# 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

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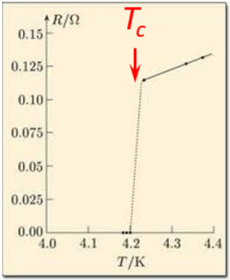
# Lecture Summary

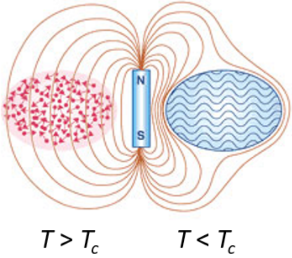
- BCS theory of superconductivity
- Allen-Dynes formula for critical temperature
- Density functional theory for superconductors
- Nambu-Gor'kov formalism
- Migdal-Eliashberg theory for superconductors

# 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

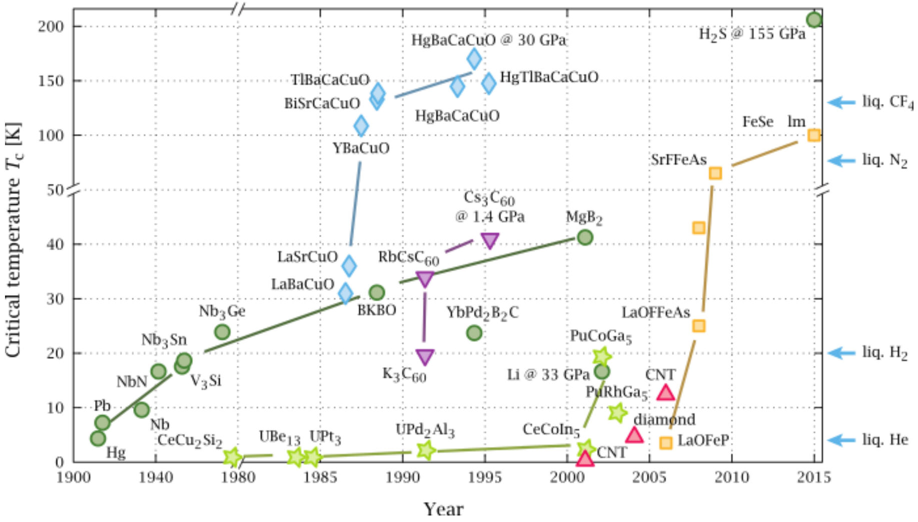
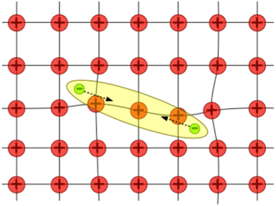


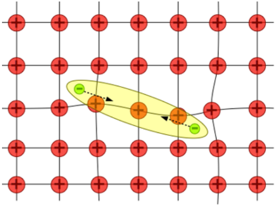

Figure from Wikipedia

# BCS Theory



electron Cooper
pairs in a lattice

# BCS Theory



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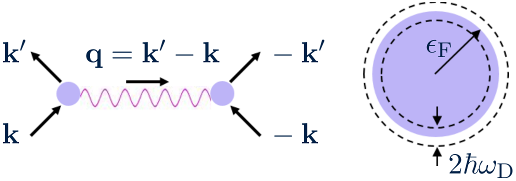
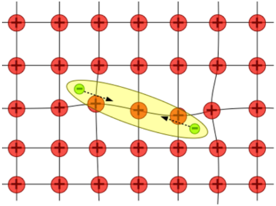



exchange of virtual phonons produces an attraction for electrons close to Fermi level



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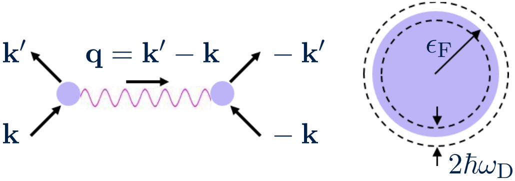


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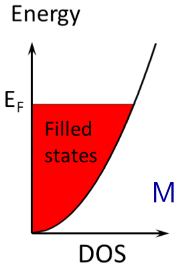
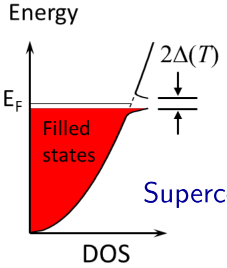



Metal




Superconductor

# BCS Theory

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

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

# BCS Theory

superconducting gap

$\downarrow$

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superconducting gap ↓ paring potential ↓

