2022 Summer School on Electron-Phonon Physics from First Principles

Austin Texas

NSF

U.S. DEPARTMENT OF ENERGY

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TEXAS ADVANCED COMPUTING CENTER

ODEN

Intro to Hands-On Tutorial Wed.6

The superconducting module of EPW

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Binghamton University - State University of New York

Lecture Summary

- Input variables
- Output files
- Structure of the code
- Additional notes

Isotropic Migdal-Eliashberg Equations on the Imaginary Axis

```
eliashberg = .true.
liso = .true.
limag = .true.
```

mass renormalization function

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

superconducting gap function

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

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isotropic e-ph coupling strength

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

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$\boxed{|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2}$ $\rightarrow$ write e-ph matrix elements to file: `ephwrite = .true.`

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$\boxed{\int \frac{d\mathbf{k}}{\Omega_{BZ}}}$ $\rightarrow$ use crystal symmetry on fine $\mathbf{k}$ grid: `mp_mesh_k = .true.`

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$\int \frac{d\mathbf{k}}{\Omega_{BZ}}, \int \frac{d\mathbf{q}}{\Omega_{BZ}} \rightarrow$ consider $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ states within an energy window around ϵ_F: `fsthick = 0.4` eV

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$\delta(\epsilon_{n\mathbf{k}} - \epsilon_\mathrm{F}) \rightarrow$ use Gaussian smearing of width: `degaussw = 0.1`

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$\boxed{\mu_c^*} \rightarrow$ Coulomb parameter: `muc = 0.1`

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$\boxed{\mu_c^*} \rightarrow$ Coulomb parameter: `muc = 0.1`

$\boxed{\sum_{j'}} \rightarrow$ upper limit over Matsubara frequency summation: `wscut = 0.1`

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

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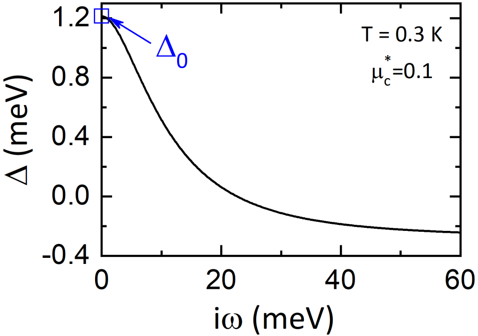
$\boxed{\mu_c^*}$ → Coulomb parameter: `muc = 0.1`

$\boxed{\sum_{j'}}$ → upper limit over Matsubara frequency summation: `wscut = 0.1`

$\boxed{T}$ → temperatures at which the Migdal-Eliashberg equations are solved: `temps = 1.0 2.0`

Isotropic case in Pb



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

liso = .true. and limag = .true.

```
! XX = temperature
prefix.imag_iso_gap0_XX
```

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

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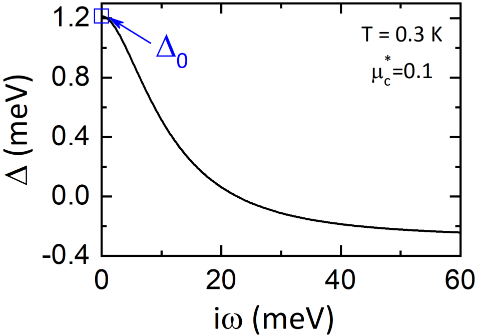

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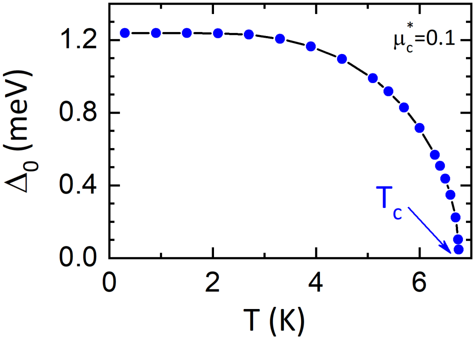

T_c is defined as the temperature at which $\Delta_0 = 0$

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

Linearized Isotropic Migdal-Eliashberg Equations on the Imaginary Axis

Isotropic case in Pb

```
tc_linear = .true.
tc_linear_solver = power
```

Near T_c, $\Delta(i\omega_j) \to 0$ and the system of equations reduces to a linear matrix equation for $\Delta(i\omega_j)$:

$$\Delta(i\omega_j) = \sum_{j'} \frac{1}{|2j'+1|}[\lambda(\omega_j - \omega_{j'}) - \mu_c^* - \delta_{jj'} \sum_{j''} \lambda(\omega_j - \omega_{j''}) s_j s_{j''}] \Delta(i\omega_{j'})$$

