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

June 14-18 2021

Hands-On Intro Thu.5

The superconducting module of EPW

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Lecture Summary

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

Isotropic Migdal-Eliashberg Equations on the Imaginary Axis

mass renormalization function

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

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eliashberg = .true.
liso = .true.
limag = .true.
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superconducting gap function

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

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isotropic e-ph coupling strength

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

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$|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \rightarrow$ write e-ph matrix elements to file: `ephwrite = .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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$\delta(\epsilon_{n\mathbf{k}} - \epsilon_F)$ → use Gaussian smearing of width: `degaussw = 0.1`

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

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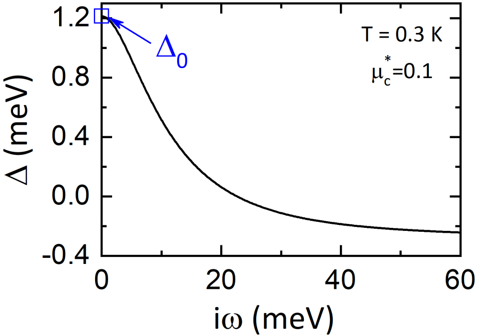
T → temperatures at which the Migdal-Eliashberg equations are solved: `temps = 1.0 2.0`

Isotropic Migdal-Eliashberg Equations on the Imaginary Axis

Isotropic case in Pb

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

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



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)

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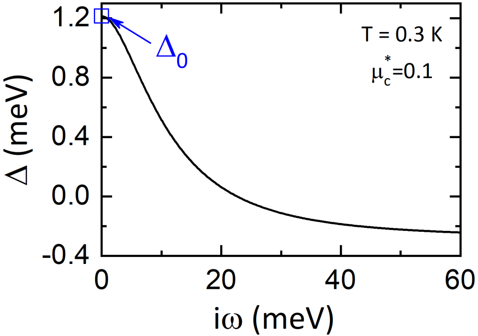

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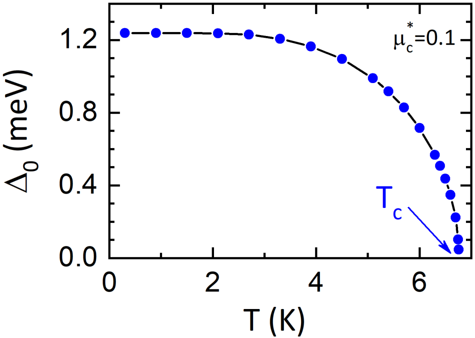

T_c is defined as the temperature at which $\Delta_0 = 0$

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

Isotropic case in Pb

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

Near T_c, $\Delta(i\omega_j) \rightarrow 0$ 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 $s_j = sign(\omega_j)$

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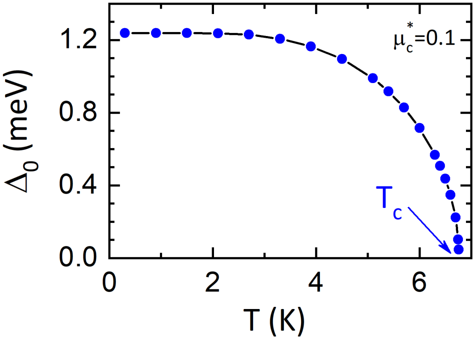

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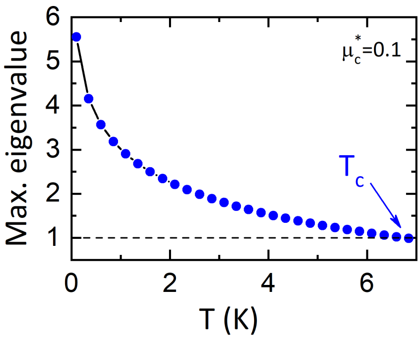

