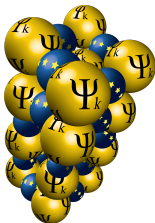


ICTP/Psi-k/CECAM School on Electron-Phonon Physics from First Principles

Trieste, 19-23 March 2018



Lecture Fri.2

Migdal-Eliashberg theory of superconductivity

Roxana Margine

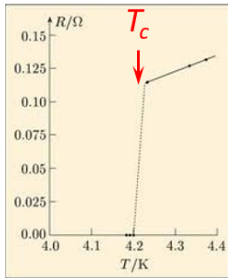
Department of Physics, Applied Physics, and Astronomy
Binghamton University - State University of New York

Lecture Summary

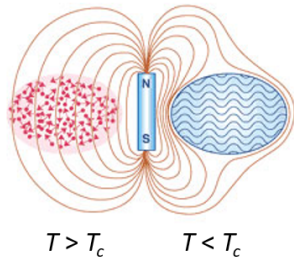
- Superconductivity
- BCS theory of superconductivity
- McMillan-Allen-Dynes formula for critical temperature
- Migdal-Eliashberg approximation
- Nambu-Gor'kov formalism
- Migdal-Eliashberg equations
- Density functional theory for superconductors

Superconductivity

A macroscopic quantum-mechanical phenomenon occurring in certain materials below a characteristic critical temperature



"zero resistivity"
1911 Kamerlingh Onnes



"perfect diamagnetism"
1933 Meissner & Ochsenfeld

Superconductivity Timeline

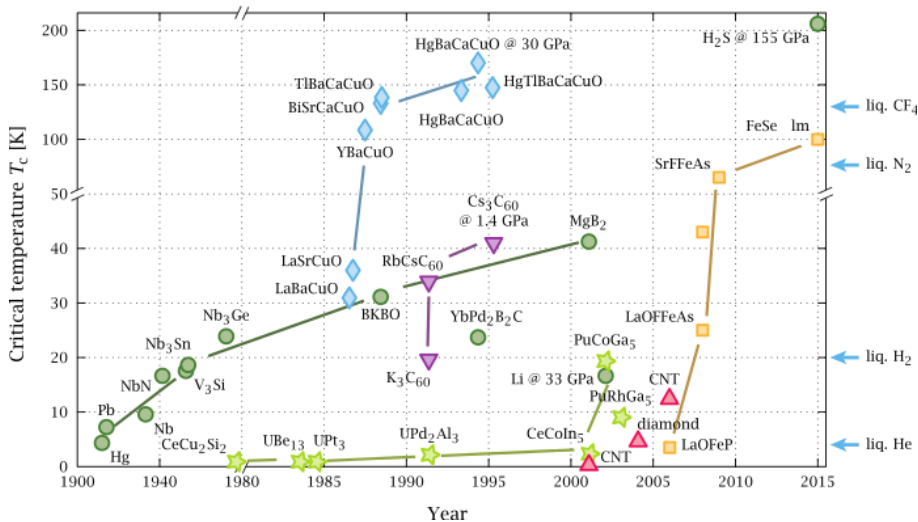
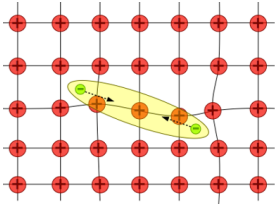


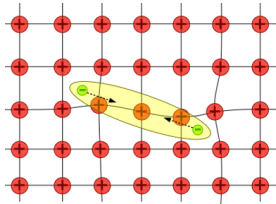
Figure from Wikipedia

BCS Theory

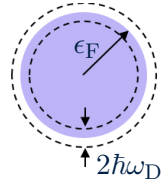
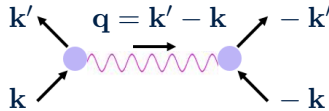


electron Cooper
pairs in a lattice

BCS Theory

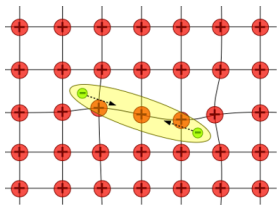


electron Cooper pairs in a lattice

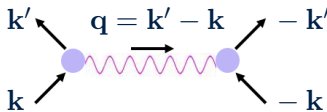


exchange of virtual phonons produces an attraction for electrons close to Fermi level

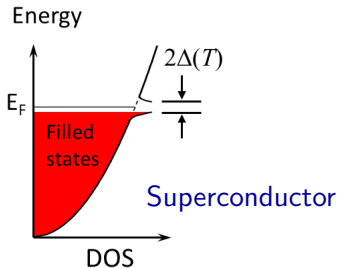
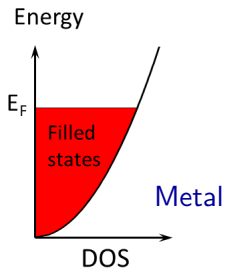
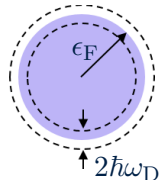
BCS Theory



electron Cooper pairs in a lattice



exchange of virtual phonons produces an attraction for electrons close to Fermi level



BCS Theory

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

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

BCS Theory

superconducting gap



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

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BCS Theory

superconducting gap



paring potential



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

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BCS Theory

superconducting gap

paring potential

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

quasiparticle
excitation energy

BCS Theory

superconducting gap



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

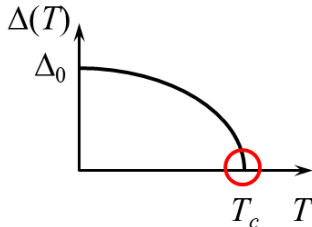
paring potential



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



quasiparticle
excitation energy



BCS Theory

superconducting gap



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

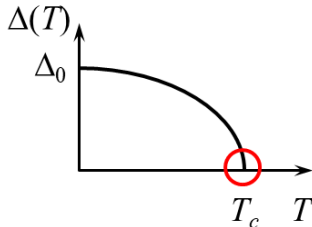
paring potential



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



quasiparticle
excitation energy



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

How can T_c be calculated beyond BCS?

