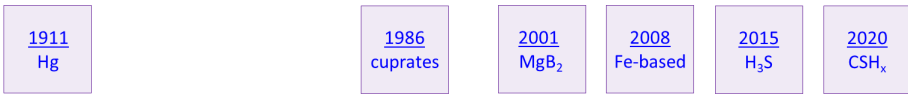


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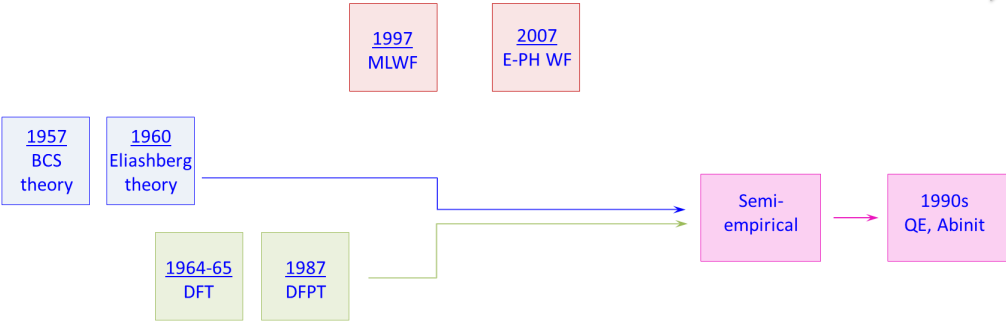