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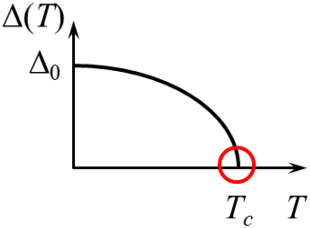

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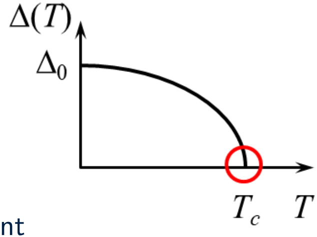


- describes in detail the phenomenology of superconductivity
- is a descriptive theory, material-independent $\rightarrow 2\Delta_0 = 3.53 k_{\rm B} T_{\rm c}$
- does not account for the retardation of the e-ph interaction

How can $T_c$ be calculated beyond BCS?

# Allen-Dynes Formula

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

# Allen-Dynes Formula

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

Coulomb pseudopotential

# Allen-Dynes Formula

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Coulomb pseudopotential ($\mu_c^*$)

e-ph coupling strength ($\lambda$)

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Coulomb pseudopotential ($\mu_c^*$)

e-ph coupling strength ($\lambda$)

- can be easily calculated (e.g., Quantum Espresso)
- works reasonably well for isotropic superconductors
- requires dense $\mathbf{k}$- and $\mathbf{q}$-meshes to converge $\lambda$
- fails for multiband and/or anisotropic superconductors
- approximates the Coulomb interaction through $\mu_c^*$

# Density Functional Theory for Superconductors (SCDFT)

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

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↑ superconducting gap function

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# Density Functional Theory for Superconductors (SCDFT)

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

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superconducting gap function

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

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

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superconducting gap function

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

- 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

# Migdal-Eliashberg Theory

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

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

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

paring self-energy

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

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

# Migdal-Eliashberg Theory

dressed phonon propagator

paring self-energy

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e-ph matrix elements

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e-ph matrix elements

interacting Green's function

# Migdal-Eliashberg Theory

paring self-energy

dressed phonon propagator

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

screened Coulomb interaction

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

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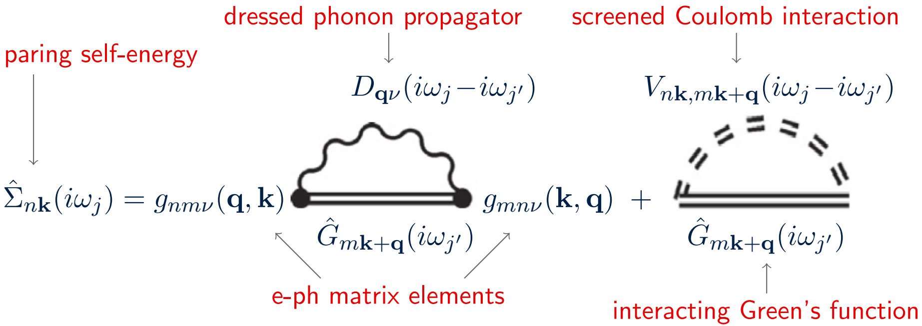


- has predictive power, material-dependent
- accounts for the retardation of the e-ph interaction
- works for multiband and/or anisotropic superconductors
- generally approximates the Coulomb interaction through $\mu_c^*$
- requires dense $\mathbf{k}$- and $\mathbf{q}$-meshes

# Nambu-Gor'kov Formalism

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

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

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imaginary time — Wick's time-ordering operator

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two-component field operator

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

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$\hat{G}_{n\mathbf{k}}(\tau)$ is periodic in the imaginary time $\tau$ 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 electronic Matsubara frequencies and $T$ is the temperature.

$$\hat{G}_{n\mathbf{k}}(i\omega_j) = \left[ \begin{array}{cc} G_{n\mathbf{k}}(i\omega_j) & F_{n\mathbf{k}}(i\omega_j) \\ F^*_{n\mathbf{k}}(i\omega_j) & -G_{-n\mathbf{k}}(-i\omega_j) \end{array} \right]$$

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- 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 (become non-zero below $T_{\rm c}$, marking the transition to the superconducting state).

