The ElectronPhononCoupling module

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Overview

Computation of temperature-dependent quantities from Abinit

- Renormalization of the eigenvalues
- Lifetimes
- Frequency-dependent self-energy
- Spectral function
- Beyond on-the-mass-shell approximation
- Double grid technique

Features

- NetCDF output
- mpi4py
  - `> mpirun -n 64 python myscript.py`
  - parallelization over q-points

Temperature renormalization and broadening of the eigenvalues

Renormalized energies

$$\varepsilon_i(T) = \varepsilon_i^0 + \Re\Sigma_{ii}(\varepsilon_i, T)$$

Broadening

$$\tau_{\mathbf{k}n}^{-1}(T) = \Im\Sigma_{ii}(\varepsilon_i, T)$$

Linearized solution

$$\varepsilon_i(T) \approx \varepsilon_i^0 + Z_i \Re\Sigma_{ii}(\varepsilon_i^0, T)$$

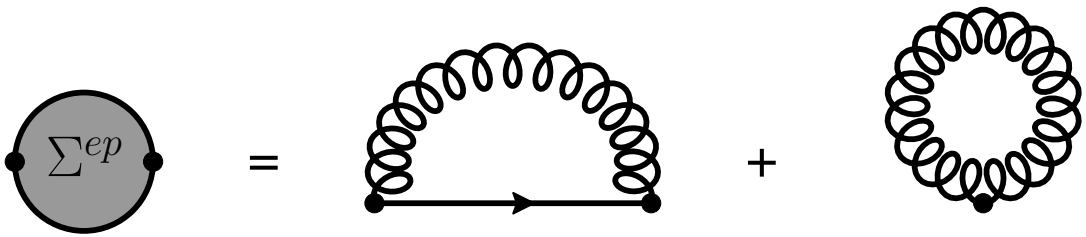
With

$$Z_i^{-1} = 1 - \Re \frac{\partial \Sigma_{ii}(\omega)}{\partial \omega}\Big|_{\varepsilon_i^0}$$

On-the-mass-shell approximation

$$\varepsilon_i(T) \approx \varepsilon_i^0 + \Re\Sigma_{ii}(\varepsilon_i^0, T)$$

Electron-phonon self-energy



$$\Sigma^{\text{ep}}_{\mathbf{k}n}(T,\omega) = \Sigma^{\text{Fan}}_{\mathbf{k}n}(T,\omega) + \Sigma^{DW}_{\mathbf{k}n}(T)$$

Dynamical Fan term

$$\begin{aligned}\Sigma^{\text{Fan}}_{\mathbf{k}n}(T,\omega) = &\sum_{\mathbf{q}\lambda}\sum_{m} |\langle \phi_{\mathbf{k}n}| V^{(1)}_{\mathbf{q}\lambda} |\phi_{\mathbf{k}+\mathbf{q}m}\rangle|^2 \\ &\times \left[\frac{n_{\mathbf{q}\lambda}(T)+f_{\mathbf{k}+\mathbf{q}m}(T)}{\omega-\varepsilon^0_{\mathbf{k}+\mathbf{q}m}+\omega_{\mathbf{q}\lambda}+i\eta_{\mathbf{k}n}} + \frac{n_{\mathbf{q}\lambda}(T)+1-f_{\mathbf{k}+\mathbf{q}m}(T)}{\omega-\varepsilon^0_{\mathbf{k}+\mathbf{q}m}-\omega_{\mathbf{q}\lambda}+i\eta_{\mathbf{k}n}}\right] \\ = &\sum_{\mathbf{q}\lambda}\sum_{m} \Sigma^{\text{Fan}}_{\mathbf{k}n,m,\mathbf{q}\lambda}(T,\omega)\end{aligned}$$