Superconductivity Milestones

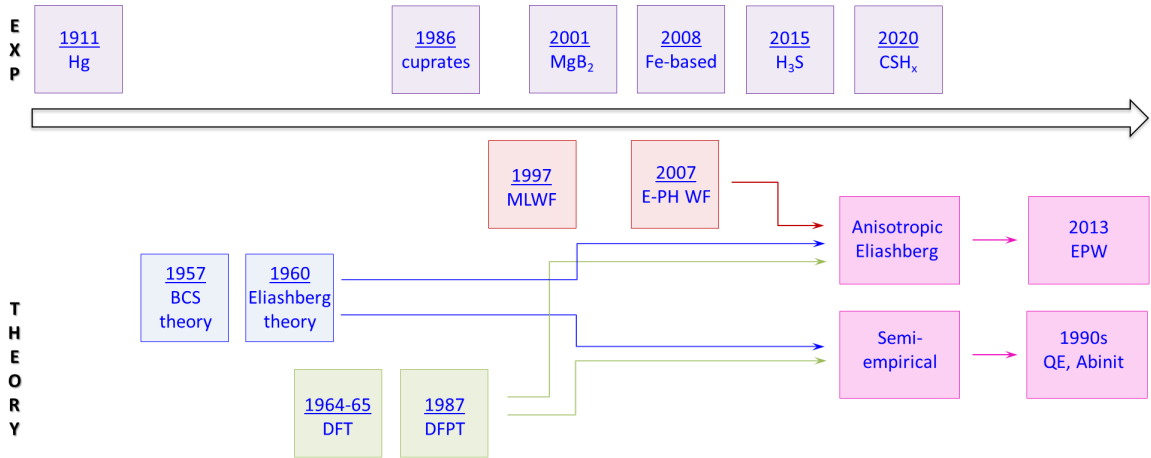
E
X
P



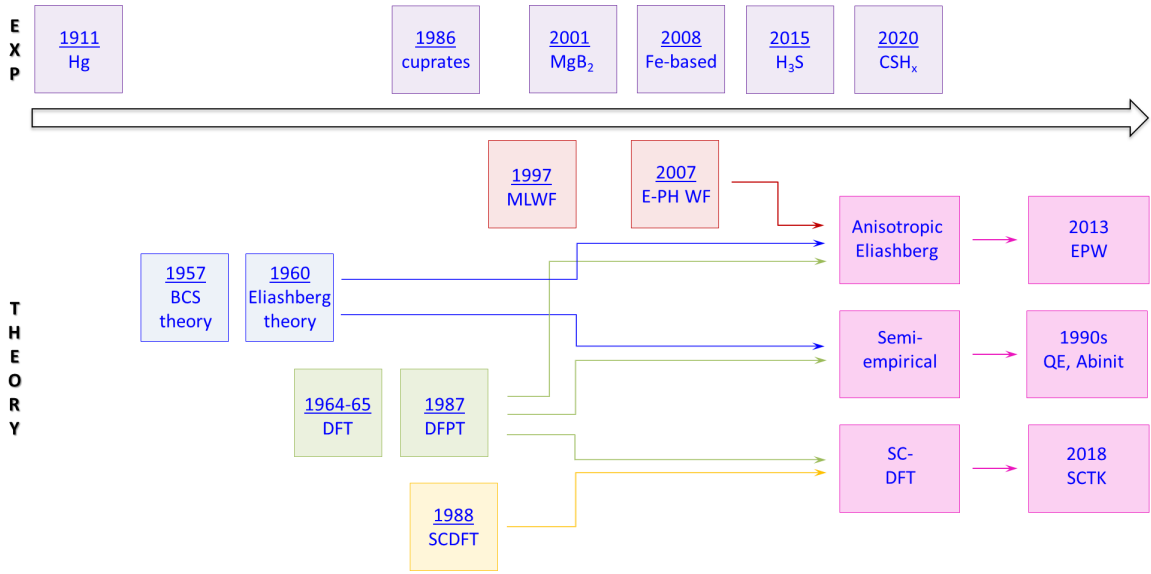
T
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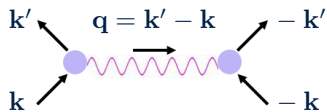
Superconductivity Milestones



Superconductivity Milestones

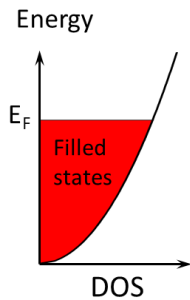
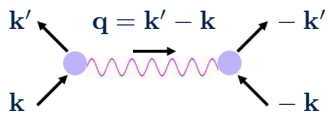


BCS Theory



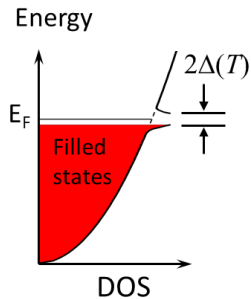
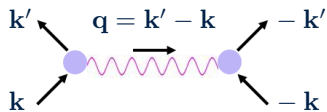
Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)

BCS Theory



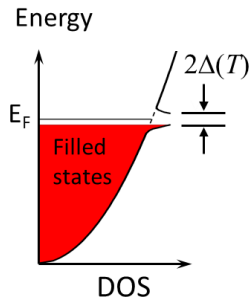
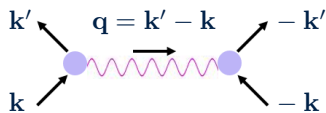
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BCS Theory



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BCS Theory



superconducting gap

paring potential

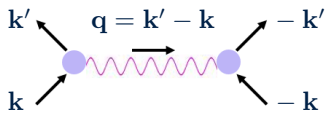
$$\Delta_{n\mathbf{k}} = \sum_m \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \tanh\left(\frac{E_{m\mathbf{k}+\mathbf{q}}}{2k_B T}\right) \frac{V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \Delta_{m\mathbf{k}+\mathbf{q}}}{2E_{m\mathbf{k}+\mathbf{q}}}$$

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

↑
quasiparticle
excitation energy

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

BCS Theory



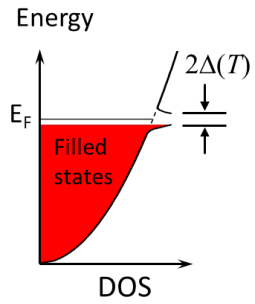
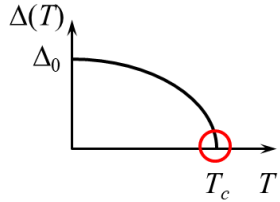
superconducting gap