T_c is defined as the value at which the maximum eigenvalue is close to 1

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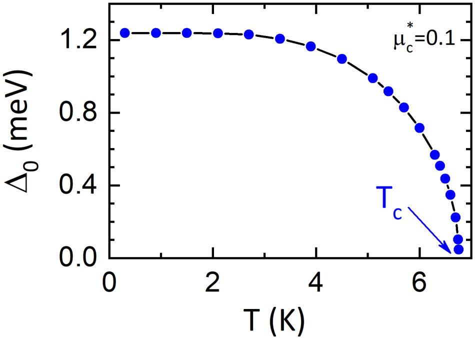

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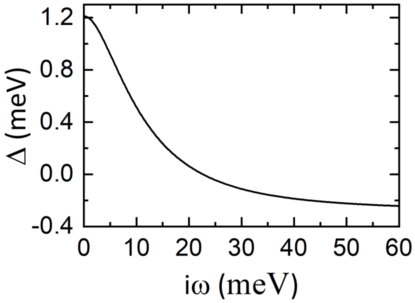

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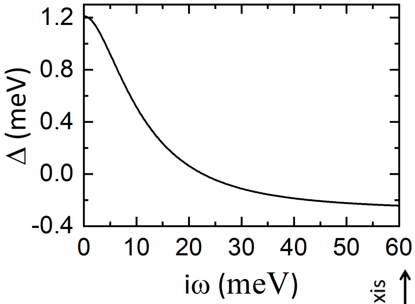
Analytic Continuation from Imaginary to Real Axis



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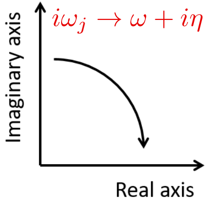

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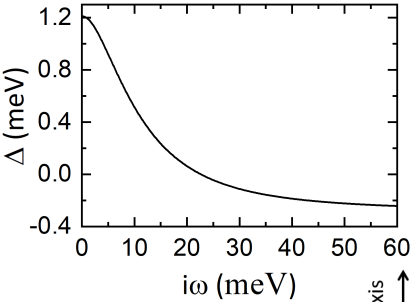

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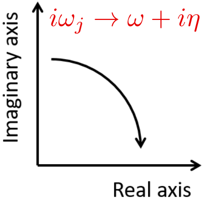

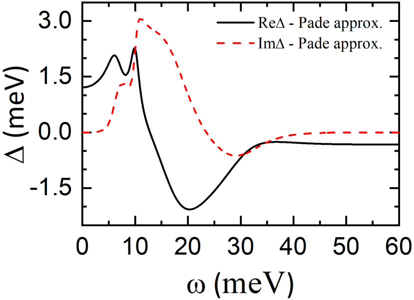

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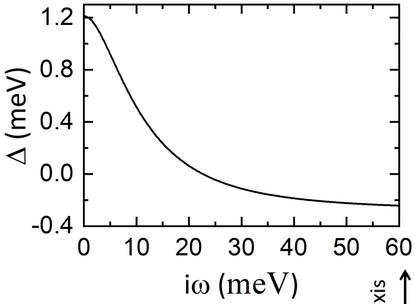

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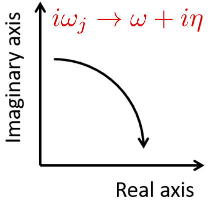

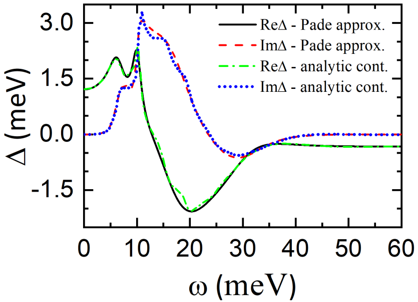

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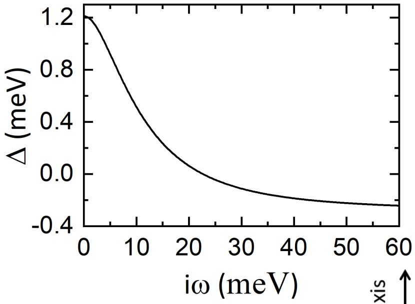