where $s_j = sign(\omega_j)$

`liso = .true.` and `limag = .true.`

```
! XX = temperature
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```

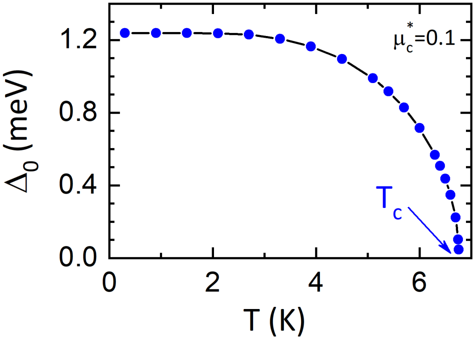

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Isotropic case in Pb

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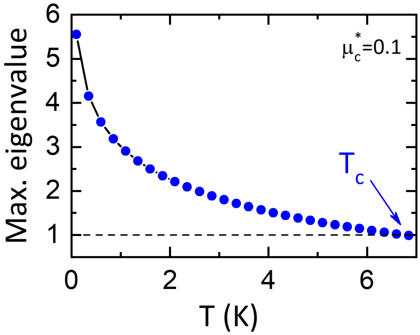

T_c is defined as the value at which the maximum eigenvalue is close to 1

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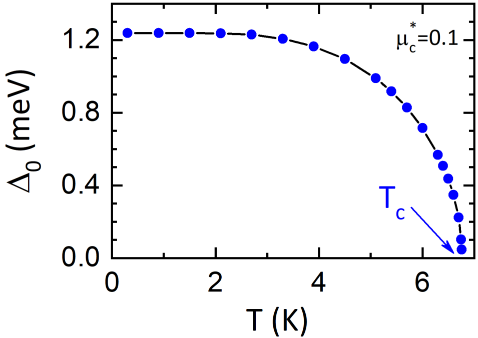
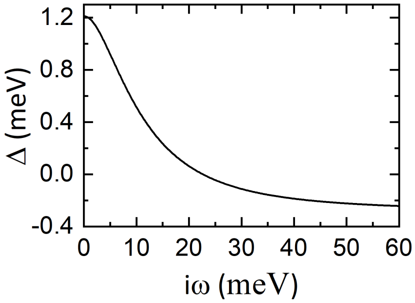


T_c is defined as the temperature at which $\Delta_0 = 0$

Analytic Continuation from Imaginary to Real Axis



`lpade = .true.` and `lacon = .true.`

```
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prefix.pade_iso_XX
prefix.acon_iso_XX
```
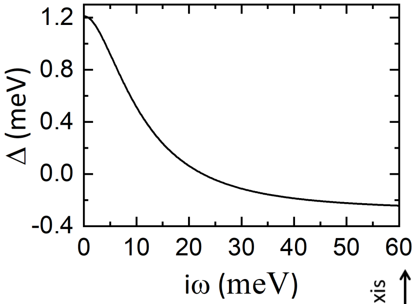

Isotropic case in Pb

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



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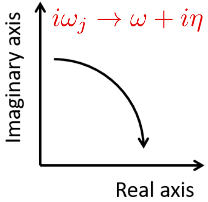
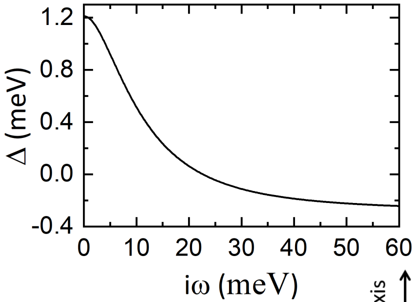


$i\omega_j \to \omega + i\eta$

Isotropic case in Pb

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

Analytic Continuation from Imaginary to Real Axis



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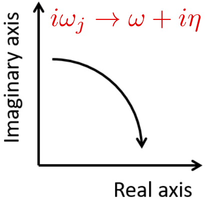

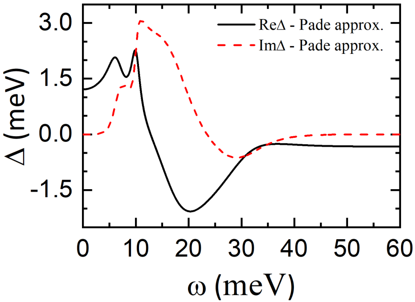

Isotropic case in Pb

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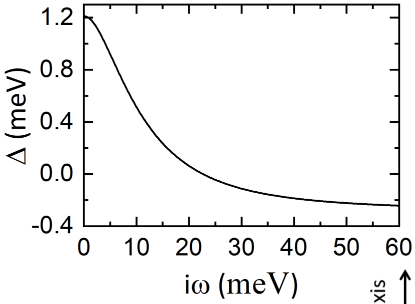

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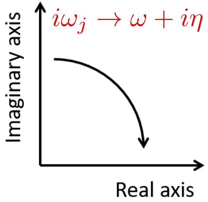

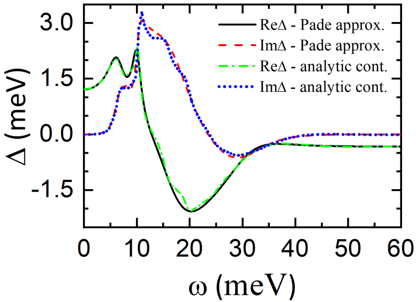

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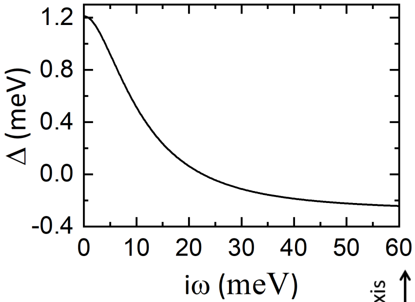

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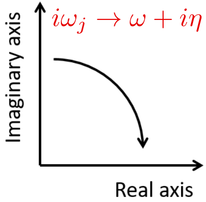
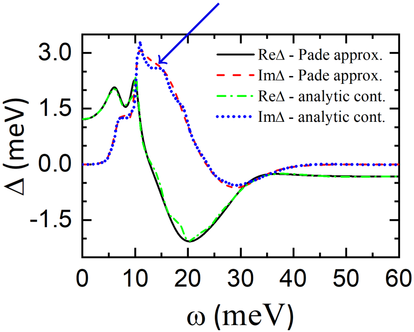


structure in the real axis solutions on the scale of the phonon energy



Isotropic case in Pb

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

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FSR

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

mass renormalization function

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

superconducting gap function

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superconducting gap function

anisotropic e-ph coupling strength

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

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```

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FSR

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

mass renormalization function

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

superconducting gap function

anisotropic e-ph coupling strength

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

$\boxed{|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2}$ $\rightarrow$ write e-ph matrix elements to file: `ephwrite = .true.`

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FSR

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

mass renormalization function

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

superconducting gap function

anisotropic e-ph coupling strength

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

$|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$ $\rightarrow$ write e-ph matrix elements to file: `ephwrite = .true.`

$\int \frac{d\mathbf{k}}{\Omega_\mathrm{BZ}}$ $\rightarrow$ use crystal symmetry on fine $\mathbf{k}$ grid: `mp_mesh_k = .true.`

$\int \frac{d\mathbf{k}}{\Omega_\mathrm{BZ}}, \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}}$ $\rightarrow$ consider $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ states within an energy window around ϵ_F: `fsthick = 0.4` eV

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FSR

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

mass renormalization function

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

superconducting gap function

anisotropic e-ph coupling strength

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FSR

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

mass renormalization function

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

superconducting gap function

anisotropic e-ph coupling strength

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

μ_c^* → Coulomb parameter: `muc = 0.1`

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

mass renormalization function

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

superconducting gap function

anisotropic e-ph coupling strength

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

$\boxed{\mu_\mathrm{c}^*}$ → Coulomb parameter: `muc = 0.1`

$\boxed{\sum_{j'}}$ → upper limit over Matsubara frequency summation: `wscut = 0.1`

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FSR

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

mass renormalization function

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

superconducting gap function

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

anisotropic e-ph coupling strength

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

$\boxed{\mu_\mathrm{c}^*}$ $\rightarrow$ Coulomb parameter: `muc = 0.1`

$\boxed{\sum_{j'}}$ $\rightarrow$ upper limit over Matsubara frequency summation: `wscut = 0.1`

$\boxed{T}$ $\rightarrow$ temperatures at which the Migdal-Eliashberg equations are solved: `temps = 1.0 2.0`

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

mass renormalization function

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

superconducting gap function

anisotropic e-ph coupling strength

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
```