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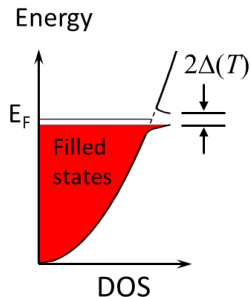
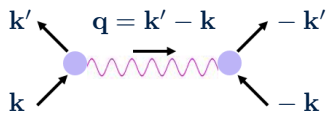
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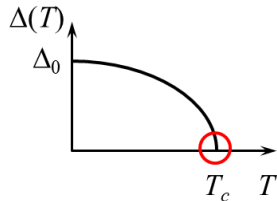
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$$E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_F)^2 + |\Delta_{n\mathbf{k}}|^2}$$

↑
quasiparticle
excitation energy



- describes in detail the phenomenology of superconductivity
- is a descriptive theory, material-independent $\rightarrow 2\Delta_0 = 3.53k_B T_c$
- does not account for the retardation of the e-ph interaction

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

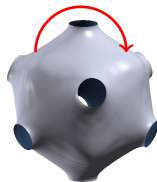
How can T_c be calculated beyond BCS?

McMillan-Allen-Dynes Formula

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

Coulomb
pseudopotential

e-ph
coupling strength



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

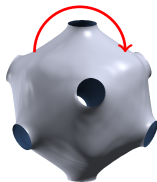
McMillan Phys. Rev. 167, 331(1968); Allen and Dynes, PRB 12, 905 (1975).

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- can be easily calculated (e.g., QE, Abinit)
- works reasonably well for isotropic superconductors
- requires dense \mathbf{k} - and \mathbf{q} -meshes to converge λ
- 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 functions $\hat{G}_{n\mathbf{k}}(\tau)$ 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

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

two-component
field operator

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

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

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

Nambu-Gor'kov Formalism

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

- 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

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

- Diagonal elements are the **normal state Green's functions** and describe single-particle electronic excitations.
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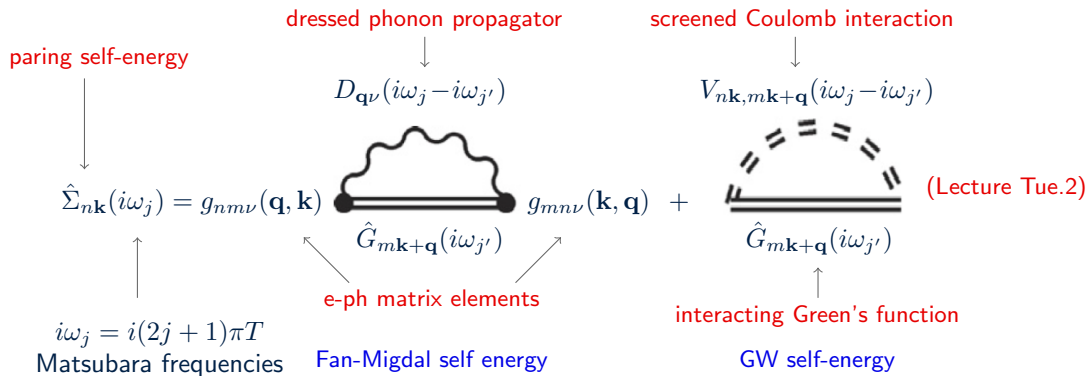
$\hat{G}_{n\mathbf{k}}(\tau)$ is periodic in τ and can be expanded in a Fourier series:

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

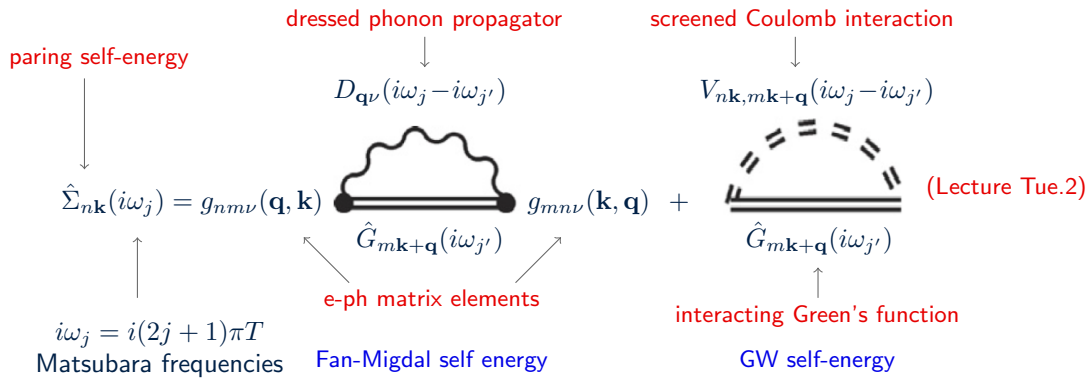
where $i\omega_j = i(2j + 1)\pi T$ (j integer) are Matsubara frequencies and T is the temperature.