McMillan-Allen-Dynes Formula

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

McMillan-Allen-Dynes Formula

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←
e-ph
coupling strength

McMillan-Allen-Dynes Formula

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


Coulomb pseudopotential e-ph coupling strength

McMillan-Allen-Dynes Formula

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


Coulomb pseudopotential e-ph coupling strength

- 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^*

Migdal-Eliashberg Theory

paring self-energy

dressed phonon propagator

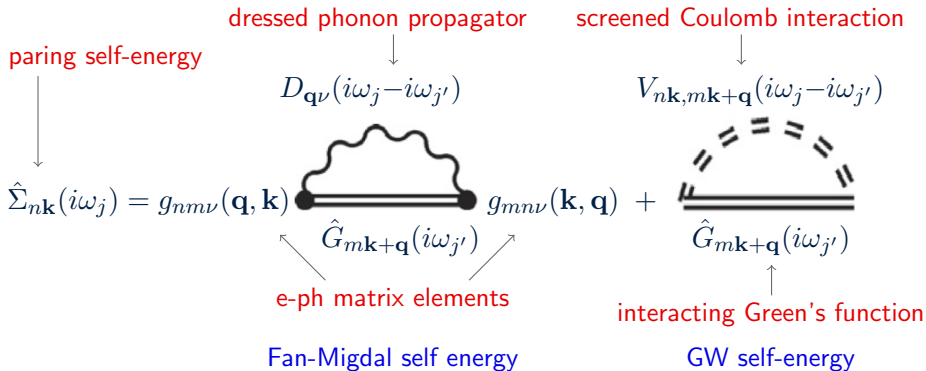
screened Coulomb interaction

$$\hat{\Sigma}_{n\mathbf{k}}(i\omega_j) = g_{nm\nu}(\mathbf{q}, \mathbf{k}) \overset{\substack{\text{dressed phonon propagator} \\ D_{\mathbf{q}\nu}(i\omega_j - i\omega_{j'})}}{\text{cloud}} \overset{\substack{\text{e-ph matrix elements} \\ \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}}{\text{line}} g_{mn\nu}(\mathbf{k}, \mathbf{q}) + \overset{\substack{\text{screened Coulomb interaction} \\ V_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})}}{\text{dashed arc}} \overset{\substack{\text{interacting Green's function} \\ \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}}{\text{line}}$$

e-ph matrix elements

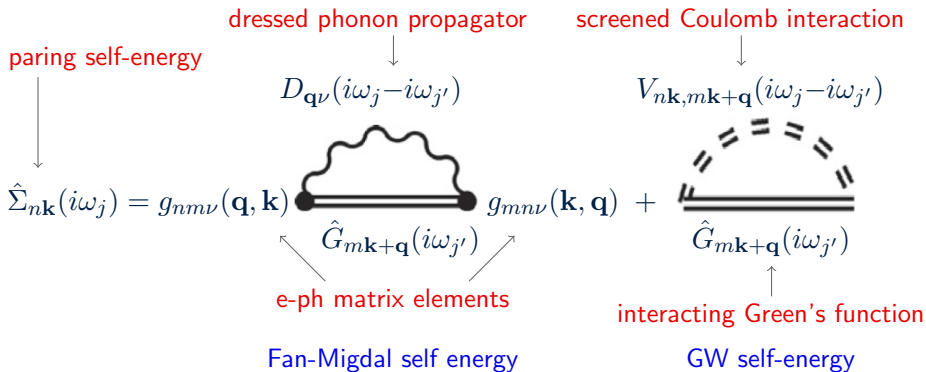
interacting Green's function

Migdal-Eliashberg Theory



(Lecture Wed.1)

Migdal-Eliashberg Theory



(Lecture Wed.1)

Migdal's theorem

Only the leading terms in Feynman diagram of the self-energy are included.

The neglected terms are of the order of $(m_e/M)^{1/2} \propto \omega_D/\epsilon_F$.

Migdal-Eliashberg Approximation

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

Migdal-Eliashberg Approximation

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Migdal-Eliashberg Approximation

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

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



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

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

Migdal-Eliashberg Approximation

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

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



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

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.

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

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


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imaginary time  Wick's time-ordering operator

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

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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- 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.
- 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.

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

Nambu-Gor'kov Formalism

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ can be evaluated by solving **Dyson's equation**:

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

Nambu-Gor'kov Formalism

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ can be evaluated by solving Dyson's equation:

non-interacting Green's function

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

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

Nambu-Gor'kov Formalism

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ can be evaluated by solving Dyson's equation:

non-interacting Green's function

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

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

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

mass renormalization
function

energy
shift

superconducting
gap function

Nambu-Gor'kov Formalism

$\hat{G}_{n\mathbf{k}}(i\omega_j)$ can be evaluated by solving Dyson's equation:

non-interacting Green's function

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

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

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

mass renormalization
function

energy
shift

superconducting
gap function

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

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

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

Migdal-Eliashberg Approximation

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

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

Migdal-Eliashberg Approximation

$$\begin{aligned}
 \hat{G}_{n\mathbf{k}}(i\omega_j) &= -\frac{1}{\Theta_{n\mathbf{k}}(i\omega_j)} \left\{ i\omega_j Z_{n\mathbf{k}}(i\omega_j) \hat{\tau}_0 + [(\epsilon_{n\mathbf{k}} - \epsilon_F) + \chi_{n\mathbf{k}}(i\omega_j)] \hat{\tau}_3 \right. \\
 &\quad \left. + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j) \hat{\tau}_1 \right\} \\
 \Theta_{n\mathbf{k}}(i\omega_j) &= [\omega_j Z_{n\mathbf{k}}(i\omega_j)]^2 + [(\epsilon_{n\mathbf{k}} - \epsilon_F) + \chi_{n\mathbf{k}}(i\omega_j)]^2 + [Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j)]^2 \\
 \hat{\Sigma}_{n\mathbf{k}}(i\omega_j) &= -T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \hat{\tau}_3 \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'}) \hat{\tau}_3 \\
 &\quad \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})]
 \end{aligned}$$