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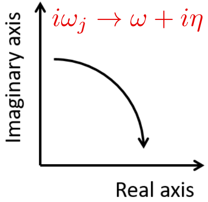
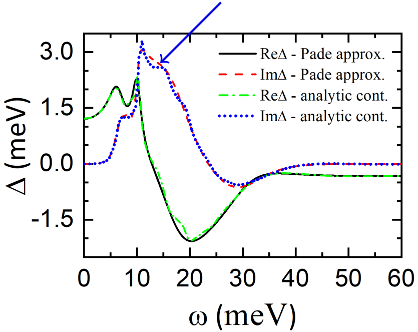
structure in the real axis solutions on the scale of the phonon energy





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

mass renormalization function

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

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

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

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.
```

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

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis

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

mass renormalization function

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

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

$|g_{mn\nu}(\mathbf{k},\mathbf{q})|^2 \rightarrow$ 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

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

mass renormalization function

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

superconducting gap function

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

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

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

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

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

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis

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

mass renormalization function

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

superconducting gap function

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

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

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis

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

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

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```

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

T → temperatures at which the Migdal-Eliashberg equations are solved: `temps = 1.0 2.0`

Anisotropic Migdal-Eliashberg Equations on the Imaginary Axis

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

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

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T → temperatures at which the Migdal-Eliashberg equations are solved: `temps = 1.0 2.0`

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

Isotropic and Anisotropic Electron-Phonon Coupling Strength

eliashberg = .true.

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

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

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

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

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

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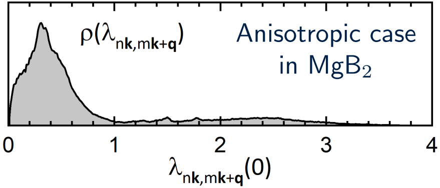

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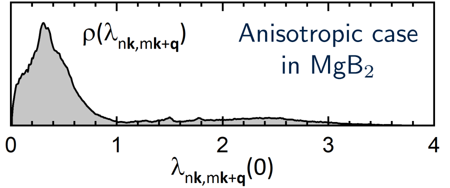
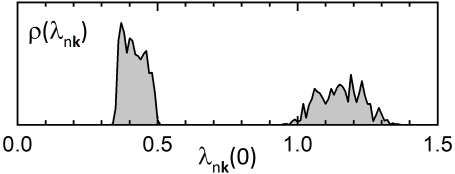
$$\times\, \delta(\omega - \omega_{\mathbf{q}\nu}) \delta(\epsilon_{n\mathbf{k}} - \epsilon_\mathrm{F}) \delta(\epsilon_{m\mathbf{k+q}} - \epsilon_\mathrm{F})$$





Isotropic and Anisotropic Electron-Phonon Coupling Strength

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

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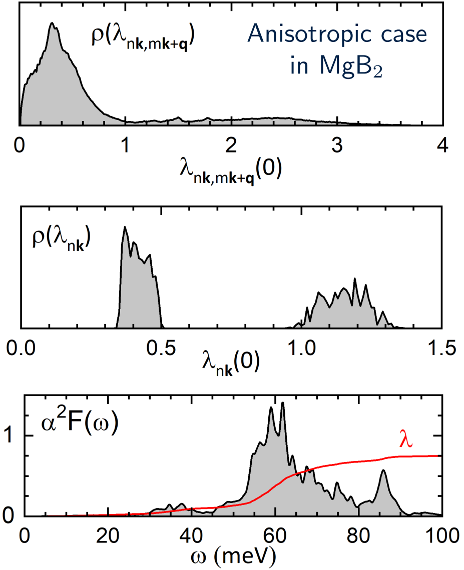
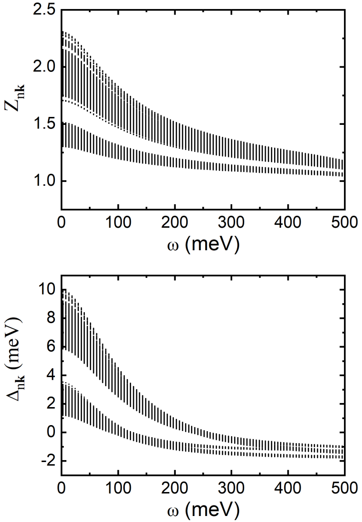


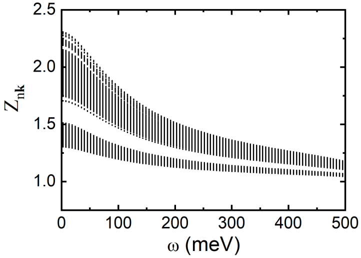


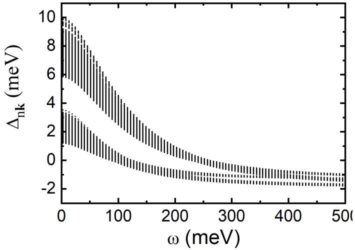
Anisotropic case in MgB_2

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
```