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

Migdal-Eliashberg Theory



Migdal-Eliashberg Theory



Migdal's theorem

E-ph vertex corrections are neglected assuming that the neglected terms are of the order of $(m_e/M)^{1/2} \propto \omega_D/\epsilon_F$.


Migdal-Eliashberg Approximation

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

Migdal-Eliashberg Approximation

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

bare phonon propagator


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

Migdal-Eliashberg Approximation

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

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

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

Migdal-Eliashberg Approximation

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

$$\times \left[\sum_{\nu} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'}) + V_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) \right]$$

bare phonon propagator

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

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

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

Migdal-Eliashberg Approximation

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

$$\times \left[\sum_{\nu} |g_{m\nu}(\mathbf{k}, \mathbf{q})|^2 D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'}) + V_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) \right]$$

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

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

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

Migdal-Eliashberg Theory

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


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

Migdal-Eliashberg Theory

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

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

non-interacting
Green's function


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

Pauli
matrices

$$\hat{\tau}_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\hat{\tau}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

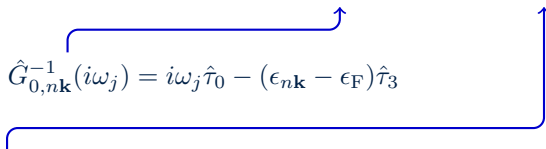
$$\hat{\tau}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Migdal-Eliashberg Theory

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

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

non-interacting
Green's function

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


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

mass renormalization
function

energy
shift

superconducting
gap function

Pauli
matrices

$$\hat{\tau}_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\hat{\tau}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

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

Migdal-Eliashberg Theory

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

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

- 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 in the superconducting state.

Migdal-Eliashberg Theory

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

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

Migdal-Eliashberg Theory

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

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

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

Migdal-Eliashberg Theory

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

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

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

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

Migdal-Eliashberg Theory

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

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

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

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

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

Migdal-Eliashberg Theory

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

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

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

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

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

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

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis: FBW

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

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

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

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis: FBW

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

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

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

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

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis: FBW

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

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

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

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

- 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

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

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

- 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
- the dynamically screened Coulomb interaction $N_{\text{F}} V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})$ is embedded into the semiempirical pseudopotential μ_{c}^*

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis: FSR

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anisotropic e-ph
coupling strength

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

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

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Coulomb
pseudopotential

$$\mu_c^* = \frac{\mu_c}{1 + \mu_c \log(\omega_{\text{el}}/\omega_{\text{ph}})}$$

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

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



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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-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).

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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

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

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

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- The pole positions are:

$$E_{n\mathbf{k}}^2 = \frac{(\epsilon_{n\mathbf{k}} - \epsilon_F)^2}{Z_{n\mathbf{k}}^2(E_{n\mathbf{k}})} + \Delta_{n\mathbf{k}}^2(E_{n\mathbf{k}})$$

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

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

$$G_{n\mathbf{k}}^{11}(\omega) = \frac{\omega Z_{n\mathbf{k}}(\omega) + (\epsilon_{n\mathbf{k}} - \epsilon_F)}{[\omega Z_{n\mathbf{k}}(\omega)]^2 - (\epsilon_{n\mathbf{k}} - \epsilon_F)^2 - [Z_{n\mathbf{k}}(\omega) \Delta_{n\mathbf{k}}(\omega)]^2}$$

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$$E_{n\mathbf{k}}^2 = \frac{(\epsilon_{n\mathbf{k}} - \epsilon_F)^2}{Z_{n\mathbf{k}}^2(E_{n\mathbf{k}})} + \Delta_{n\mathbf{k}}^2(E_{n\mathbf{k}})$$