Migdal-Eliashberg Approximation

$$\begin{aligned} \hat{G}_{n\mathbf{k}}(i\omega_j) &= -\frac{1}{\Theta_{n\mathbf{k}}(i\omega_j)} \left\{ i\omega_j Z_{n\mathbf{k}}(i\omega_j) \hat{\tau}_0 + [(\epsilon_{n\mathbf{k}} - \epsilon_F) + \chi_{n\mathbf{k}}(i\omega_j)] \hat{\tau}_3 \right. \\ &\quad \left. + \Delta_{n\mathbf{k}}(i\omega_j) Z_{n\mathbf{k}}(i\omega_j) \hat{\tau}_1 \right\} \\ \Theta_{n\mathbf{k}}(i\omega_j) &= [\omega_j Z_{n\mathbf{k}}(i\omega_j)]^2 + [(\epsilon_{n\mathbf{k}} - \epsilon_F) + \chi_{n\mathbf{k}}(i\omega_j)]^2 + [Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j)]^2 \\ \hat{\Sigma}_{n\mathbf{k}}(i\omega_j) &= -T \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \hat{\tau}_3 \hat{G}_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'}) \hat{\tau}_3 \\ &\quad \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) + V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'})] \\ \hat{\tau}_0 &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \hat{\tau}_1 &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \hat{\tau}_3 &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ \hat{\tau}_3 \hat{\tau}_0 \hat{\tau}_3 &= \hat{\tau}_0 & \text{and} & \hat{\tau}_3 \hat{\tau}_1 \hat{\tau}_3 &= -\hat{\tau}_1 \end{aligned}$$

Migdal-Eliashberg Approximation

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

Migdal-Eliashberg Approximation

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

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

Migdal-Eliashberg Approximation

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

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

Migdal-Eliashberg Approximation

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

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

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

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

Anisotropic Migdal-Eliashberg Equations

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

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

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

Anisotropic Migdal-Eliashberg Equations

Standard approximations

- 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

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$$Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{T}{\omega_j N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\omega_{j'} Z_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\Theta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})} \\ \times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - N_F V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(i\omega_j - i\omega_{j'}) \right]$$

Anisotropic Migdal-Eliashberg Equations

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- 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

Anisotropic Migdal-Eliashberg Equations

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Anisotropic Migdal-Eliashberg Equations

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- 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 is assumed to be constant
- the dynamically screened Coulomb interaction $N_F V_{n\mathbf{k},m\mathbf{k}'}$ is embedded into the semiempirical pseudopotential μ_c^*

Anisotropic Migdal-Eliashberg Equations

$$\begin{aligned}
 Z_{n\mathbf{k}}(i\omega_j) &= 1 + \frac{\pi T}{\omega_j N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 \text{mass renormalization} & \quad \times \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \\
 \text{function} & \\
 Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j) &= \frac{\pi T}{N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 \text{superconducting} & \quad \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_c^*] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \\
 \text{gap function} &
 \end{aligned}$$

Anisotropic Migdal-Eliashberg Equations

$$\begin{aligned}
 & Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 & \text{mass renormalization function} \quad \times \lambda_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \\
 \\
 & Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 & \text{superconducting gap function} \quad \times \left[\lambda_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_c^* \right] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F)
 \end{aligned}$$

Anisotropic Migdal-Eliashberg Equations

$$\begin{aligned}
 & \text{mass renormalization function} \quad Z_{n\mathbf{k}}(i\omega_j) = 1 + \frac{\pi T}{\omega_j N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 & \quad \times \lambda_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \\
 & \text{superconducting gap function} \quad Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j) = \frac{\pi T}{N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 & \quad \times [\lambda_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_c^*] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \\
 & \lambda_{n\mathbf{k}, m\mathbf{k}+\mathbf{q}}(\omega_j) = N_F \sum_{\nu} \int_0^{\infty} d\omega \frac{2\omega}{\omega_j^2 + \omega^2} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \delta(\omega - \omega_{\mathbf{q}\nu})
 \end{aligned}$$

↑
anisotropic e-ph coupling strength

Anisotropic Migdal-Eliashberg Equations

$$\begin{aligned}
 Z_{n\mathbf{k}}(i\omega_j) &= 1 + \frac{\pi T}{\omega_j N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 \text{mass renormalization} & \quad \times \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \\
 \text{function} & \\
 Z_{n\mathbf{k}}(i\omega_j) \Delta_{n\mathbf{k}}(i\omega_j) &= \frac{\pi T}{N_F} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
 \text{superconducting} & \quad \times [\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_c^*] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \\
 \text{gap function} &
 \end{aligned}$$

$$\begin{aligned}
 \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j) &= N_F \sum_{\nu} \int_0^{\infty} d\omega \frac{2\omega}{\omega_j^2 + \omega^2} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \delta(\omega - \omega_{\mathbf{q}\nu}) \\
 \text{anisotropic e-ph} & \quad \uparrow \\
 \text{coupling strength} & \\
 &= \int_0^{\infty} d\omega \alpha^2 F_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega) \frac{2\omega}{\omega_j^2 + \omega^2} \\
 & \quad \uparrow \\
 & \quad \text{anisotropic Eliashberg} \\
 & \quad \text{spectral function}
 \end{aligned}$$

Anisotropic Migdal-Eliashberg Equations

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

Anisotropic Migdal-Eliashberg Equations

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

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

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

Anisotropic Migdal-Eliashberg Equations

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

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

- The coupled nonlinear equations need to be solved self-consistently at each **temperature T**
- The equations must be evaluated on dense electron **$\mathbf{k}$ -** and phonon **$\mathbf{q}$ -meshes** to properly describe anisotropic effects

Anisotropic Migdal-Eliashberg Equations

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

- The coupled nonlinear equations need to be solved self-consistently at each **temperature T**
- The equations must be evaluated on dense electron **$\mathbf{k}$ -** and phonon **$\mathbf{q}$ -meshes** to properly describe anisotropic effects
- The sum over **Matsubara frequencies** must be truncated (typically set to four to ten times the largest phonon energy)