- $\boxed{\mu_\mathrm{c}^*}$ → Coulomb parameter: `muc = 0.1`
- $\boxed{\sum_{j'}}$ → upper limit over Matsubara frequency summation: `wscut = 0.1`
- $\boxed{T}$ → temperatures at which the Migdal-Eliashberg equations are solved: `temps = 1.0 2.0`
- $\boxed{\delta(\epsilon_{n\mathbf{k}} - \epsilon_\mathrm{F})}$ → use Gaussian smearing of width: `degaussw = 0.1`

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FBW

mass renormalization function

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

energy shift

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

superconducting gap function

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
fbw = .true.
```

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FBW

mass renormalization function

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

energy shift

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

superconducting gap function

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

electron number

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
fbw = .true.
muchem = .true.
```

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis: FBW

mass renormalization function

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

energy shift

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

superconducting gap function

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

electron number

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

```
eliashberg = .true.
laniso = .true.
limag = .true.
fbw = .true.
muchem = .true.
```

$\boxed{\mu_\mathrm{c}^*}$ $\rightarrow$ Coulomb parameter: `muc = 0.1`

$\boxed{\sum_{j'}}$ $\rightarrow$ upper limit over Matsubara frequency summation: `wscut = 0.1`

$\boxed{T}$ $\rightarrow$ temperatures at which the Migdal-Eliashberg equations are solved: `temps = 1.0 2.0` eliashberg = .true.

```
prefix.lambda_pairs ! (iverbosity = 2)
prefix.lambda_k_pairs
prefix.a2f
```

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

$$\lambda_{n\mathbf{k}}(\omega_j) = \sum_m \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_\mathrm{F})}{N_\mathrm{F}} \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j)$$

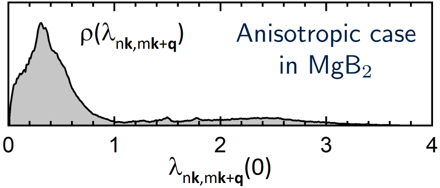
$$\lambda(\omega_j) = \sum_n \int \frac{d\mathbf{k}}{\Omega_\mathrm{BZ}} \frac{\delta(\epsilon_{n\mathbf{k}} - \epsilon_\mathrm{F})}{N_\mathrm{F}} \lambda_{n\mathbf{k}}(\omega_j)$$