# Nambu-Gor'kov Formalism

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

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

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non-interacting Green's function

$$\downarrow$$

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

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

mass renormalization function — energy shift — superconducting gap function

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mass renormalization function — energy shift — superconducting gap function

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

# Migdal-Eliashberg Approximation

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

# Migdal-Eliashberg Approximation

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

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

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

# Migdal-Eliashberg Approximation

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

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

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

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

# Migdal-Eliashberg Approximation

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

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

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

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

Migdal's theorem

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

The neglected terms are of the order of $(m_{\rm e}/M)^{1/2} \propto \omega_{\rm D}/\epsilon_{\rm F}$.

# Migdal-Eliashberg Approximation

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

# Migdal-Eliashberg Approximation

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

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

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

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

$$\hat{\tau}_3\hat{\tau}_0\hat{\tau}_3 = \hat{\tau}_0 \qquad \text{and} \qquad \hat{\tau}_3\hat{\tau}_1\hat{\tau}_3 = -\hat{\tau}_1$$

# Migdal-Eliashberg Approximation

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

# Migdal-Eliashberg Approximation

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

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# Migdal-Eliashberg Approximation

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$$\times\left\{i\omega_{j'}Z_{m\mathbf{k+q}}(i\omega_{j'})\hat{\tau}_0 + \left[(\epsilon_{m\mathbf{k+q}}-\epsilon_{\mathrm{F}}) + \chi_{m\mathbf{k+q}}(i\omega_{j'})\right]\hat{\tau}_3 - \Delta_{m\mathbf{k+q}}(i\omega_{j'})Z_{m\mathbf{k+q}}(i\omega_{j'})\hat{\tau}_1\right\}$$

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

# Migdal-Eliashberg Approximation

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

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

# Anisotropic Migdal-Eliashberg Equations

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

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

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

# 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

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

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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 $\omega_j$
- the electron density of states is assumed to be constant
- the dynamically screened Coulomb interaction $N_{\mathrm{F}} V_{n\mathbf{k},m\mathbf{k}'}$ is embedded into the semiempirical pseudopotential $\mu_{\mathrm{c}}^{*}$

# Anisotropic Migdal-Eliashberg Equations

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

mass renormalization function

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

superconducting gap function

# Anisotropic Migdal-Eliashberg Equations

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

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superconducting gap function

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

↑ anisotropic e-ph coupling strength

# Anisotropic Migdal-Eliashberg Equations

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

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superconducting gap function

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

↑ anisotropic e-ph coupling strength

↑ anisotropic Eliashberg spectral function

# 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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$W$ can be calculated within the random phase approximation in ⟨S⟩GW

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$W$ can be calculated within the random phase approximation in SternheimerGW

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

Giustino, Cohen, Louie, PRB 81, 115105 (2010);
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Screened Coulomb interaction

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

$W$ can be calculated within the random phase approximation in SGW

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

Morel-Anderson semiempirical pseudopotential

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

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# Anisotropic Migdal-Eliashberg Equations

$$
\begin{aligned}
Z_{n\mathbf{k}}(i\omega_j) \;&=\; 1 + \frac{\pi T}{\omega_j N_{\rm F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{\omega_{j'}}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
&\quad \times \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\rm F}) \\
Z_{n\mathbf{k}}(i\omega_j)\Delta_{n\mathbf{k}}(i\omega_j) \;&=\; \frac{\pi T}{N_{\rm F}} \sum_{mj'} \int \frac{d\mathbf{q}}{\Omega_{\rm BZ}} \frac{\Delta_{m\mathbf{k}+\mathbf{q}}(i\omega_{j'})}{\sqrt{\omega_{j'}^2 + \Delta_{m\mathbf{k}+\mathbf{q}}^2(i\omega_{j'})}} \\
&\quad \times \left[\lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j - \omega_{j'}) - \mu_{\rm c}^*\right] \delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\rm F})
\end{aligned}
$$

# Anisotropic Migdal-Eliashberg Equations

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

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

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- The equations must be evaluated on dense electron $\mathbf{k}$- and phonon $\mathbf{k}'$-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

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

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Isotropic e-ph coupling strength