Anisotropic Migdal-Eliashberg Equations

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

- The coupled nonlinear equations need to be solved self-consistently at each **temperature T**
- The equations must be evaluated on dense electron **$\mathbf{k}$ -** and phonon **$\mathbf{q}$ -meshes** to properly describe anisotropic effects
- The sum over **Matsubara frequencies** must be truncated (typically set to four to ten times the largest phonon energy)
- $Z_{n\mathbf{k}}$ and $\Delta_{n\mathbf{k}}$ are only meaningful for **$n\mathbf{k}$ at or near the Fermi surface**

Isotropic Migdal-Eliashberg Equations

$$Z(i\omega_j) = 1 + \frac{\pi T}{\omega_j} \sum_{j'} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta(i\omega_j)}} \lambda(\omega_j - \omega_{j'})$$

$$Z(i\omega_j) \Delta(i\omega_j) = \pi T \sum_{j'} \frac{\Delta(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta^2(i\omega_{j'})}} [\lambda(\omega_j - \omega_{j'}) - \mu_c^*]$$

Isotropic Migdal-Eliashberg Equations

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Isotropic e-ph coupling strength

$$\lambda(\omega_j) = \int_0^\infty d\omega \alpha^2 F(\omega) \frac{2\omega}{\omega_j^2 + \omega^2}$$

Isotropic Eliashberg spectral function

$$\begin{aligned} \alpha^2 F(\omega) = & \frac{1}{N_F} \sum_{nm\nu} \int \frac{d\mathbf{k}}{\Omega_{\text{BZ}}} \int \frac{d\mathbf{q}}{\Omega_{\text{BZ}}} |g_{mn\nu}(\mathbf{k}, \mathbf{q})|^2 \\ & \times \delta(\omega - \omega_{\mathbf{q}\nu}) \delta(\epsilon_{n\mathbf{k}} - \epsilon_F) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_F) \end{aligned}$$

What about the Coulomb Interaction?

Screened Coulomb interaction

$$V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} = \langle n\mathbf{k}, -n\mathbf{k} | W | m\mathbf{k}+\mathbf{q}, -m\mathbf{k}+\mathbf{q} \rangle$$



Giustino, Cohen, Louie, PRB 81, 115105 (2010);
Lambert and Giustino, PRB 88, 075117 (2013)

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$$\mu_c = N_F \langle \langle V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \rangle \rangle_{\text{FS}}$$

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W can be calculated within the random phase approximation

$$\mu_c = N_F \langle \langle V_{n\mathbf{k},m\mathbf{k}+\mathbf{q}} \rangle \rangle_{\text{FS}}$$

Morel-Anderson semiempirical pseudopotential

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

Migdal-Eliashberg Theory

- 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)

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

Density Functional Theory for Superconductors (SCDFT)

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↑
superconducting
gap function

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

Density Functional Theory for Superconductors (SCDFT)

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

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

↑
superconducting
gap function

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

Density Functional Theory for Superconductors (SCDFT)

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

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

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

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Density Functional Theory for Superconductors (SCDFT)

$\mathcal{Z}$ accounts for
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↑
superconducting
gap function

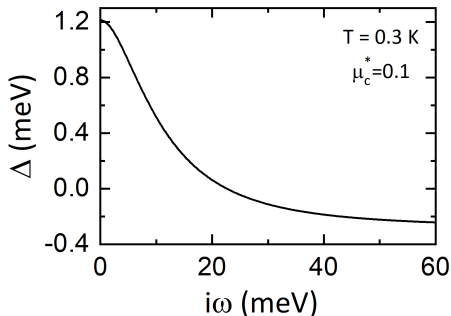
$$E_{n\mathbf{k}} = \sqrt{(\epsilon_{n\mathbf{k}} - \epsilon_{\text{F}})^2 + |\Delta_{n\mathbf{k}}|^2}$$

- 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

Examples from calculations and experiments

Supeconductivity in Pb

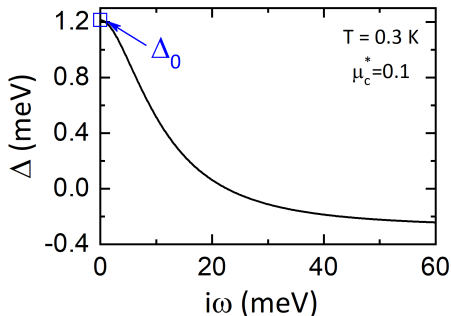
- Isotropic Migdal-Eliasbergh formalism (EPW)



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

Supeconductivity in Pb

- Isotropic Migdal-Eliasbergh formalism (EPW)

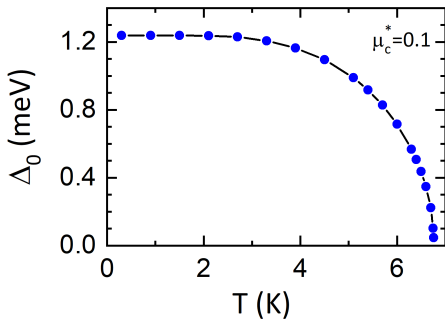
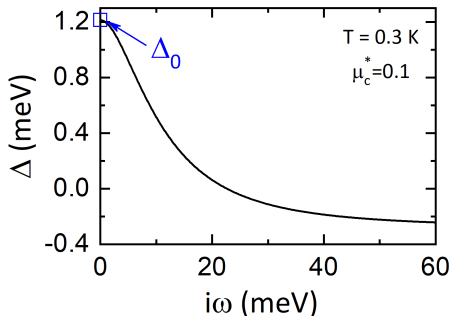


superconducting gap edge Δ_0
is defined as $\Delta_0 = \Delta(i\omega = 0)$

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

Supeconductivity in Pb

- Isotropic Migdal-Eliasbergh formalism (EPW)

