2021 Virtual School on Electron-Phonon Physics and the EPW code

June 14-18 2021

Lecture Thu.1

Superconductors and Migdal-Eliashberg theory

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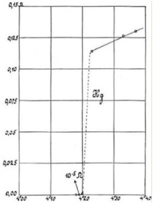
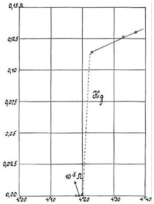
Lecture Summary

- Superconductivity milestones
- BCS theory of superconductivity
- McMillan-Allen-Dynes formula for critical temperature
- 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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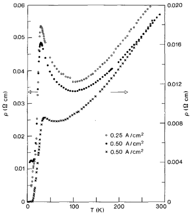
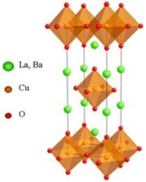
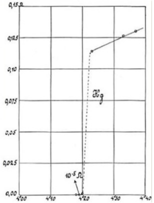




Bednorz and Müller, Z. Phys. B - Cond. Matter 64, 189 (1986)

Superconductivity Milestones



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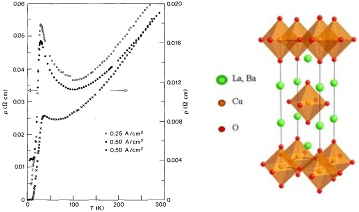

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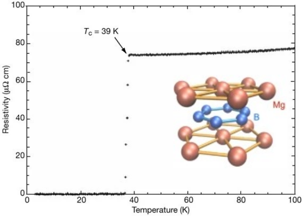

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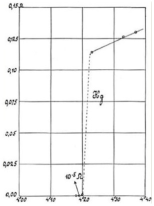

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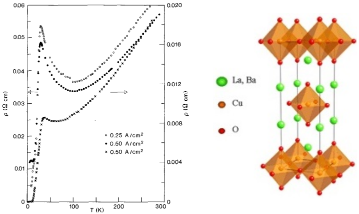

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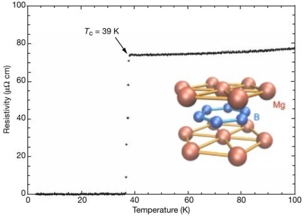

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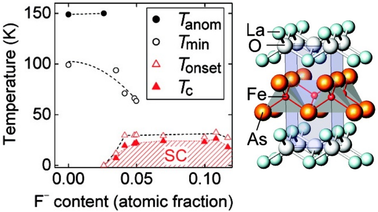

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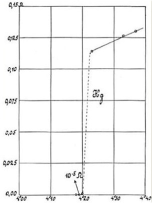
Superconductivity Milestones



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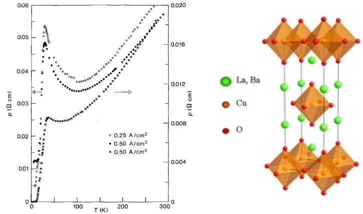

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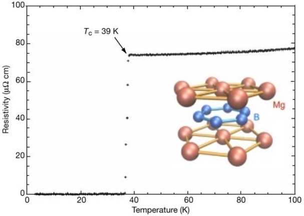

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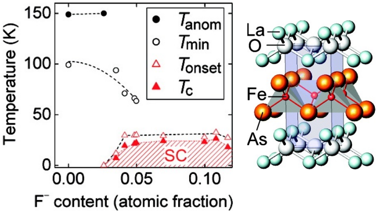

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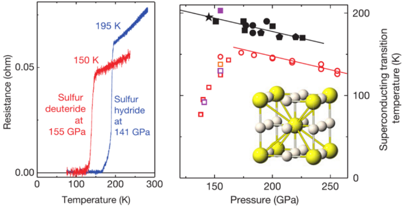

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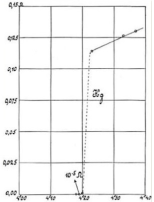
Superconductivity Milestones



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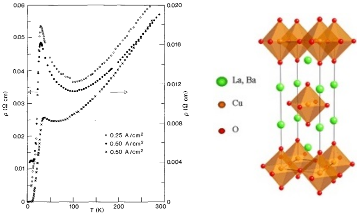

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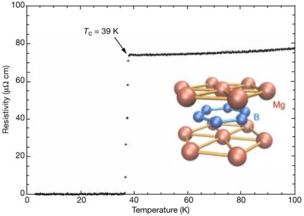