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

Isotropic and Anisotropic Electron-Phonon Coupling Strength

eliashberg = .true.

```
prefix.lambda_pairs ! (iverbosity = 2)
prefix.lambda_k_pairs
prefix.a2f
```



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

$$\lambda_{n\mathbf{k}}(\omega_j) = \sum_m \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\delta(\epsilon_{m\mathbf{k}+\mathbf{q}} - \epsilon_{\mathrm{F}})}{N_{\mathrm{F}}} \lambda_{n\mathbf{k},m\mathbf{k}+\mathbf{q}}(\omega_j)$$

$$\lambda(\omega_j) = \sum_n \int \frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}} \frac{\delta(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})}{N_{\mathrm{F}}} \lambda_{n\mathbf{k}}(\omega_j)$$

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

eliashberg = .true.

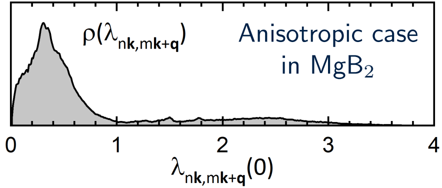
```
prefix.lambda_pairs ! (iverbosity = 2)
prefix.lambda_k_pairs
prefix.a2f
```

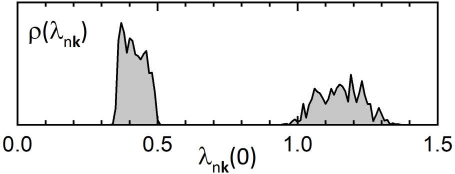
$$\lambda_{n\mathbf{k},m\mathbf{k+q}}(\omega_j) = N_{\mathrm{F}} \sum_{\nu} \frac{2\omega_{\mathbf{q}\nu}}{\omega_j^2 + \omega_{\mathbf{q}\nu}^2} |g_{mn\nu}(\mathbf{k},\mathbf{q})|^2$$

$$\lambda_{n\mathbf{k}}(\omega_j) = \sum_{m} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} \frac{\delta(\epsilon_{m\mathbf{k+q}} - \epsilon_{\mathrm{F}})}{N_{\mathrm{F}}} \lambda_{n\mathbf{k},m\mathbf{k+q}}(\omega_j)$$

$$\lambda(\omega_j) = \sum_{n} \int \frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}} \frac{\delta(\epsilon_{n\mathbf{k}} - \epsilon_{\mathrm{F}})}{N_{\mathrm{F}}} \lambda_{n\mathbf{k}}(\omega_j)$$

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





Isotropic and Anisotropic Electron-Phonon Coupling Strength

```
eliashberg = .true.
```

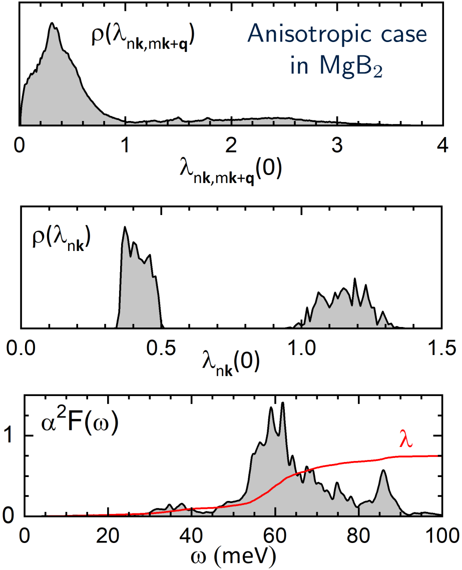
```
prefix.lambda_pairs ! (iverbosity = 2)
prefix.lambda_k_pairs
prefix.a2f
```

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

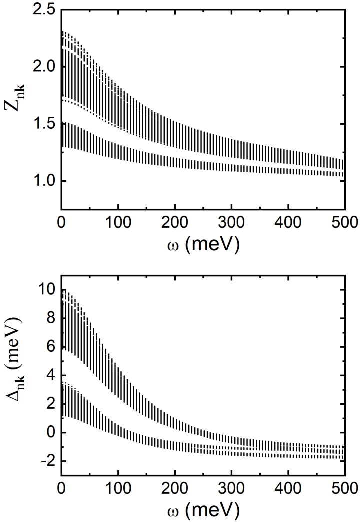
$$\lambda_{n\mathbf{k}}(\omega_j) = \sum_m \int \frac{d\mathbf{q}}{\Omega_\mathrm{BZ}} \frac{\delta(\epsilon_{m\mathbf{k+q}} - \epsilon_\mathrm{F})}{N_\mathrm{F}} \lambda_{n\mathbf{k},m\mathbf{k+q}}(\omega_j)$$

$$\lambda(\omega_j) = \sum_n \int \frac{d\mathbf{k}}{\Omega_\mathrm{BZ}} \frac{\delta(\epsilon_{n\mathbf{k}} - \epsilon_\mathrm{F})}{N_\mathrm{F}} \lambda_{n\mathbf{k}}(\omega_j)$$