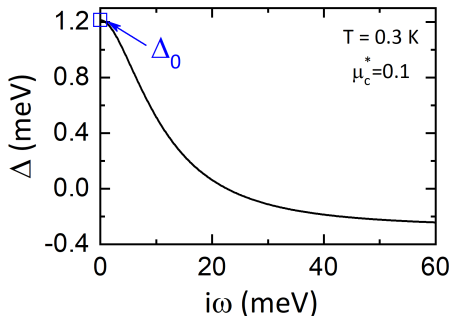


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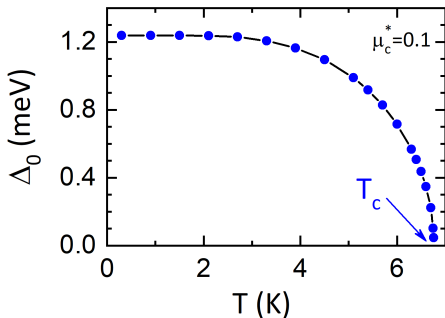
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Supeconductivity in Pb

- Isotropic Migdal-Eliasbergh formalism (EPW)



superconducting gap edge Δ_0
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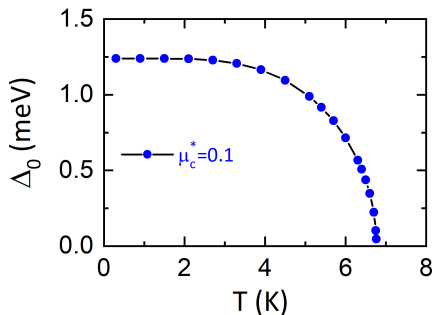


T_c is defined as the temperature
at which $\Delta_0 = 0$

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

Supecductivity in Pb

- Comparison between Migdal-Eliashberg and SCDFT formalism

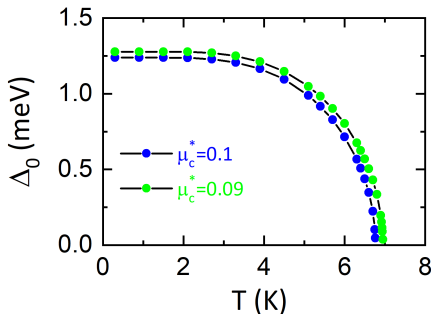


Right top and bottom figures from Marques et al, Phys. Rev. B 72, 024546 (2005) and

Floris et al, Phys. Rev. B 75, 054508 (2007)

Supeconductivity in Pb

- Comparison between Migdal-Eliashberg and SCDFT formalism

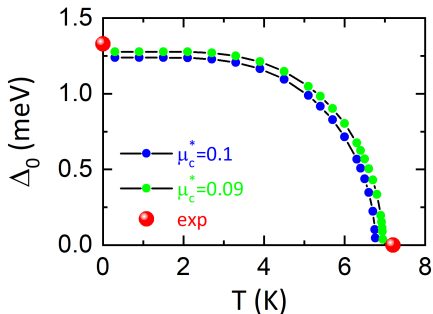


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Supeconductivity in Pb

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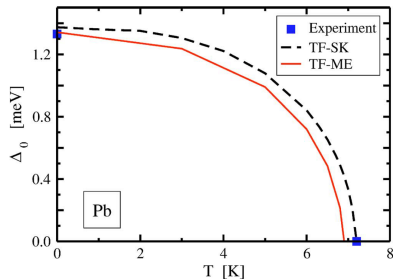
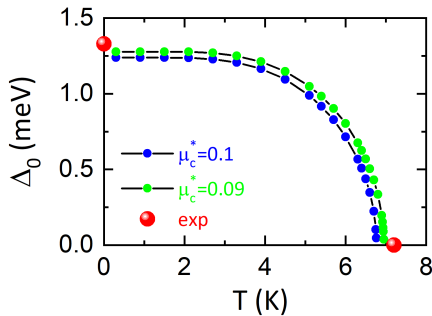


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Supeconductivity in Pb

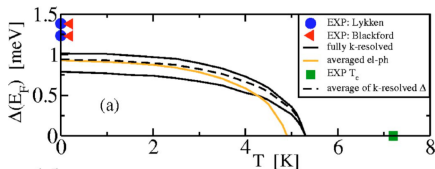
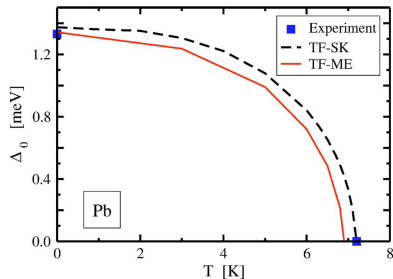
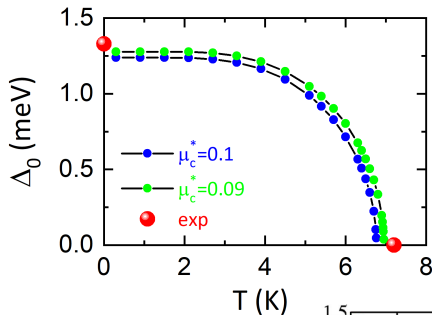
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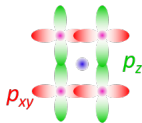
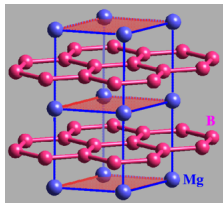
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Right top and bottom figures from Marques et al, Phys. Rev. B 72, 024546 (2005) and

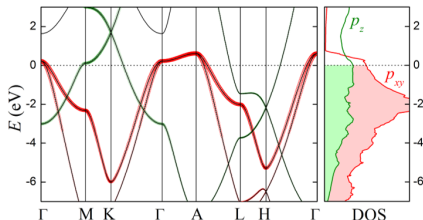
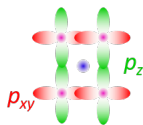
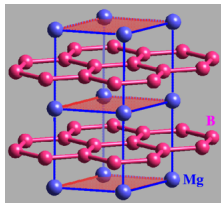
Floris et al, Phys. Rev. B 75, 054508 (2007)