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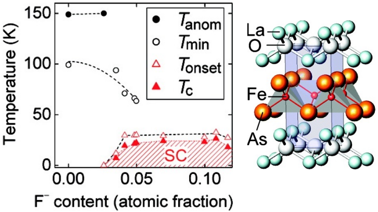

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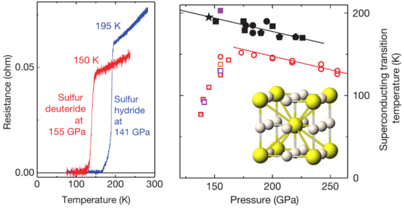

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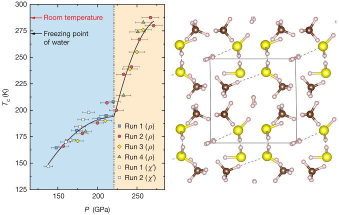
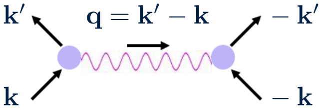
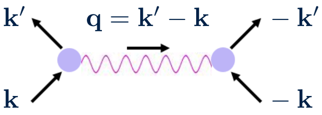
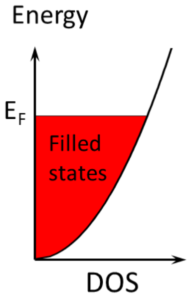


Snider *et. al.* Nature 583, 373 (2020)



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





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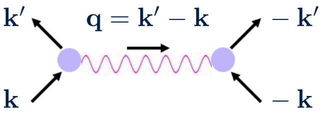

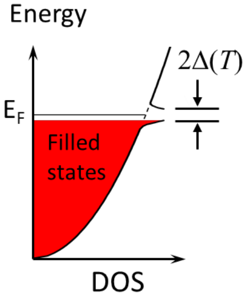

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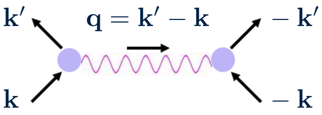
BCS Theory



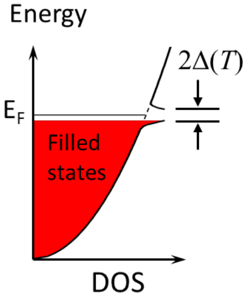
superconducting gap

paring potential

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

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

quasiparticle excitation energy



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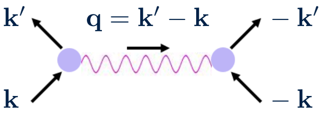


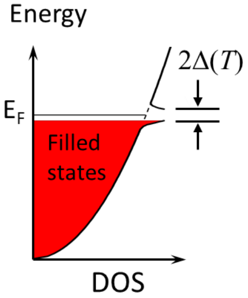
superconducting gap

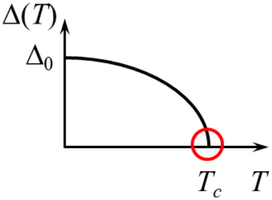
paring potential

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

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

quasiparticle
excitation energy





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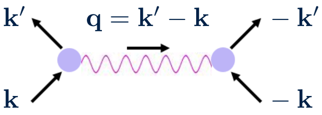

superconducting gap

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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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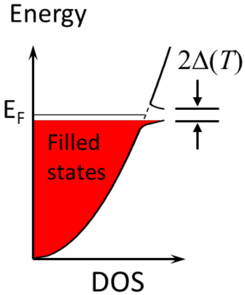
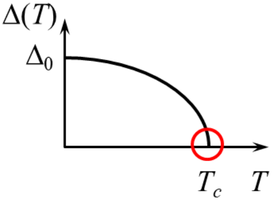




- describes in detail the phenomenology of superconductivity
- is a descriptive theory, material-independent $\rightarrow 2\Delta_0 = 3.53 k_{\mathrm{B}} T_{\mathrm{c}}$
- does not account for the retardation of the e-ph interaction

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

How can T_c be calculated beyond BCS?

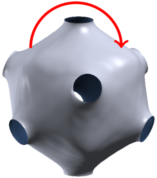
McMillan-Allen-Dynes Formula

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

(Lecture Mon.1)

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).