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



Anisotropic Migdal-Eliashberg Equations



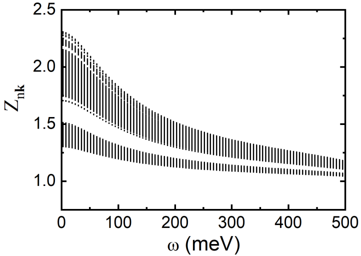
Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Anisotropic case in MgB_2

laniso = .true. and limag = .true.

```
! XX = temperature, YY = band index
prefix.imag_aniso_XX
prefix.imag_aniso_gap0_XX
prefix.imag_aniso_gap0_XX_YY.cube
```

Anisotropic Migdal-Eliashberg Equations



Anisotropic case in MgB_2

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prefix.imag_aniso_gap0_XX
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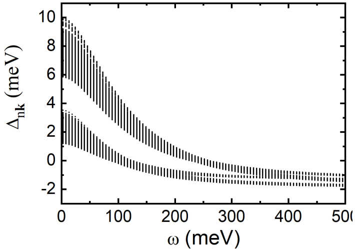

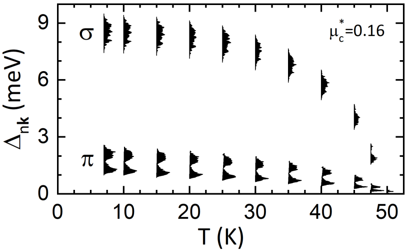

Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Anisotropic Migdal-Eliashberg Equations

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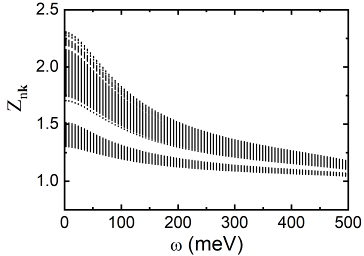
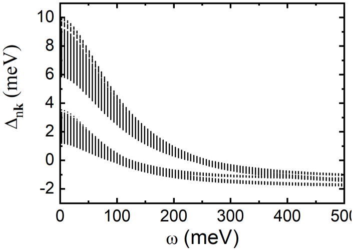
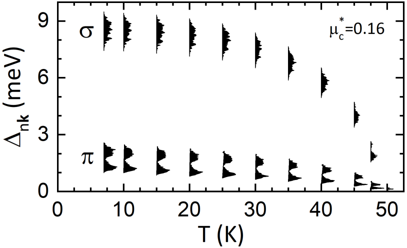
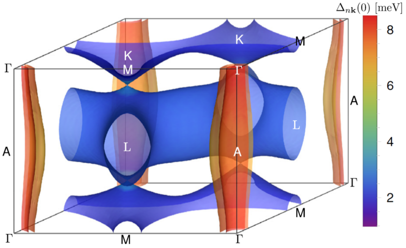




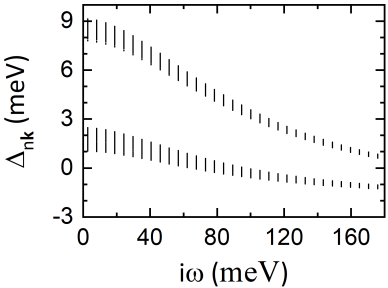




Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

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

Anisotropic Migdal-Eliashberg Equations



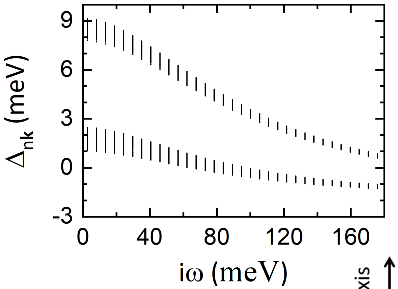

```
lpade = .true.
```

```
! XX = temperature
prefix.pade_aniso_gap0_XX
```

Anisotropic case in MgB_2

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

Anisotropic Migdal-Eliashberg Equations



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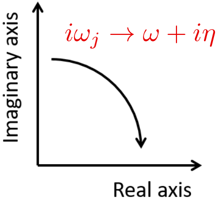


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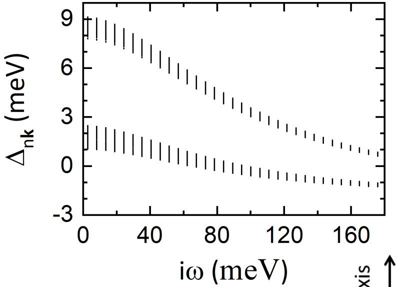
Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Anisotropic Migdal-Eliashberg Equations

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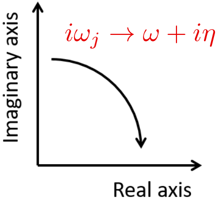
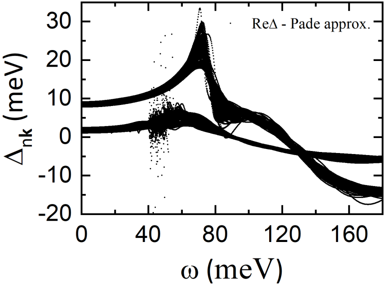
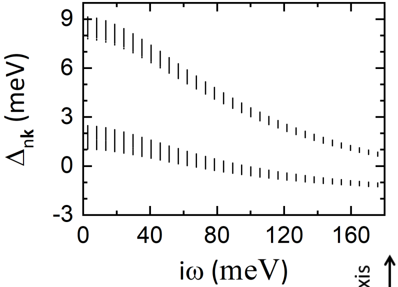