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binding energy of electrons
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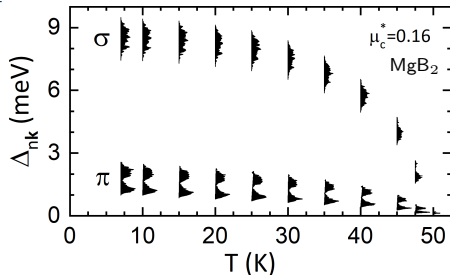
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Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Superconducting Quasiparticle Density of States and Spectral Function

- Superconducting quasiparticle density of states:

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

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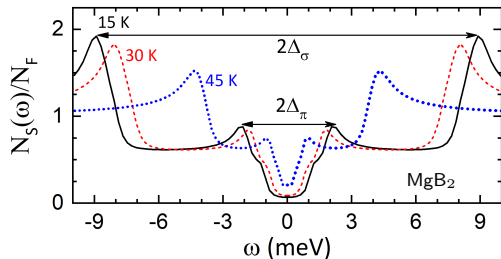
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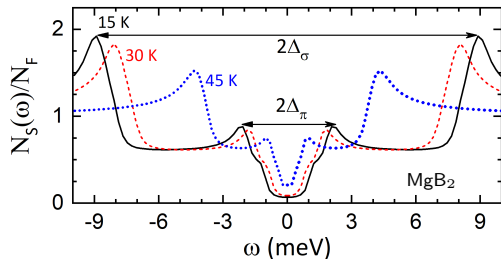
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Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

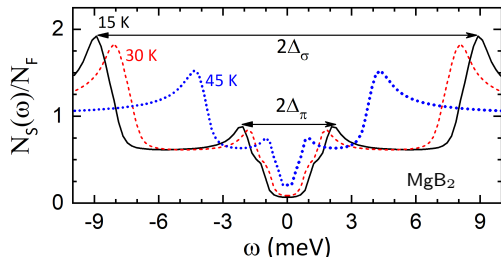
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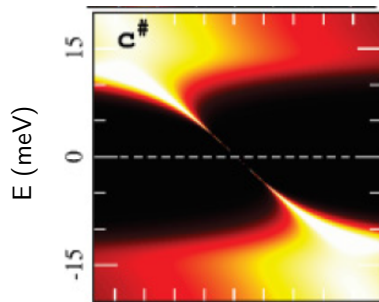
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CaC₆ normal state

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

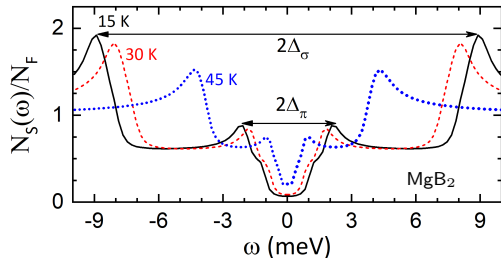
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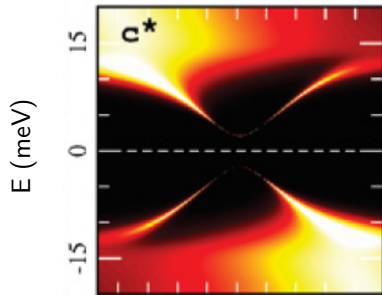
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CaC₆ superconducting state

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Migdal-Eliashberg Theory

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

$$Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} [\lambda_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_c^*] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F)$$

- has predictive power, material-dependent
- accounts for the retardation of the e-ph interaction
- works for multiband and/or anisotropic superconductors
- generally approximates the Coulomb interaction through μ_c^*
- requires dense \mathbf{k} - and \mathbf{q} -meshes

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

quasiparticle excitation energy $\rightarrow E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_{\text{F}})^2 + |\Delta_{n\mathbf{k}}|^2}$

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)