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

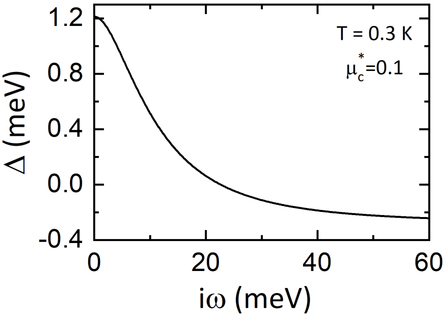
Isotropic Eliashberg spectral function

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

# 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)

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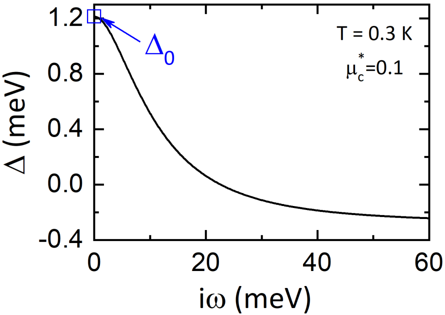


superconducting gap edge $\Delta_0$
is defined as $\Delta_0 = \Delta(i\omega = 0)$

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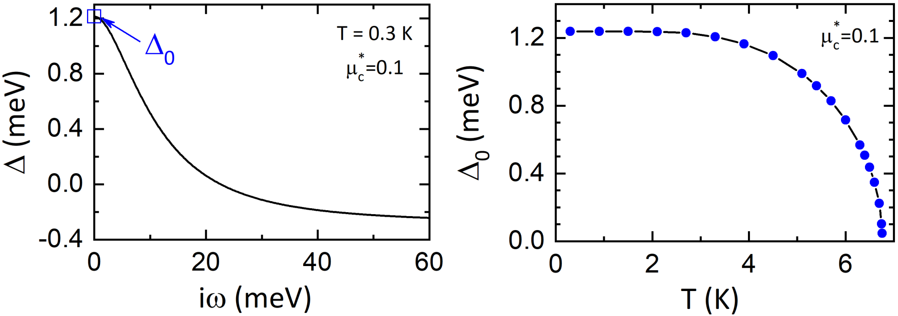


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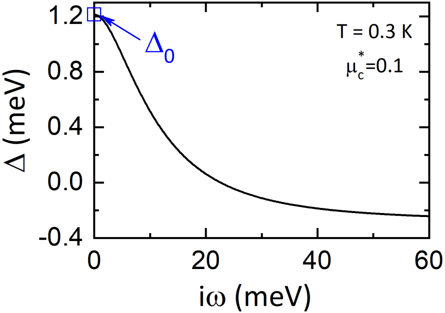
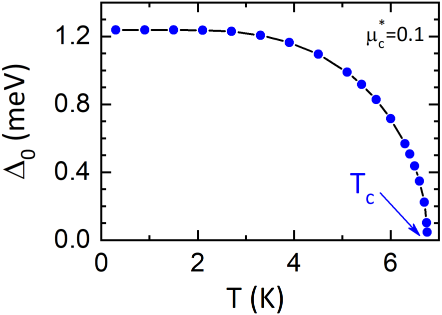


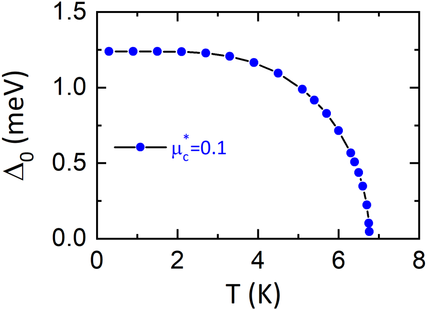

superconducting gap edge $\Delta_0$ is defined as $\Delta_0 = \Delta(i\omega = 0)$

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

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

# Supeconductivity 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)

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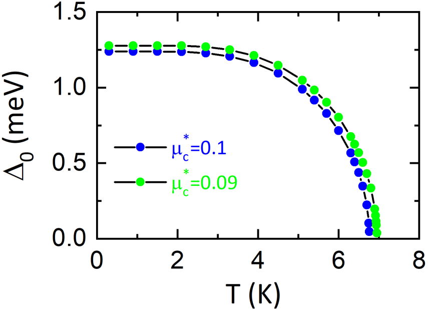


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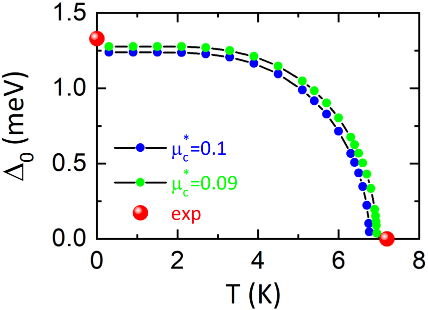