Anisotropic case in MgB_2

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

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lpade = .true.
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! XX = temperature
prefix.pade_aniso_gap0_XX
```
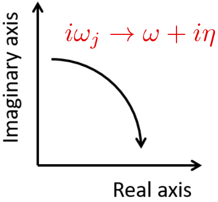
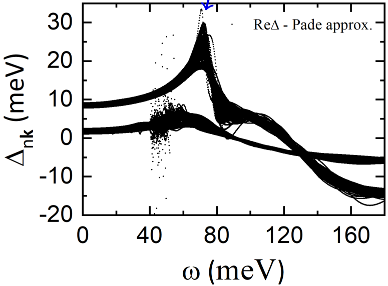

structure in the real axis solutions
on the scale of the phonon energy





Anisotropic case in MgB_2

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

Superconducting Quasiparticle Density of States

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

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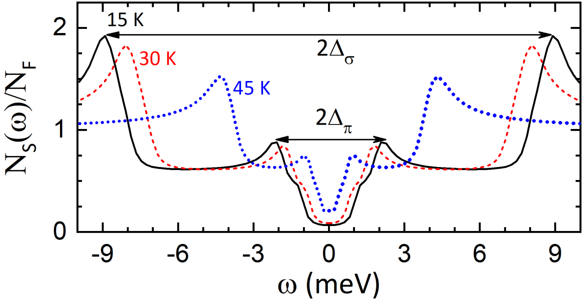

Anisotropic case in MgB_2

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

Superconductivity Calculations: Input Variables

```
mp_mesh_k = .true. ! irreducible k-points
nkf1 = 60
nkf2 = 60
nkf3 = 60
nqf1 = 20
nkf2 = 20
nkf3 = 20
```

The fine $\mathbf{k}$ and $\mathbf{q}$ grids need to be uniform and commensurate such that the $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ grid maps into the $\mathbf{k}$ grid.

Superconductivity Calculations: Input Variables

```
mp_mesh_k = .true. ! irreducible k-points
nkf1 = 60
nkf2 = 60
nkf3 = 60
nqf1 = 20
nkf2 = 20
nkf3 = 20

ephwrite = .true.
fsthick  = 0.4 ! eV Fermi window thickness
degaussw = 0.1 ! eV smearing

```

The fine $\mathbf{k}$ and $\mathbf{q}$ grids need to be uniform and commensurate such that the $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ grid maps into the $\mathbf{k}$ grid.

The ephmatXX (one per CPU), freq, egnv, and ikmap files are written in prefix.ephmat directory (used for solving the Migdal-Eliashberg equations).

Superconductivity Calculations: Input Variables

```
mp_mesh_k = .true. ! irreducible k-points
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nkf3 = 20

ephwrite = .true.
fsthick  = 0.4 ! eV Fermi window thickness
degaussw = 0.1 ! eV smearing

eliashberg = .true.
```

The fine $\mathbf{k}$ and $\mathbf{q}$ grids need to be uniform and commensurate such that the $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ grid maps into the $\mathbf{k}$ grid.

The ephmatXX (one per CPU), freq, egnv, and ikmap files are written in prefix.ephmat directory (used for solving the Migdal-Eliashberg equations).

Calculate isotropic and anisotropic e-ph coupling strength.

Superconductivity Calculations: Input Variables

```
mp_mesh_k = .true. ! irreducible k-points
nkf1 = 60
nkf2 = 60
nkf3 = 60
nqf1 = 20
nkf2 = 20
nkf3 = 20

ephwrite = .true.
fsthick  = 0.4 ! eV Fermi window thickness
degaussw = 0.1 ! eV smearing

eliashberg = .true.

laniso = .true.
limag  = .true.
lpade  = .true.

wscut   = 1.0  ! eV Matsubara cutoff freq.
muc     = 0.16 ! Coulomb parameter

temps   = 10.0 20.0 ! K

conv_thr_iaxis = 1.0d-4
nsiter = 100
```

The fine $\mathbf{k}$ and $\mathbf{q}$ grids need to be uniform and commensurate such that the $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ grid maps into the $\mathbf{k}$ grid.

The ephmatXX (one per CPU), freq, egnv, and ikmap files are written in prefix.ephmat directory (used for solving the Migdal-Eliashberg equations).

Calculate isotropic and anisotropic e-ph coupling strength.

Solve the anisotropic FSR ME eqs. on imaginary axis at specific temperatures and perform an analytic continuation to real axis with Padé approximants.

Superconductivity Calculations: Input Variables

```
mp_mesh_k = .true. ! irreducible k-points
nkf1 = 60
nkf2 = 60
nkf3 = 60
nqf1 = 20
nkf2 = 20
nkf3 = 20

ephwrite = .true.
fsthick  = 0.4 ! eV Fermi window thickness
degaussw = 0.1 ! eV smearing

eliashberg = .true.