Electron-phonon self-energy

Static approximation

$$\Sigma^{\text{Stat.Fan}}_{\mathbf{k}n}(T,\varepsilon^0_{\mathbf{k}n}) = \sum_{\mathbf{q}\lambda}\sum_{m} \frac{|\langle\phi_{\mathbf{k}n}|\, V^{(1)}_{\mathbf{q}\lambda}\,|\phi_{\mathbf{k}+\mathbf{q}m}\rangle|^2}{\varepsilon^0_{\mathbf{k}n} - \varepsilon^0_{\mathbf{k}+\mathbf{q}m} + i\eta_{\mathbf{k}n}} \left[2n_{\mathbf{q}\lambda}(T)+1\right]$$
$$= \sum_{\mathbf{q}\lambda}\sum_{m} \Sigma^{\text{Stat.Fan}}_{\mathbf{k}n,m,\mathbf{q}\lambda}(T,\varepsilon^0_{\mathbf{k}n})$$

For the bands above a certain cutoff M, we can use

$$\sum_{m>M} \Sigma^{\text{Stat.Fan}}_{\mathbf{k}n,m,\mathbf{q}\lambda}(T,\varepsilon^0_{\mathbf{k}n}) = \langle\phi_{\mathbf{k}n}|\, V^{(1)}_{\mathbf{q}\lambda}\,|\phi^{(1)}_{\mathbf{k}n,\mathbf{q}\lambda}\rangle \left[2n_{\mathbf{q}\lambda}(T)+1\right]$$

With the Sternheimer equation

$$(H-\varepsilon^0_{\mathbf{k}n})P_M\,|\phi^{(1)}_{\mathbf{k}n,\mathbf{q}\lambda}\rangle = -P_M V^{(1)}_{\mathbf{q}\lambda}\,|\phi_{\mathbf{k}n}\rangle$$

Semi-static approximation

$$\Sigma^{\text{Fan}}_{\mathbf{k}n}(T,\omega) = \sum_{\mathbf{q}\lambda}\sum_{m\leq M}\Sigma^{\text{Fan}}_{\mathbf{k}n,m,\mathbf{q}\lambda}(T,\omega) + \sum_{m>M}\Sigma^{\text{Stat.Fan}}_{\mathbf{k}n,m,\mathbf{q}\lambda}(T,\varepsilon^0_{\mathbf{k}n})$$
$$= \Sigma^{\text{Fan Active}}_{\mathbf{k}n}(T,\omega) + \Sigma^{\text{Fan Sternheimer}}_{\mathbf{k}n}(T)$$

- Eliminates sum over bands
- The frequency range of interest ω is typically less than 0.2 eV away from $\varepsilon^0_{\mathbf{k}n}$.
- By choosing a cutoff band M that lies more than 20 eV above $\varepsilon^0_{\mathbf{k}n}$, the relative error on Σ is less than 1%.

Calculation with Abinit

For each q-point...

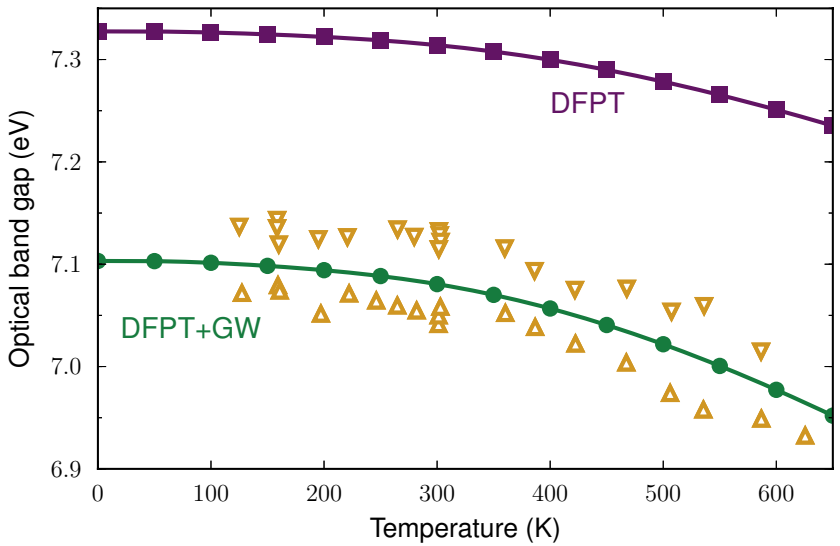
kpts	**variables**	**files**	**quantities**
mesh	`rfphon=1`	`_DDB.nc`	Φ
set	`iscf=-2`	`_EIG.nc`	$\varepsilon^0_{\mathbf{k}n}$
set	`iscf=-2` `nqpt=1`	`_EIG.nc`	$\varepsilon^0_{\mathbf{k}+\mathbf{q}m}$
set	`ieig2rf=5`	`_EIGR2D.nc` `_GKK.nc`	$\langle \phi_{\mathbf{k}n} \vert V^{(1)}_{\mathbf{q}\lambda} \vert \phi^{(1)}_{\mathbf{k}n,\mathbf{q}\lambda} \rangle$ $\langle \phi_{\mathbf{k}n} \vert V^{(1)}_{\mathbf{q}\lambda} \vert \phi_{\mathbf{k}+\mathbf{q}m} \rangle$
set	`optdriver=7` `eph_task=2`	`_GKK.nc`	