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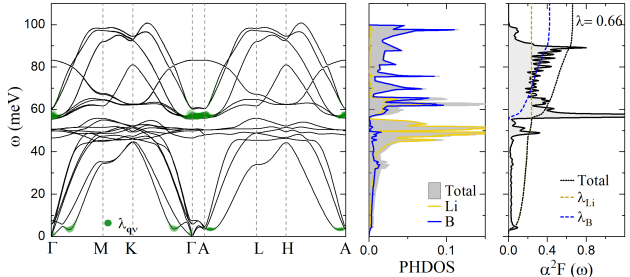
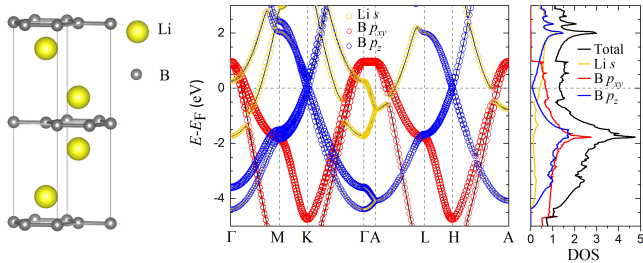
- has predictive power, material-dependent
- accounts for retardation effects through the XC functionals
- works for multiband and/or anisotropic superconductors
- treats e-ph and e-e interactions on equal footing
- requires development of new functionals for e-ph interactions
- requires dense \mathbf{k} - and \mathbf{q} -meshes

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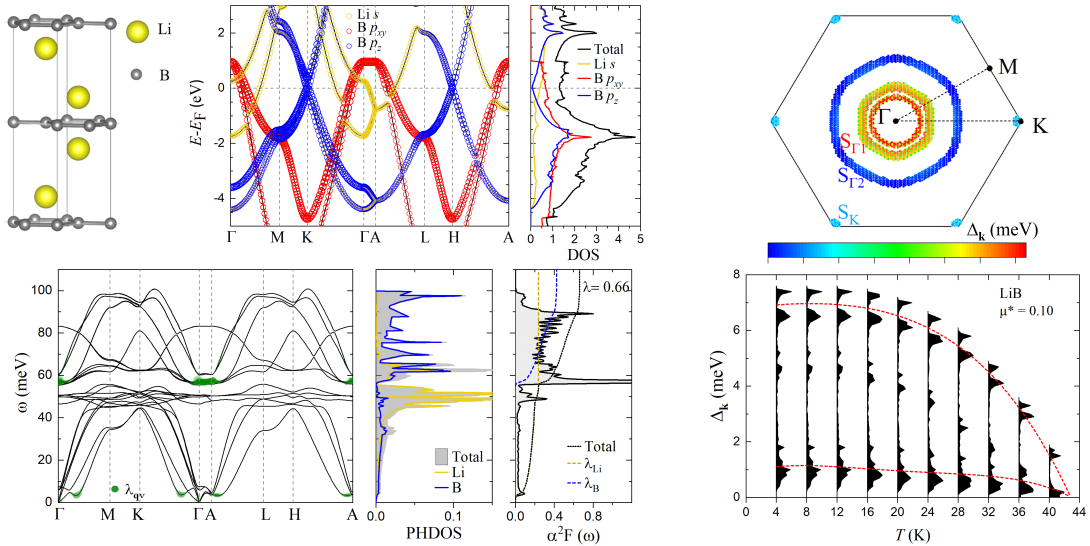
Examples from calculations

Supeconductivity in LiB: FSR



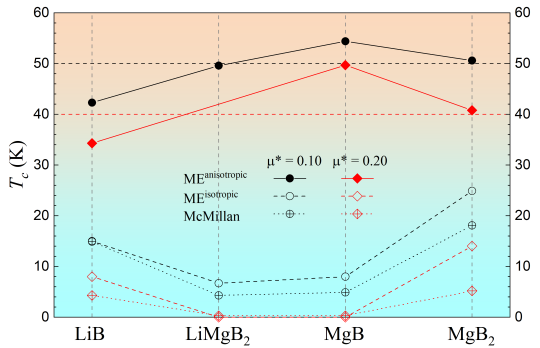
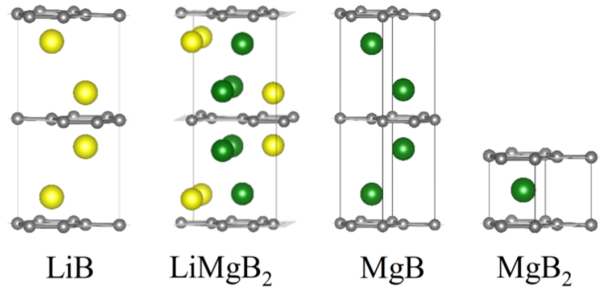
Kolmogorov and Curtarolo, Phys. Rev. B 73, 180501(R) (2006); Kafle et al, Phys. Rev. Materials (under review).