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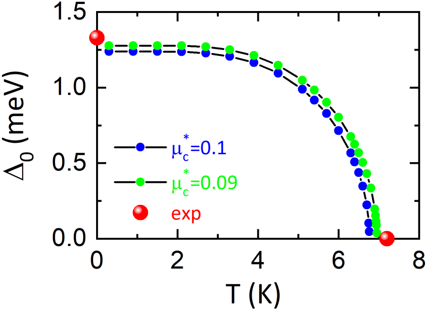


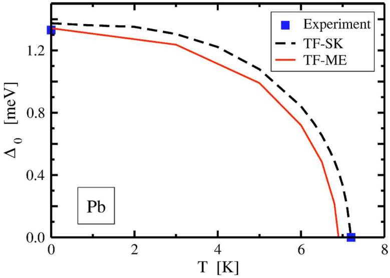


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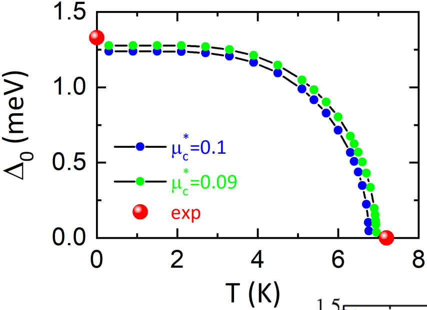


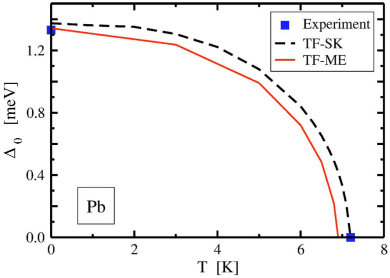


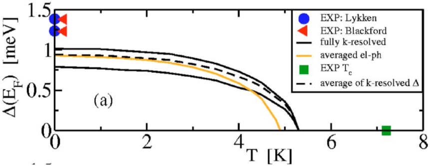


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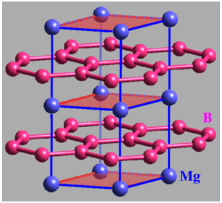


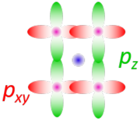


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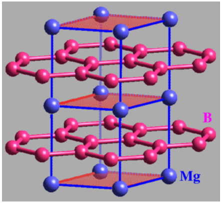


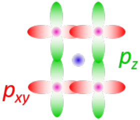


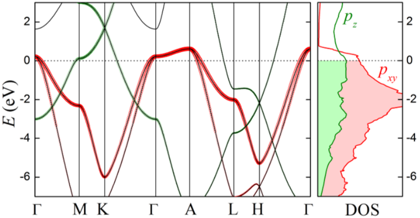


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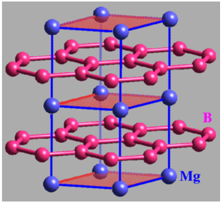


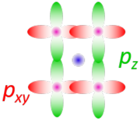


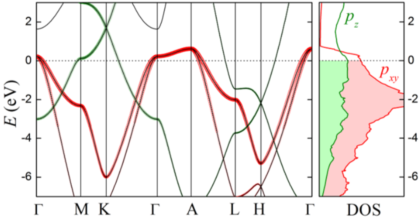


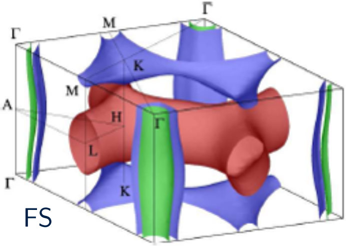


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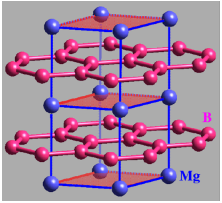