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





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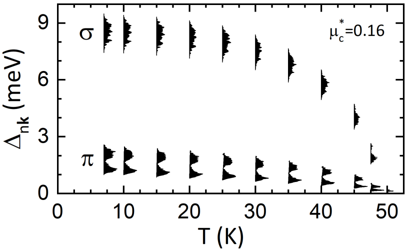
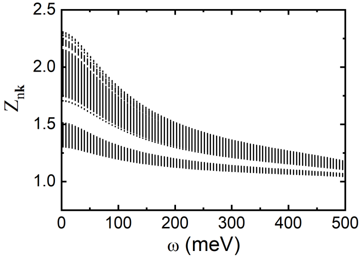


Margine and Giustino, Phys. Rev. B 87, 024505 (2013)



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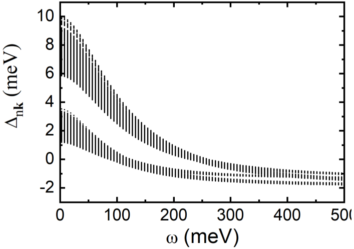
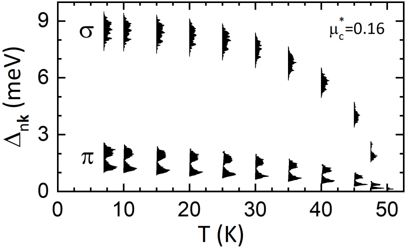
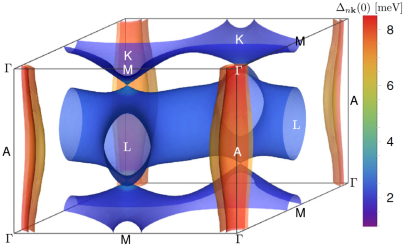


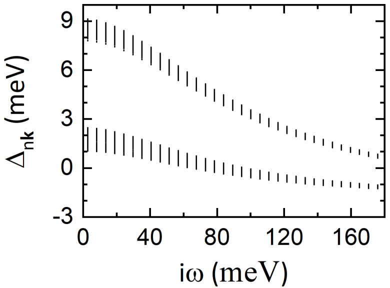




Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

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

Anisotropic Migdal-Eliashberg Equations

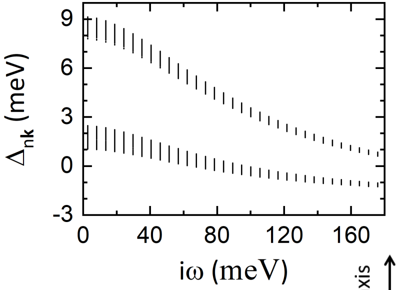


lpade = .true.