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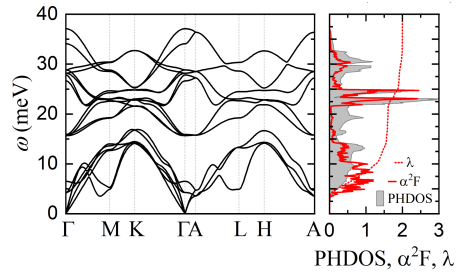
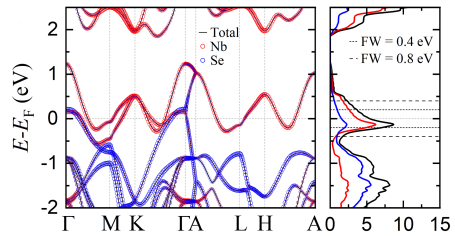
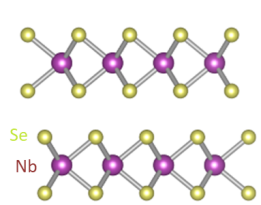
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Superconductivity in Li-Mg-B phases

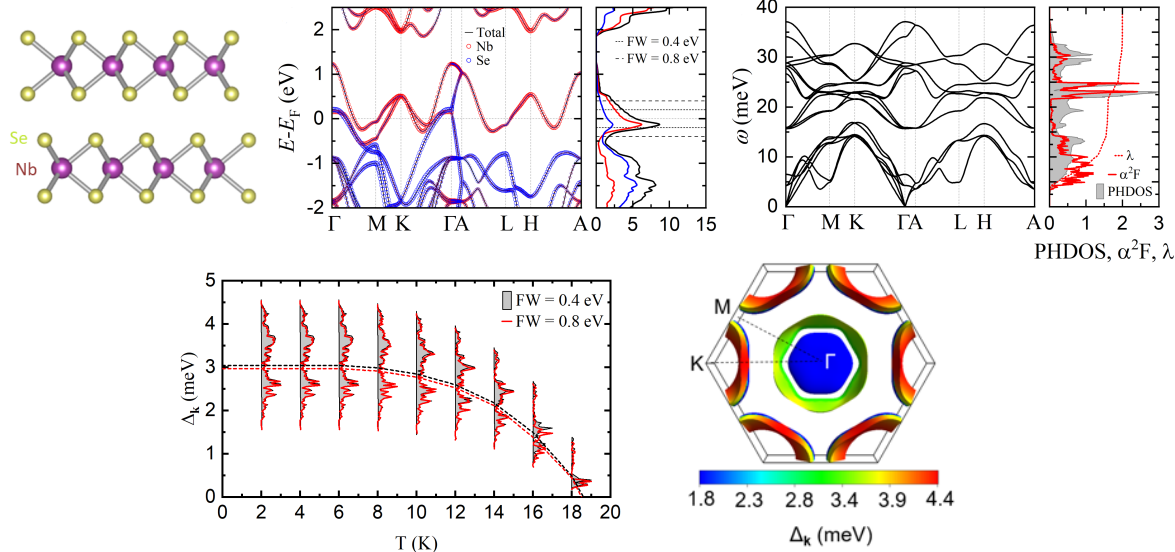


Kafle, Tomassetti, Mazin, Kolmogorov and Margine, Phys. Rev. Materials (under review).