laniso = .true.
limag  = .true.
lpade  = .true.

wscut  = 1.0  ! eV Matsubara cutoff freq.
muc    = 0.16 ! Coulomb parameter

temps  = 10.0 20.0 ! K

fbw    = .true.
```

The fine $\mathbf{k}$ and $\mathbf{q}$ grids need to be uniform and commensurate such that the $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ grid maps into the $\mathbf{k}$ grid.

The ephmatXX (one per CPU), freq, egnv, and ikmap files are written in prefix.ephmat directory (used for solving the Migdal-Eliashberg equations).

Calculate isotropic and anisotropic e-ph coupling strength.

Solve the anisotropic FBW ME eqs. with chemical potential fixed at the Fermi level on imaginary axis at specific temperatures and perform an analytic continuation to real axis with Padé approximants.

```
mp_mesh_k = .true. ! irreducible k-points
nkf1  = 60
nkf2  = 60
nkf3  = 60
nqf1  = 20
nkf2  = 20
nkf3  = 20

ephwrite = .true.
fsthick  = 0.4 ! eV Fermi window thickness
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eliashberg = .true.

laniso = .true.
limag  = .true.
lpade  = .true.

wscut    = 1.0  ! eV Matsubara cutoff freq.
muc      = 0.16 ! Coulomb parameter

temps    = 10.0 20.0 ! K

fbw      = .true.
muchem = .true.
```

The fine $\mathbf{k}$ and $\mathbf{q}$ grids need to be uniform and commensurate such that the $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ grid maps into the $\mathbf{k}$ grid.

The ephmatXX (one per CPU), freq, egnv, and ikmap files are written in prefix.ephmat directory (used for solving the Migdal-Eliashberg equations).

Calculate isotropic and anisotropic e-ph coupling strength.

Solve the anisotropic FBW ME eqs. with variable chemical potential on imaginary axis at specific temperatures and perform an analytic continuation to real axis with Padé approximants.

```
mp_mesh_k = .true. ! irreducible k-points
nkf1 = 60
nkf2 = 60
nkf3 = 60
nqf1 = 20
nkf2 = 20
nkf3 = 20

ephwrite = .true.
fsthick  = 0.4 ! eV Fermi window thickness
degaussw = 0.1 ! eV smearing
```

epw.f90 file:

```
CALL elphon_shuffle_wrap()
  --> CALL ephwann_shuffle(nqc, xqc)
        --> CALL write_ephmat(iqq, iq, totq)
```

Superconductivity Module in EPW: Workflow

```
mp_mesh_k = .true. ! irreducible k-points
nkf1  = 60
nkf2  = 60
nkf3  = 60
nqf1  = 20
nkf2  = 20
nkf3  = 20

ephwrite  = .true.
fsthick   = 0.4 ! eV Fermi window thickness
degaussw  = 0.1 ! eV smearing

eliashberg = .true.
```

epw.f90 file:

```
CALL elphon_shuffle_wrap()
  --> CALL ephwann_shuffle(nqc, xqc)
        --> CALL write_ephmat(iqq, iq, totq)
...
IF (eliashberg) THEN
  CALL eliashberg_eqs()
ENDIF
```

eliashberg.f90 file:

```
IF (.NOT. liso .AND. .NOT. laniso) THEN
  CALL eliashberg_init()
  CALL read_frequencies()
  CALL read_eigenvalues()
  CALL read_kqmap()
  CALL read_ephmat()
  CALL find_a2f()
    -->CALL evaluate_a2f_lambda()
  CALL read_a2f()
  CALL estimate_tc_gap()
ENDIF
```

```
mp_mesh_k = .true. ! irreducible k-points
nkf1 = 60
nkf2 = 60
nkf3 = 60
nqf1 = 20
nkf2 = 20
nkf3 = 20

ephwrite = .true.
fsthick  = 0.4 ! eV Fermi window thickness
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eliashberg = .true.

laniso = .true.
limag  = .true.
lpade  = .true.

wscut    = 1.0  ! eV Matsubara cutoff freq.
muc      = 0.16 ! Coulomb parameter

temps    = 10.0 20.0 ! K

conv_thr_iaxis = 1.0d-4
nsiter = 100
```

epw.f90 file:

```
CALL elphon_shuffle_wrap()
  --> CALL ephwann_shuffle(nqc, xqc)
        --> CALL write_ephmat(iqq, iq, totq)
...
IF (eliashberg) THEN
  CALL eliashberg_eqs()
ENDIF
```

eliashberg.f90 file:

```
IF (laniso) THEN
  CALL eliashberg_init()
  CALL read_frequencies()
  CALL read_eigenvalues()
  CALL read_kqmap()
  CALL read_ephmat()
  CALL find_a2f()
    -->CALL evaluate_a2f_lambda()
  CALL read_a2f()
  CALL estimate_tc_gap()
  IF (gap_edge > 0.d0) THEN
    gap0 = gap_edge
  ENDIF
  CALL eliashberg_aniso_iaxis()
ENDIF
```

Superconductivity Module in EPW: Output Files

eliashberg = .true.