McMillan-Allen-Dynes Formula

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

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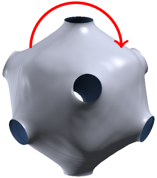

$$\lambda = N_F \left\langle\!\!\left\langle \sum_\nu \frac{|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2}{\hbar\omega_{\mathbf{q}\nu}} \right\rangle\!\!\right\rangle_{FS}$$

- can be easily calculated (e.g., Quantum Espresso)
- 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).

Migdal-Eliashberg Theory

dressed phonon propagator

screened Coulomb interaction

paring self-energy

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

$V_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j - i\omega_{j'})$

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

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

(Lecture Tue.2)

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

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

e-ph matrix elements

interacting Green's function

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

Matsubara frequencies

Fan-Migdal self energy

GW self-energy

Migdal-Eliashberg Theory

paring self-energy

dressed phonon propagator

screened Coulomb interaction

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

$V_{n\mathbf{k},m\mathbf{k+q}}(i\omega_j - i\omega_{j'})$

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

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

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

e-ph matrix elements

interacting Green's function

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

Matsubara frequencies

Fan-Migdal self energy

GW self-energy

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

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

Migdal-Eliashberg Approximation

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

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

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\begin{aligned}
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&\times \left[\sum_{\nu}\boxed{|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]
\end{aligned}
$$

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

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

Migdal-Eliashberg Approximation

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

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

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

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

Migdal-Eliashberg Approximation

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

bare phonon propagator

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

anisotropic e-ph coupling strength

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

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

Migdal-Eliashberg Theory

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

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

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ 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:

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non-interacting Green's function

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

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

mass renormalization function

energy shift

superconducting gap function

Pauli matrices

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

Migdal-Eliashberg Theory

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

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

Migdal-Eliashberg Theory

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

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

- 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.

Migdal-Eliashberg Theory

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

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

- 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

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

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

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

Migdal-Eliashberg Theory

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

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

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

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

Migdal-Eliashberg Theory

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

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

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

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

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

Migdal-Eliashberg Theory

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

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

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

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

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

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

Anisotropic Migdal-Eliashberg Equations

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

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

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

Anisotropic Migdal-Eliashberg Equations

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

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

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

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

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis

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

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

- only the off-diagonal contributions of the Coulomb self-energy are retained in order to avoid double counting of Coulomb effects
- 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 $V_{n\mathbf{k},m\mathbf{k}'}$ is embedded into the semiempirical pseudopotential μ_{c}^*

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis

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

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

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis

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

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

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis

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

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

anisotropic e-ph coupling strength

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

Anisotropic Migdal-Eliashberg Equations on Imaginary Axis

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

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

anisotropic e-ph coupling strength

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

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Anisotropic Migdal-Eliashberg Equations on Imaginary Axis

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

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anisotropic e-ph coupling strength

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

EPW

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

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Coulomb pseudopotential

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

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

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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

- The Migdal-Eliasberg equations on the imaginary frequency axis are computationally efficient (only involve sums over a finite number of Matsubara frequencies) and they are adequate for calculating the critical temperature and the superconducting gap.

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

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- The Migdal-Eliasberg equations on the imaginary frequency axis are computationally efficient (only involve sums over a finite number of Matsubara frequencies) and they are adequate for calculating the critical temperature and the superconducting gap.
- To extract information about the spectral properties (e.g., the quasi particle density of states or the single particle excitation spectrum), the Migdal-Eliashberg equations need to be solved on the real energy axis.

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- Direct evaluation of the Migdal-Eliashberg equations on the real energy axis is in principle possible but very demanding computationally since it involves the evaluation of many principal value integrals.
- As an alternative, the solutions on the real energy axis can be obtained by analytic continuation of the solutions along the imaginary frequency axis. The analytic continuation can be performed 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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This identity defines the leading edge $\Delta_{n\mathbf{k}}$ of the superconducting gap:

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binding energy of electrons in a Cooper pair

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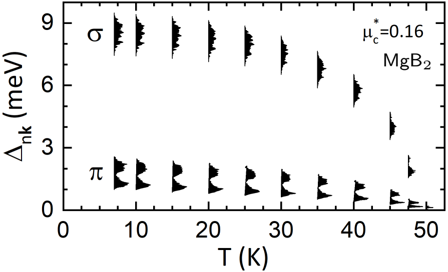

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Superconducting Quasiparticle Density of States and Spectral Function

- Superconducting quasiparticle density of states:

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

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- In the BCS limit $Z_{n\mathbf{k}} = 1$, and integrating over $\epsilon_{n\mathbf{k}}$ and averaging over the Fermi surface leads to:

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

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

Superconducting Quasiparticle Density of States and Spectral Function

- Superconducting quasiparticle density of states:

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

- In the BCS limit $Z_{n\mathbf{k}} = 1$, and integrating over $\epsilon_{n\mathbf{k}}$
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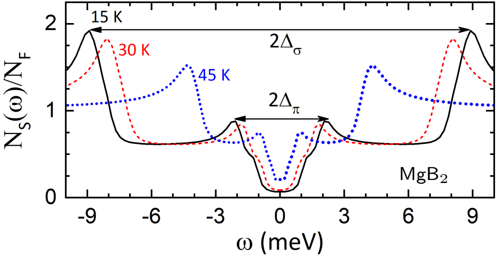

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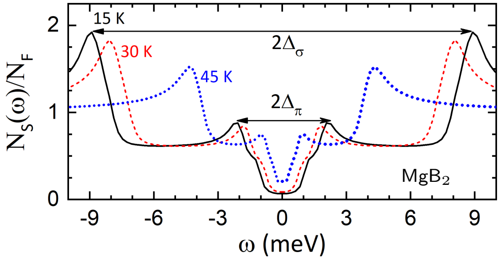

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

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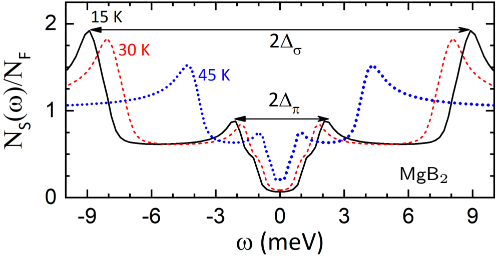

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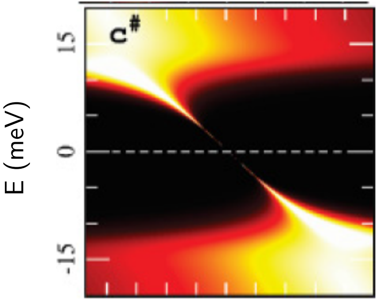

CaC_6 normal state

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

- Superconducting quasiparticle density of states:

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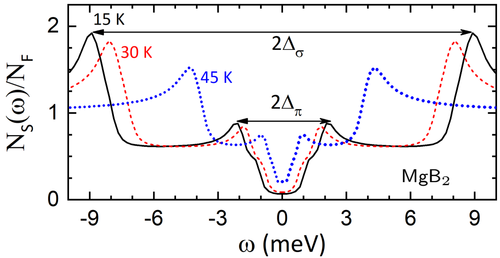

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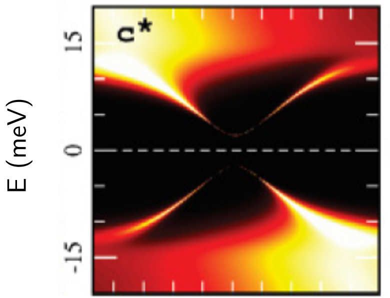

CaC_6 superconducting state

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

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

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

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

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)

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

- 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

Lüders et al, Phys. Rev. B 72, 024545 (2005); Marques et al, Phys. Rev. B 72, 024546 (2005);
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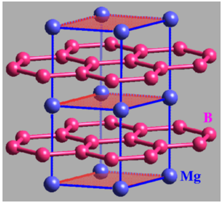
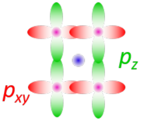
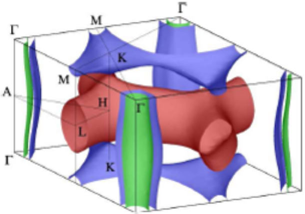
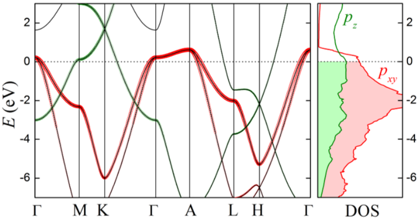
Examples from calculations