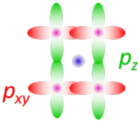


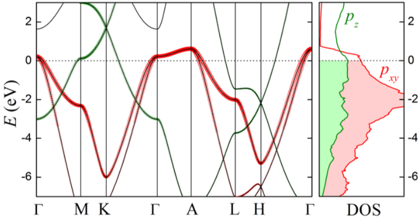


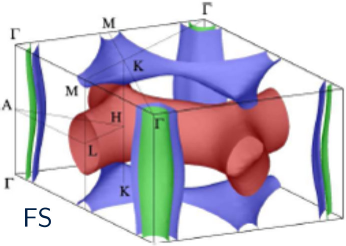


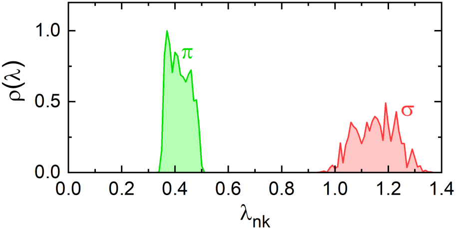


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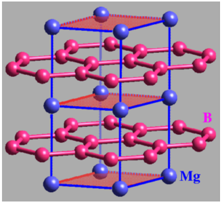
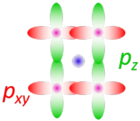
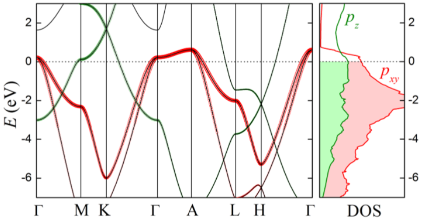
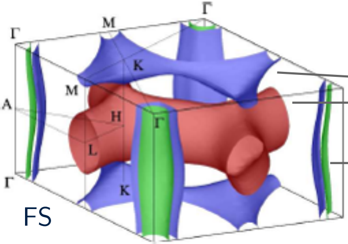
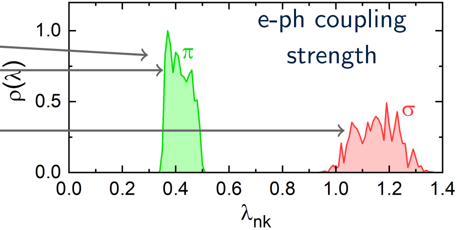
# Supeconductivity in $MgB_2$

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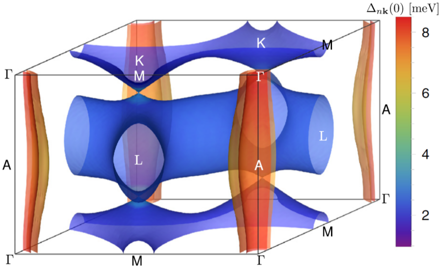
- Anisotropic Migdal-Eliasbergh formalism (EPW)




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)

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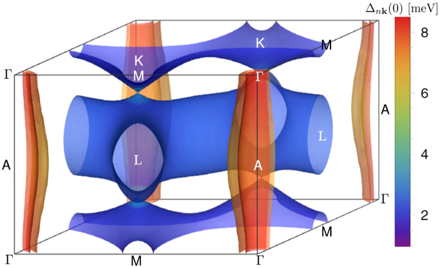


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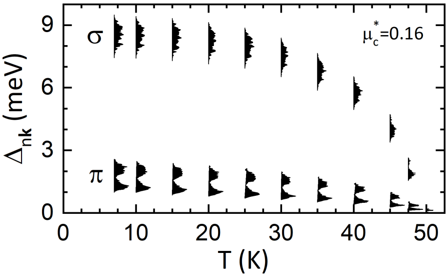


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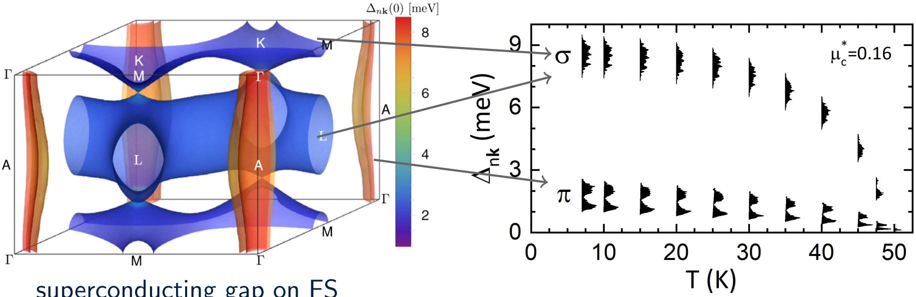


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# Supeconductivity in $MgB_2$