Superconductivity in MgB_2



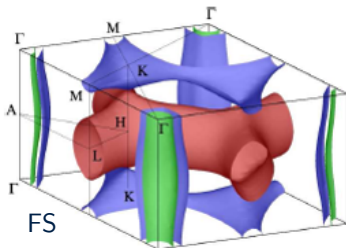
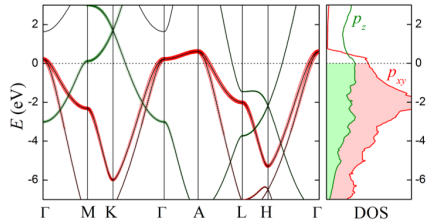
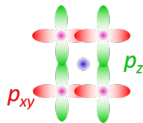
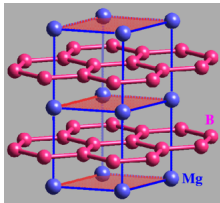
Bottom left and right figures from Kortus et al, Phys. Rev. Lett. 86, 4656 (2001) and Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Supeconductivity in MgB_2



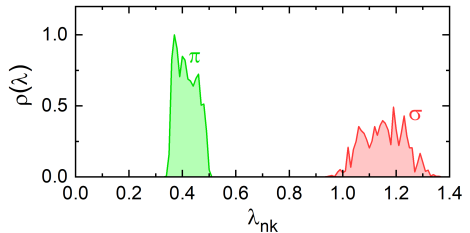
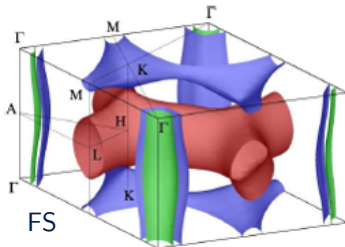
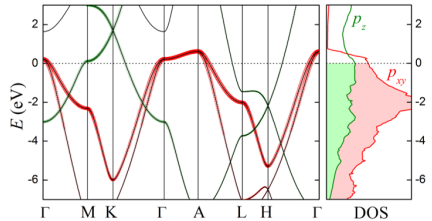
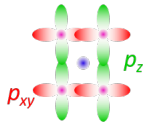
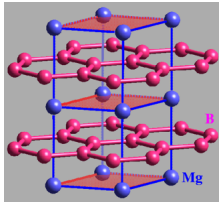
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Supeconductivity in MgB_2



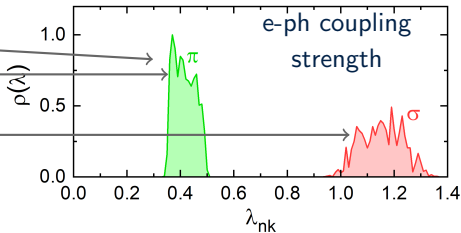
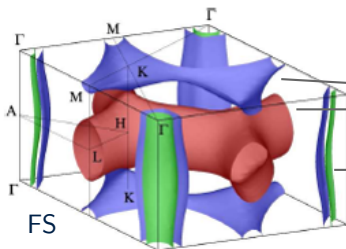
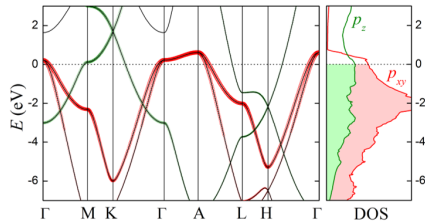
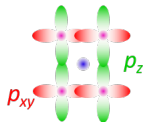
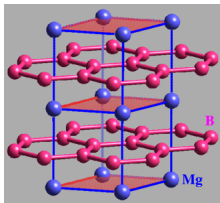
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Supeconductivity in MgB_2



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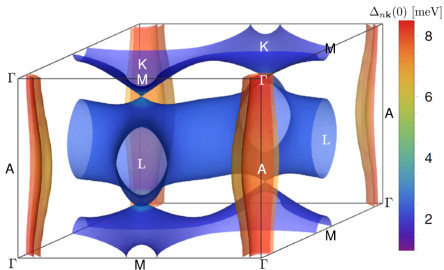
Supeconductivity in MgB_2



Bottom left and right figures from Kortus et al, Phys. Rev. Lett. 86, 4656 (2001) and Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Supeconductivity in MgB_2

- Anisotropic Migdal-Eliasbergh formalism (EPW)

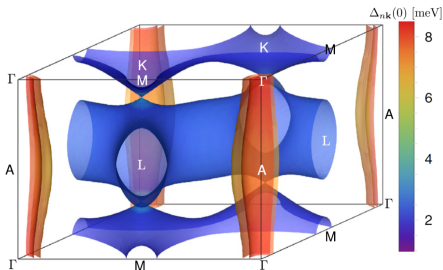


superconducting gap on FS

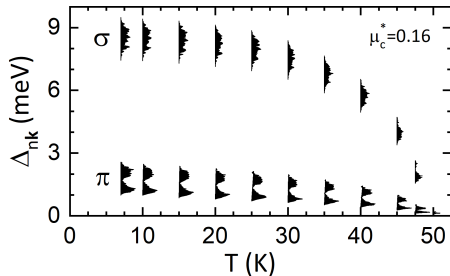
Left and right figures from Poncé et al, Comp. Phys. Commun. 209, 116 (2016) and Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Supeconductivity in MgB_2

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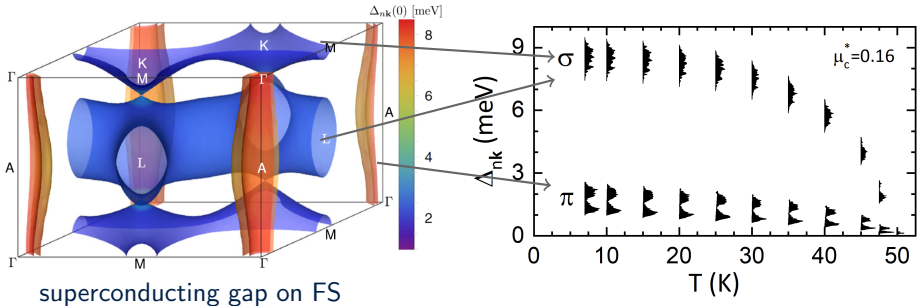
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Left and right figures from Poncé et al, Comp. Phys. Commun. 209, 116 (2016) and Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Supeconductivity in MgB_2