Supeconductivity in MgB_2

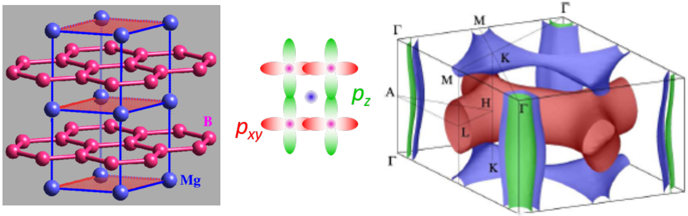


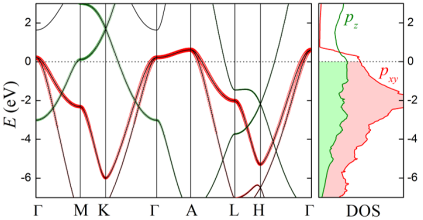






Kortus et al, Phys. Rev. Lett. 86, 4656 (2001)





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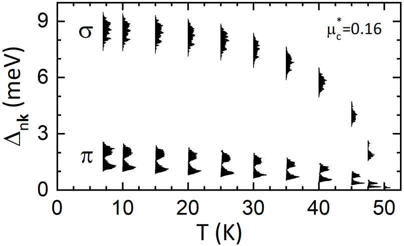
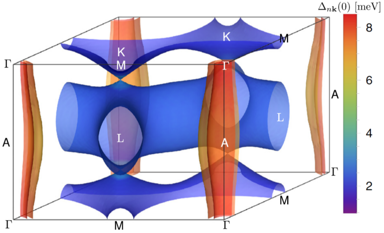
Anisotropic
Migdal-Eliashberg
formalism (EPW)

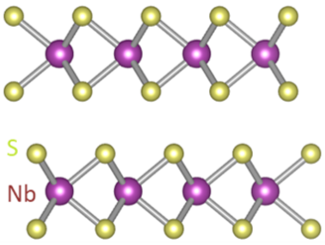




Margine and Giustino, Phys. Rev. B 87, 024505

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

Superconductivity in 2H-NbS_2



Heil, Poncé, Lambert, Schlipf, Margine, and Giustino, Phys. Rev. Lett., 119, 087003 (2017)

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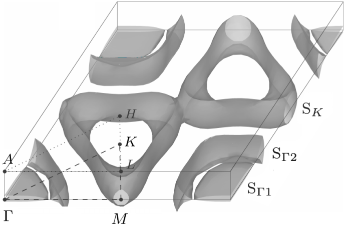

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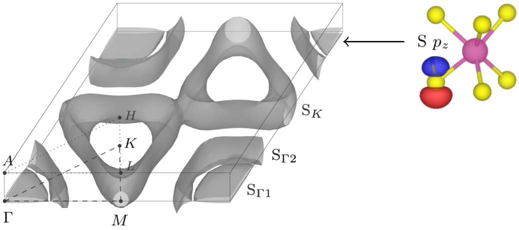

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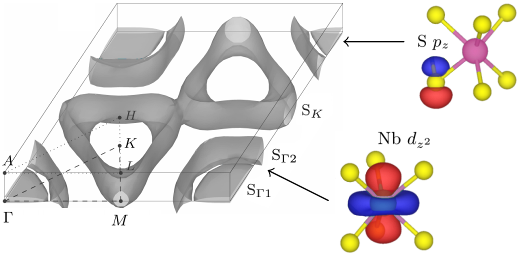

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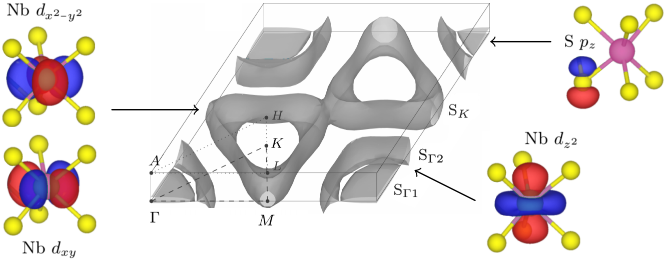

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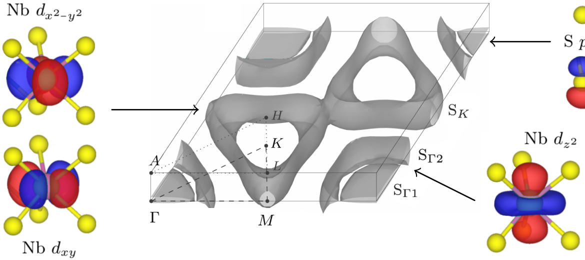