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

Anisotropic case in MgB_2

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




```
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```

```
! XX = temperature
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```
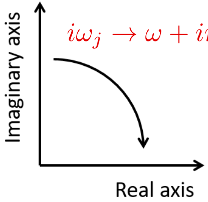
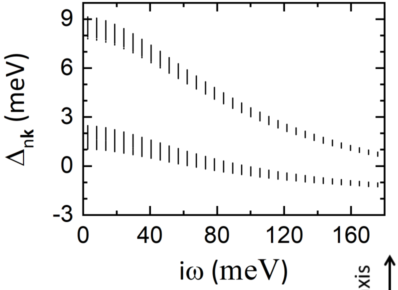



Anisotropic case in MgB_2

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



`lpade = .true.`

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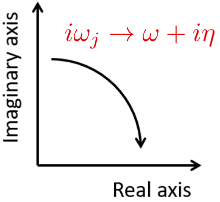
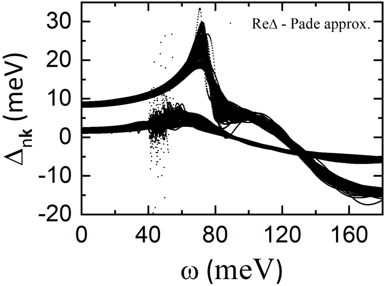
```





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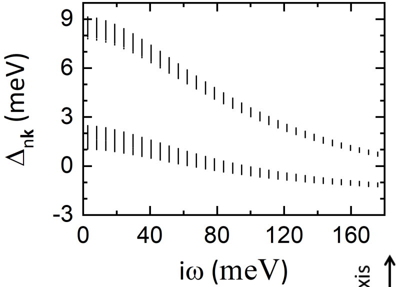
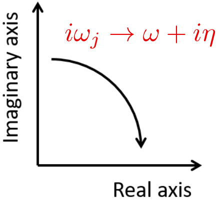
Margine and Giustino, Phys. Rev. B 87, 024505 (2013)

Anisotropic Migdal-Eliashberg Equations

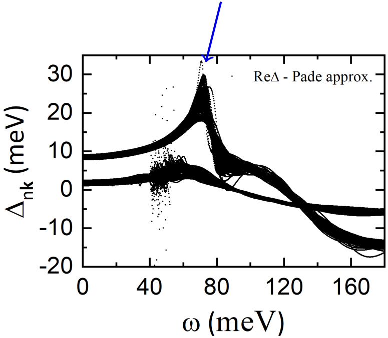



```
lpade = .true.
```

```
! 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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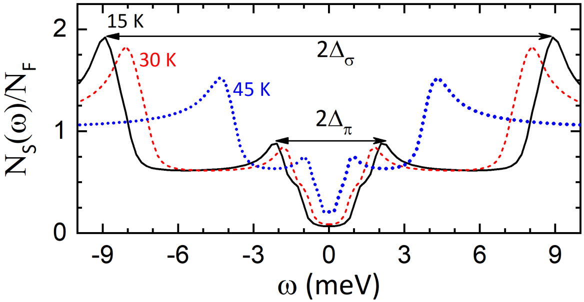

Anisotropic case in MgB_2

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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.

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

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Calculate isotropic and anisotropic e-ph coupling strength.

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

Superconductivity Module in EPW: Workflow

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

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

epw.f90 file:

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

Superconductivity Module in EPW: Workflow

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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 evaluate_a2f_lambda()
  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
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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 evaluate_a2f_lambda()
  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_iso          ! 2nd column is the Eliashberg spectral function corresponding to the
                        ! first smearing in .a2f. Remaining columns are the mode-resolved
                        ! Eliashberg spectral function (there is no specific information on
                        ! which modes correspond to which 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_iso)
```

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; YY = band index within the energy window
```

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

```
! XX = temperature
prefix.imag_iso_XX          ! w_j[eV], Z_nk, \Delta_nk[eV], Z^N_nk
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.fe_XX                ! Free energy in the superconducting state
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], Z^N_nk
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 energy 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.fe_XX                 ! Free energy in the superconducting state
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.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
- Allen-Dynes T_c can be used as a guide for defining the temperatures at which to evaluate the ME eqs.
- 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 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

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