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Left and right figures from Poncé et al, Comp. Phys. Commun. 209, 116 (2016) and Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Supeconductivity in MgB_2

- SCDFT formalism

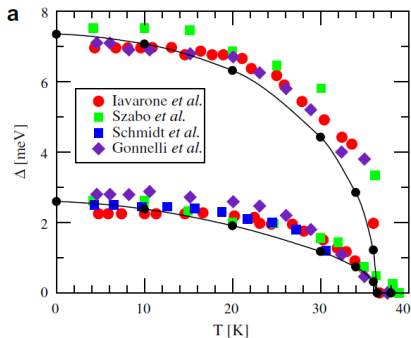
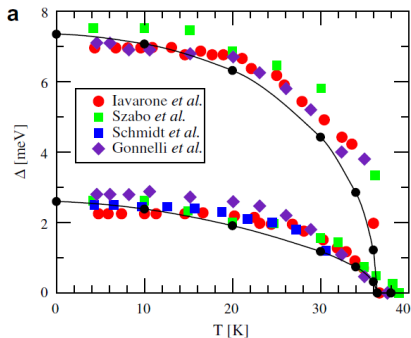


Figure and table from Floris *et al.*, Physics C 456, 45 (2007)

Supeconductivity in MgB_2

- SCDFT formalism



Summary of calculated T_c (K) and gaps (meV)

Coulomb e-e	$\alpha^2 F_{m'}(\omega)$			$\alpha^2 F(\omega)$		
	T_c	Δ_σ	Δ_π	T_c	Δ_σ	Δ_π
RPA	36.5	7.3	2.6	20.8	3.8	3.8
av-RPA	50.2	9.4	1.5	20.8		3.7
RPA-DIAG	30.0	5.9	2.2		—	
HL	34.1	6.8	2.5		—	
TF-ME	31.0	6.1	2.3		—	
exp	38.2	7.1	2.9		—	

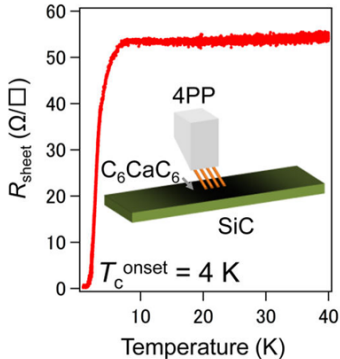
Coulomb e-e: RPA = RPA dielectric matrix with local fields (LF); RPA-DIAG = RPA diagonal dielectric matrix (no LF); HL = model dielectric matrix from Ref. [44] (with LF); TF-ME = Thomas-Fermi screening; av-RPA = average of RPA ME (Eq. (27)). Experimental values are taken from Ref. [24].

A fully anisotropic calculation gave $T_c = 22$ K.

Figure and table from Floris et al, Physics C 456, 45 (2007)

Superconductivity in C_6CaC_6

resistance vs temperature
in C_6CaC_6

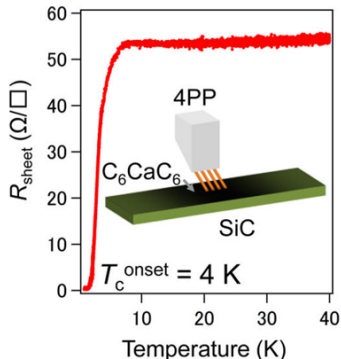


Left and right figures from Ichinokura et al, ACS Nano 10, 2761 (2016) and Chapman et al, Sci.

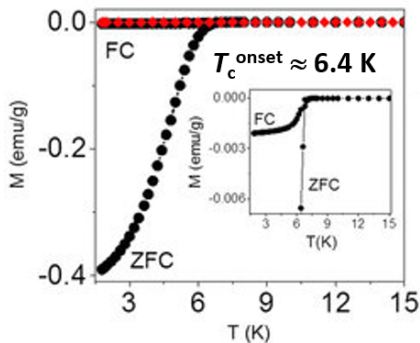
Rep. 6, 23254 (2016)

Superconductivity in C_6CaC_6

resistance vs temperature
in C_6CaC_6



magnetisation vs temperature
in Ca-doped graphite laminates



Left and right figures from Ichinokura et al, ACS Nano 10, 2761 (2016) and Chapman et al, Sci.

Rep. 6, 23254 (2016)

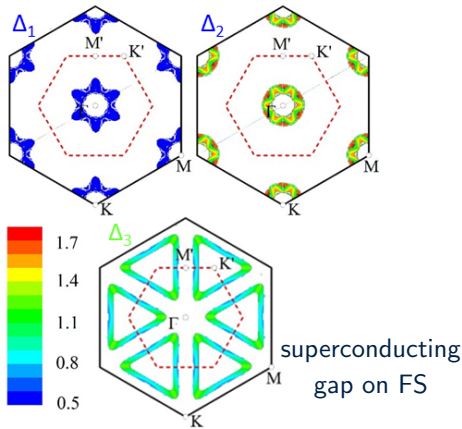
Supeconductivity in C_6CaC_6

- Anisotropic Migdal-Eliasbergh formalism with *ab initio* Coulomb pseudopotential $\mu_c^* = 0.155$ (EPW and SternheimerGW)

Figures adapted from Margine et al, Sci. Rep. 6, 21414 (2016)

Superconductivity in C_6CaC_6

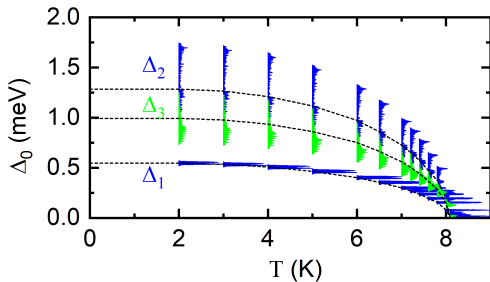
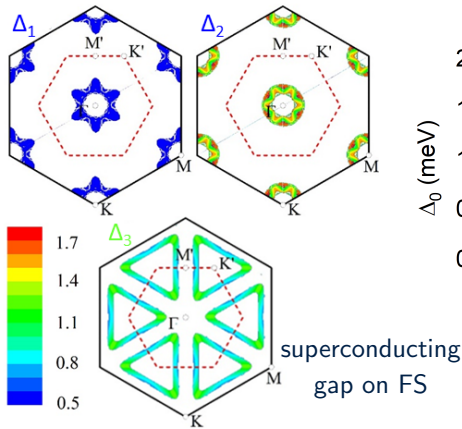
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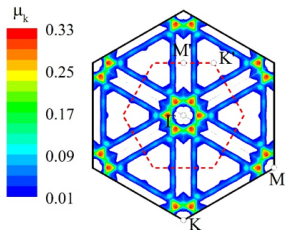
Superconductivity in C_6CaC_6