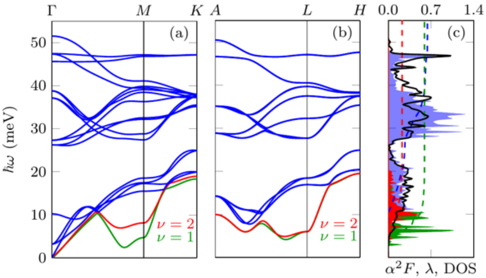

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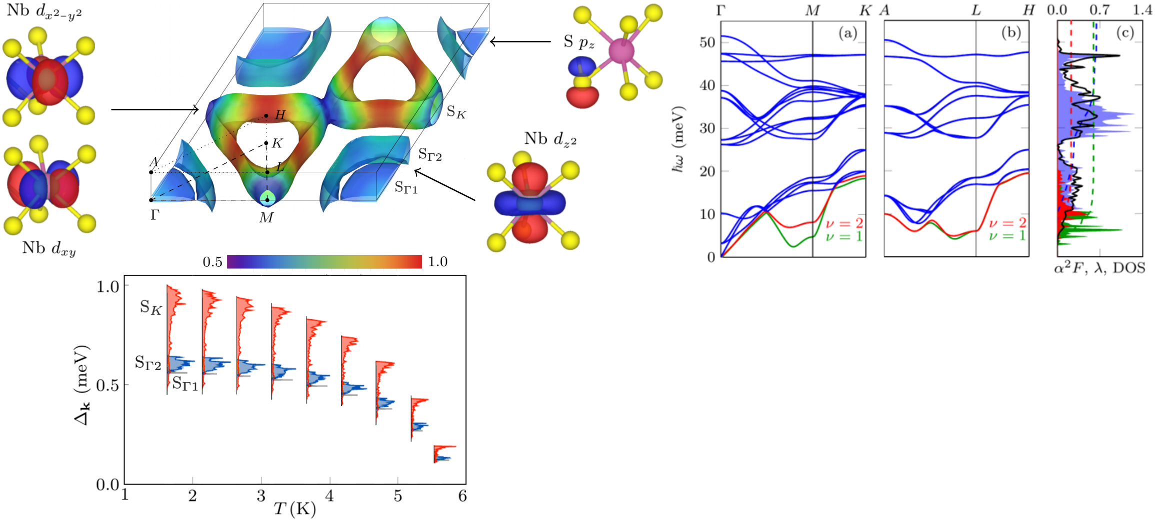
Superconductivity in 2H-NbS$_2$



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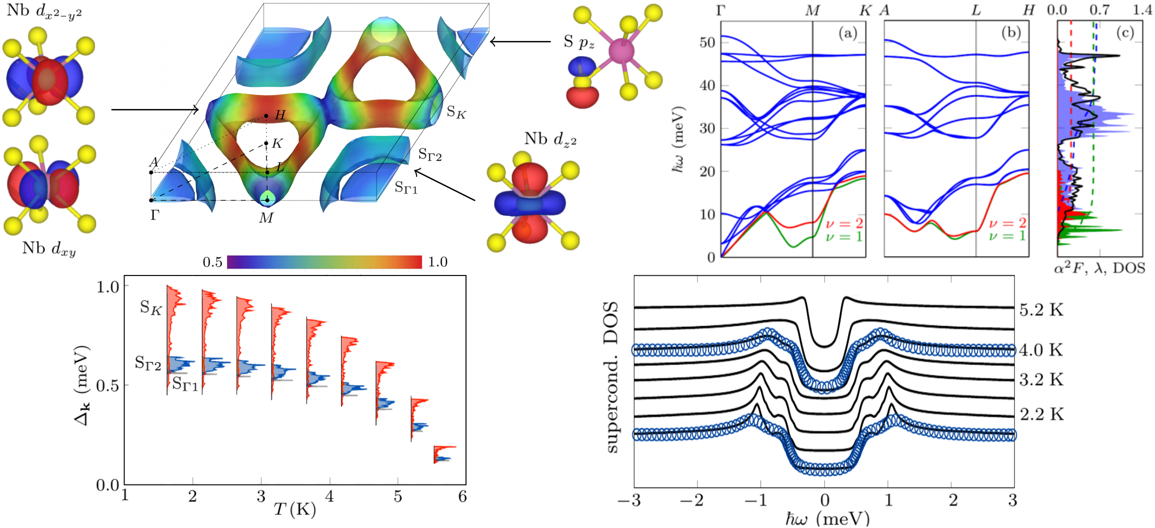