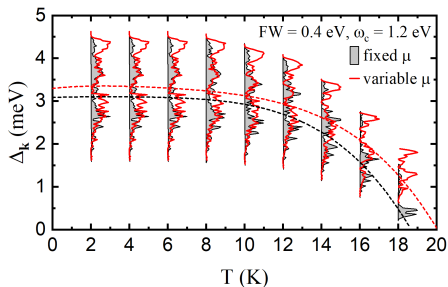
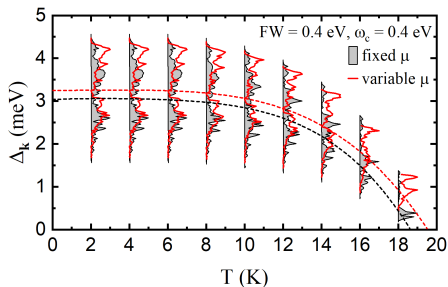
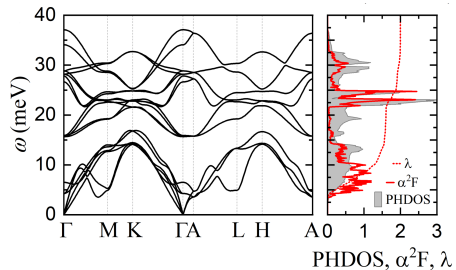
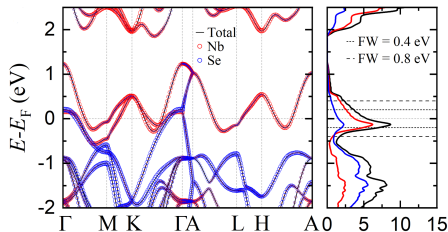
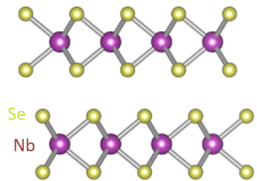
Superconductivity in 2H-NbSe₂: FBW



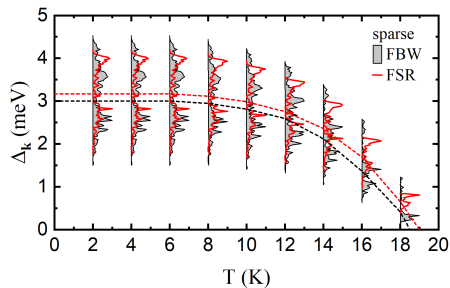
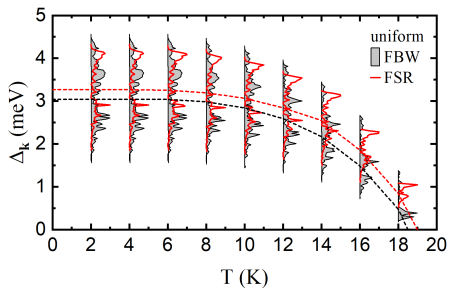
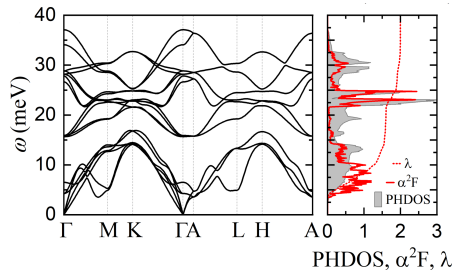
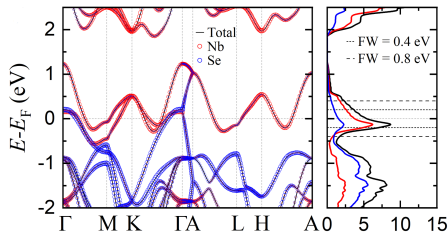
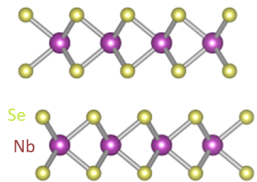
Superconductivity in 2H-NbSe₂: FBW



Superconductivity in 2H-NbSe₂: FBW



Superconductivity in 2H-NbSe₂: FBW vs. FSR



Take-home Messages

- We can obtain measurable superconducting properties with anisotropic resolution using the Migdal-Eliashberg theory
- The solutions of the anisotropic Migdal-Eliashberg equations invariably require a fine sampling of the electron-phonon matrix elements across the Brillouin zone

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