- SCDFT formalism

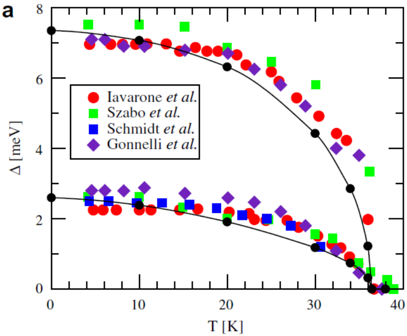
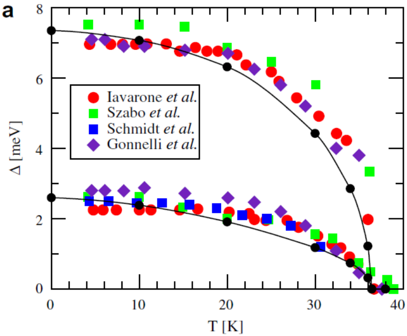



Figure and table from Floris et al, Physics C 456, 45 (2007)

# Supeconductivity in $MgB_2$

- SCDFT formalism




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

| Coulomb e–e | $\alpha^2F_{nn'}(\omega)$ | | | $\alpha^2F(\omega)$ | | |
|---|---|---|---|---|---|---|
| | $T_c$ | $\Delta_\sigma$ | $\Delta_\pi$ | $T_c$ | $\Delta_\sigma$ | $\Delta_\pi$ |
| 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 | | – | |

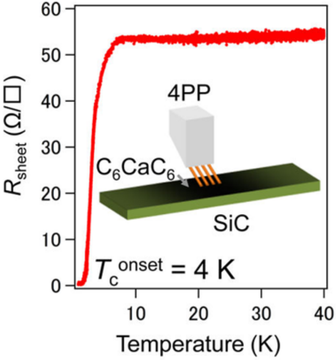
Coulomb e–e: RPA = RPA dielectric matrix with local fields (LF); RPA-DIAG = RPA diagonal dielectric matrix (no LF); HL = model dielectric matrix from Ref. [44] (with LF); TF-ME = Thomas–Fermi screening; av-RPA = average of RPA ME (Eq. (27)). Experimental values are taken from Ref. [24].

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

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

# Supeconductivity 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)

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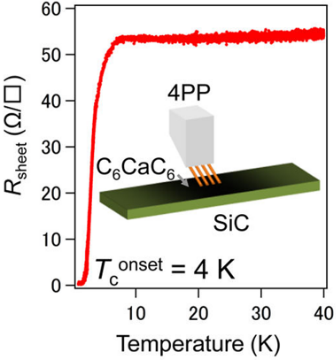
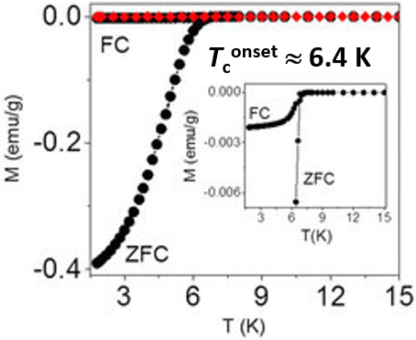
resistance vs temperature in $C_6CaC_6$




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)

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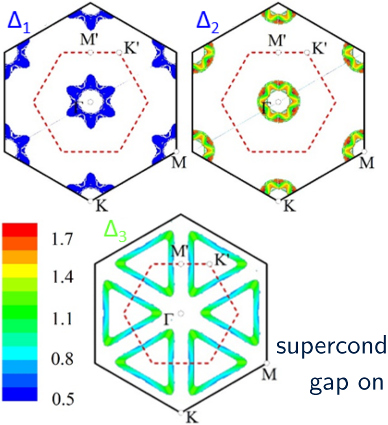


superconducting gap on FS

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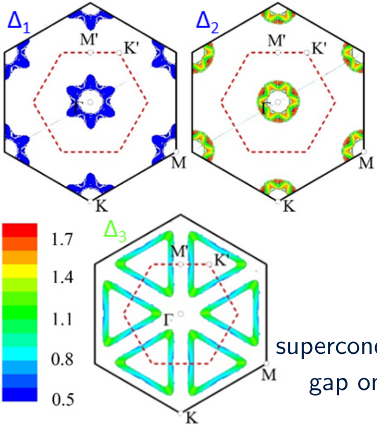


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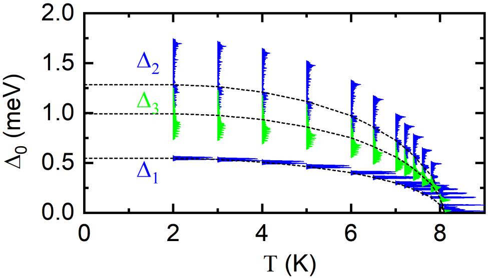