- Screened Coulomb interaction within the random phase approximation using the Sternheimer approach

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Superconductivity in C_6CaC_6

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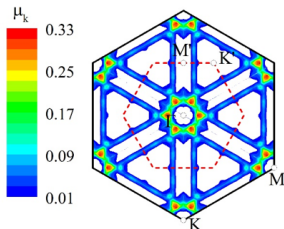
screened Coulomb interaction

$$\mu_c = N_F \langle \langle V_{n\mathbf{k}, m\mathbf{k}'} \rangle \rangle_{\text{FS}} \text{ on FS}$$

Figures adapted from Margine et al, Sci. Rep. 6, 21414 (2016)

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screened Coulomb interaction

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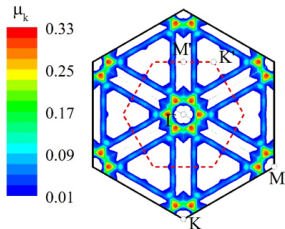
$$\mu_c = 0.254; \omega_{\text{el}} = 2.5 \text{ eV}; \omega_{\text{ph}} = 200 \text{ meV}$$

$$\mu_c^* = \mu_c / [1 + \mu_c \log(\omega_{\text{el}}/\omega_{\text{ph}})] = 0.155$$

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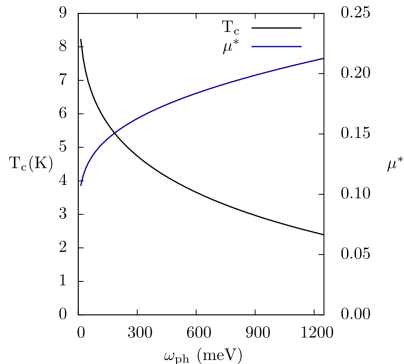


screened Coulomb interaction

$$\mu_c = N_F \langle \langle V_{n\mathbf{k}, m\mathbf{k}'} \rangle \rangle_{\text{FS}} \text{ on FS}$$

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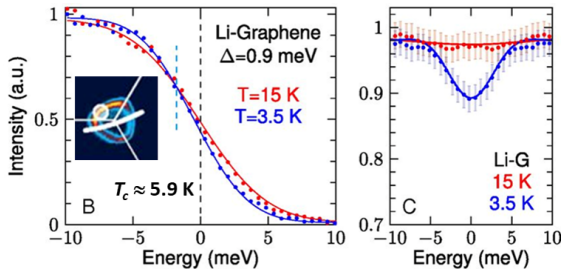
$$\mu_c^* = \mu_c / [1 + \mu_c \log(\omega_{\text{el}}/\omega_{\text{ph}})] = 0.155$$



Figures adapted from Margine et al, Sci. Rep. 6, 21414 (2016)

Supeconductivity in Li-decorated Monolayer Graphene

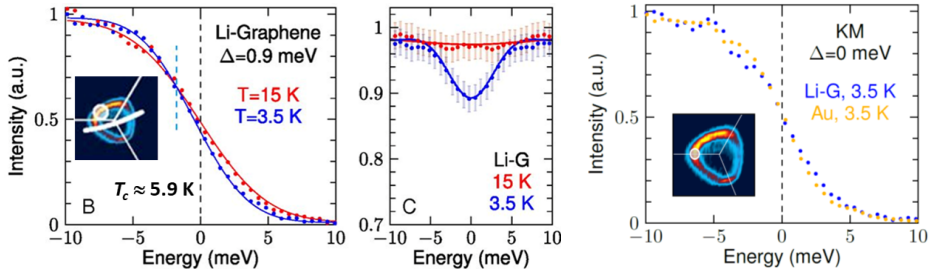
- Spectroscopic observation of a pairing gap in Li-decorated graphene



Figures from Ludbrook et al. PNAS 112, 11795 (2015)

Supeconductivity in Li-decorated Monolayer Graphene

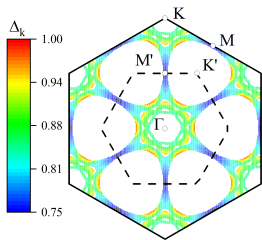
- Spectroscopic observation of a pairing gap in Li-decorated graphene



Figures from Ludbrook et al. PNAS 112, 11795 (2015)

Supeconductivity in Li-decorated Monolayer Graphene

- Anisotropic Migdal-Eliasbergh formalism (EPW)

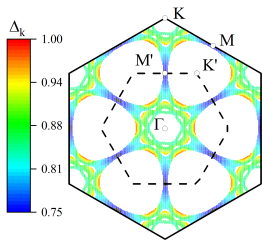


superconducting gap on FS

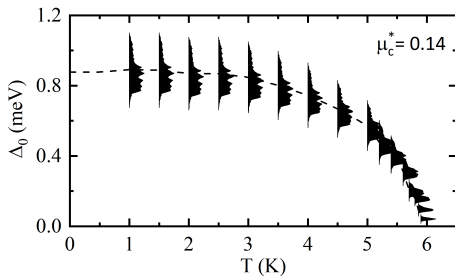
Figures adapted from Zheng and Margine, Phys. Rev. B 94, 064509 (2016)

Supeconductivity in Li-decorated Monolayer Graphene

- Anisotropic Migdal-Eliasbergh formalism (EPW)



superconducting gap on FS



Figures adapted from Zheng and Margine, Phys. Rev. B 94, 064509 (2016)

Take-home Messages

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

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