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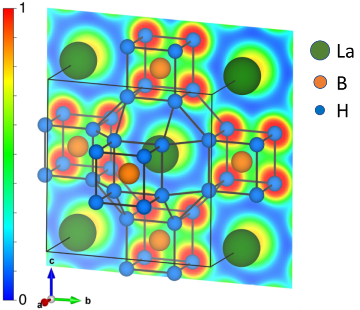
Superconductivity in $LaBH_8$



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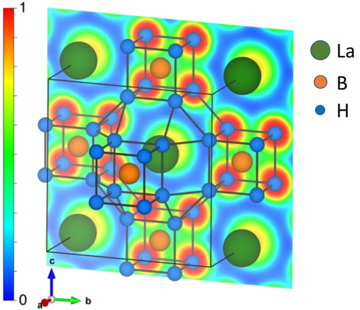

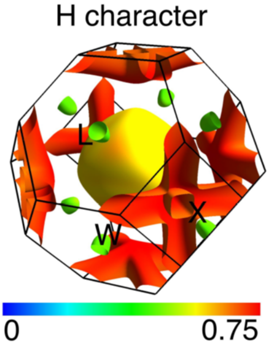

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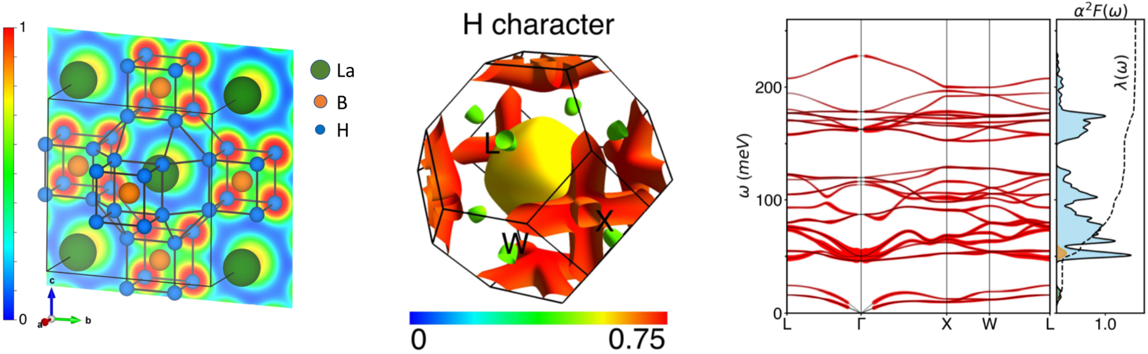

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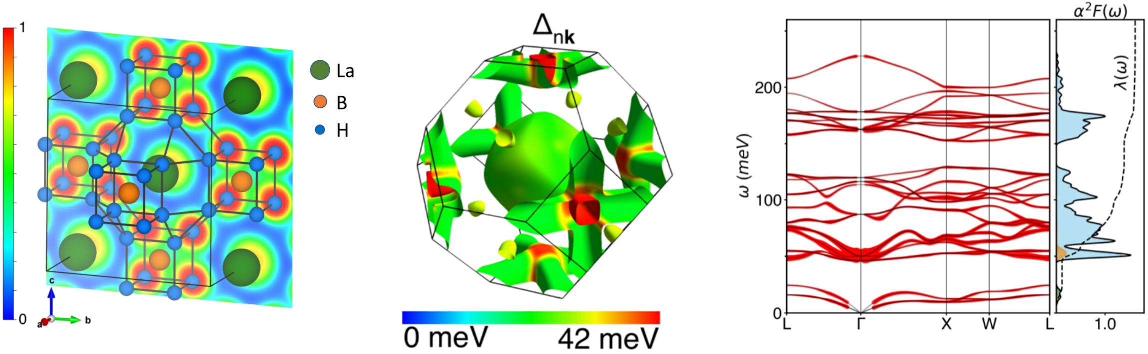

LaBH$_8$ predicted to be a conventional HTSC with a T_c of 126 K at 50 GPa

Di Cataldo, Heil, von der Linden, and Boeri, arXiv:2102.11227v2 (2021)

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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Supplemental Slides

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

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

two-component field operator

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

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

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.

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