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• Screened Coulomb interaction within the random phase approximation using the Sternheimer approach

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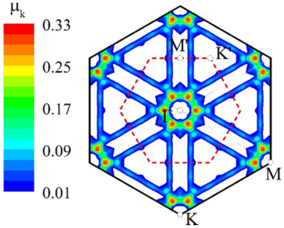


screened Coulomb interaction
$\mu_{\mathrm{c}} = N_{\mathrm{F}} \langle\langle V_{n\mathbf{k},m\mathbf{k}'} \rangle\rangle_{\mathrm{FS}}$ on FS

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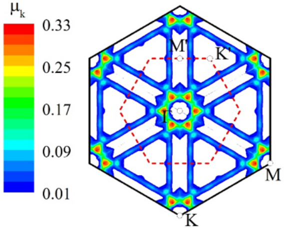


screened Coulomb interaction
$\mu_c = N_F \langle\langle V_{n\mathbf{k},m\mathbf{k}'} \rangle\rangle_{FS}$ on FS

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

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

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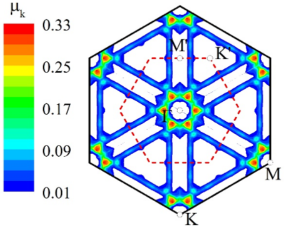


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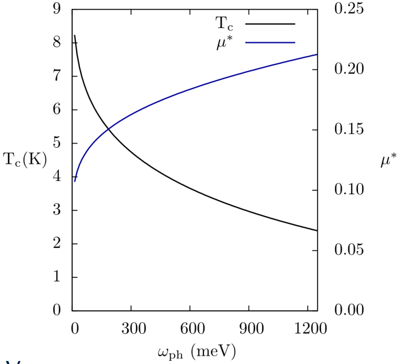


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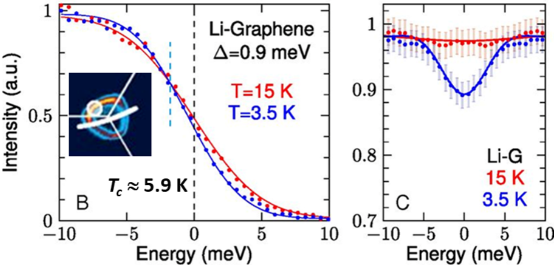
# Supeconductivity in Li-decorated Monolayer Graphene

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




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

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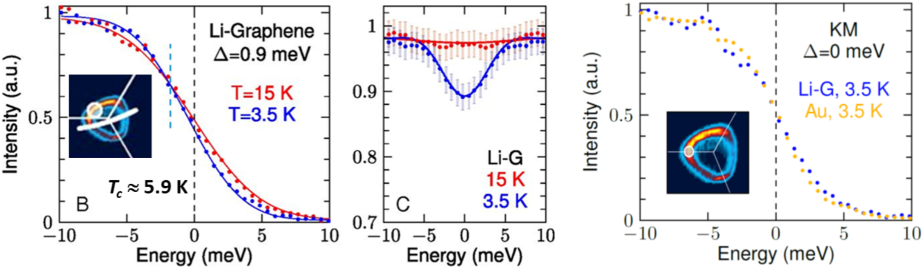


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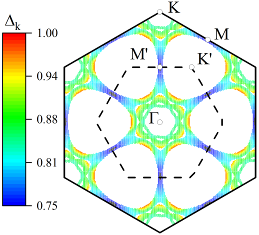
- Anisotropic Migdal-Eliasbergh formalism (EPW)

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

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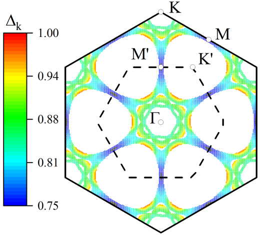


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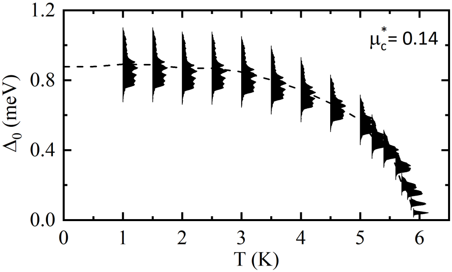


Figures adapted from Zheng and Margine, Phys. Rev. B 94, 064509 (2016)

# 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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