```
prefix.a2f             ! Eliashberg spectral function as a function of frequency (meV) for
                       ! various smearings
prefix.a2f_proj        ! columns 1 and 2 same as .a2f; remaining columns contain the mode-
                       ! resolved Eliashberg spectral functions corresponding to 1st smearing
                       ! in .a2f (no specific information on atomic species)
prefix.lambda_k_pairs  ! \lambda_nk distribution on FS
prefix.lambda_FS       ! k-point Cartesian coords, n, E_nk-E_F[eV], \lambda_nk
prefix.phdos           ! Phonon DOS (same as .a2f)
prefix.phdos_proj      ! Phonon DOS (same as .a2f_proj)
```

eliashberg = .true. and iverbosity = 2

```
prefix.lambda_aniso    ! E_nk-E_F[eV], \lambda_nk, k, n
prefix.lambda_pairs    ! \lambda_nk,mk+q distribution on FS
prefix.lambda_YY.cube  ! Same as *.lambda_FS for VESTA; YY = band index within Fermi window
prefix.lambda.frmsf    ! Same as *.lambda_FS for FermiSurfer; all YY band indices
```

liso = .true., limag = .true., lpade = .true., and lacon = .true.

```
! XX = temperature
prefix.imag_iso_XX           ! w_j[eV], Z_nk, \Delta_nk[eV]
prefix.pade_iso_XX           ! Re[\Delta_nk(0)][eV] distribution on FS
prefix.acon_iso_XX           ! Re[\Delta_nk(0)][eV] distribution on FS
prefix.qdos_XX               ! Quasiparticle DOS in the superconducting state
```

Superconductivity Module in EPW: Output Files

laniso = .true., limag = .true., lpade = .true., and lacon = .true.

```
! XX = temperature
prefix.imag_aniso_XX         ! w_j[eV], E_nk-E_F[eV], Z_nk, \Delta_nk[eV]
prefix.imag_aniso_gap0_XX    ! \Delta_nk(0)[meV] distribution on FS
prefix.imag_aniso_gap_FS_XX  ! k-point Cartesian coords, band index within Fermi window,
                             ! E_nk- E_F[eV], \Delta_nk(0)[eV]
prefix.pade_aniso_gap0_XX    ! Re[\Delta_nk(0)][eV] distribution on FS
prefix.acon_aniso_gap0_XX    ! Re[\Delta_nk(0)][eV] distribution on FS
prefix.qdos_XX               ! Quasiparticle DOS in the superconducting state
```

laniso = .true., limag = .true., lpade = .true., lacon = .true., and iverbosity= 2

```
! XX = temperature, YY = band index within the Fermi window
prefix.imag_aniso_gap0_XX_YY.cube ! Same as prefix.imag_aniso_gap_FS_XX for VESTA plotting
prefix.imag_aniso_gap0_XX.frmsf ! Same as prefix.imag_aniso_gap_FS_XX for FermiSurfer plotting
prefix.pade_aniso_XX ! w[eV], E_nk-E_F[eV], RE[Z_nk], Im[Z_nk], Re[\Delta_nk][eV],
                     ! Im[\Delta_nk][eV]
prefix.acon_aniso_XX ! w[eV], E_nk-E_F[eV], RE[Z_nk], Im[Z_nk], Re[\Delta_nk][eV],
                     ! Im[\Delta_nk][eV]
```

Additional Notes

- `ephwrite` requires uniform fine **k** or **q** grids and `nkf1,nkf2,nkf3` to be multiple of `nqf1,nqf2,nqf3`
- `ephmatXX`, egnv, `freq`, and `ikmap` files need to be generated whenever **k** or **q** fine grid is changed
- `wscut` is ignored if the frequencies on the imaginary axis are given with `nswi`
- `laniso/liso` requires `eliashberg`
- `lpade` requires `limag`
- `lacon` requires `limag` and `lpade`
- `muchem` solve the anisotropic FBW ME eqs. with variable chemical potential.
- `gridsamp = 0` generates a uniform Matsubara frequency grid (default).
- `gridsamp = 1` generates a sparse Matsubara frequency grid.
- Allen-Dynes T_c can be used as a guide for defining the temperatures at which to evaluate the ME eqs.

Additional Notes

- `imag_read` requires `limag` and `laniso`
- `imag_read` allows the code to read from file the superconducting gap and renormalization function on the imaginary axis at specific temperature `XX` from file `.imag_aniso_XX`. The temperature is specified as `temps = XX` or `temps(1) = XX`.
- `imag_read` can be used to: (1) solve the anisotropic ME eqs. on the imag. axis at temperatures greater than `XX` starting from the superconducting gap estimated at temperature `XX`; (2) solve the anisotropic ME eqs. on the real axis with lpade or lacon starting from the imag axis solutions at temperature `XX`; (3) write to file the superconducting gap on the FS in cube format at temperature `XX` for `iverbosity = 2`.

References

- E. R. Margine and F. Giustino, Phys. Rev. B 87, 024505 (2013) [link]
- S. Poncé, E. R. Margine, C. Verdi, and F. Giustino, Comput. Phys. Commun. 209, 116 (2016) [link]
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