Usage: renormalization and broadening

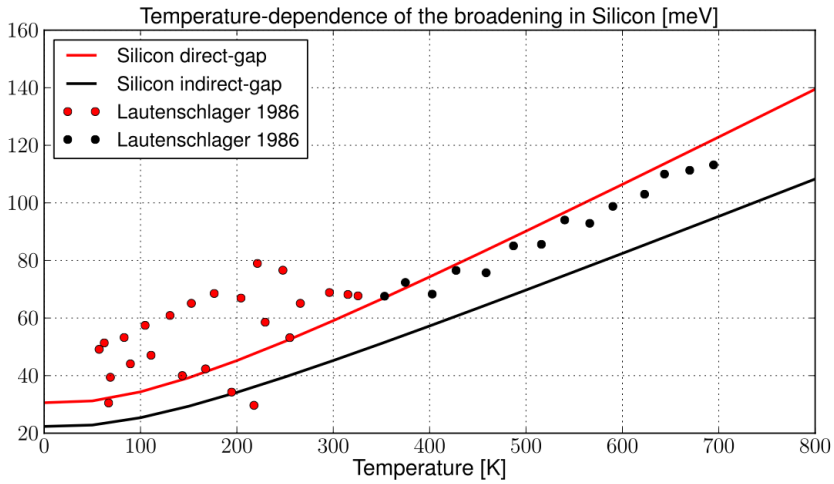
```
import ElectronPhononCoupling as epc

analyzer = epc.compute(
    renormalization = True,  # Compute the eigenvalues renormalization
    broadening = True,       # Compute broadening
    temperature = True,      # Compute at several temperatures

    write = True,          # Do write the results
    rootname = 'output',   # Rootname for the output

    smearing_eV = 0.01,            # Imaginary broadening parameter
    temp_range = [0, 1000, 250],   # Temperatures (min, max, step)

    nqpt = 3,                    # Number of q-points
    wtq = [0.125, 0.5, 0.375],   # Weights of the q-points.

    eigk_fname    = EIG_nc_at_k,           # All the netcdf files
    eigq_fnames   = list_of_EIG_nc_at_kq,  # produced by Abinit.
    ddb_fnames    = list_of_DDB_nc,        #
    eigr2d_fnames = list_of_EIGR2D_nc,     #
    gkk_fnames    = list_of_GKK_nc,        #
    )
```

Temperature-dependent renormalization/broadening

Direct band gap of diamond[1]



Broadening of the band gap of silicon[2]



[1] G. Antonius et al. (2014). *Physical Review Letters* 112.21, p. 215501

[2] S. Poncé et al. (2015). *The Journal of Chemical Physics* 143.10, p. 102813

Spectral function

Dyson equation for the Green's function

$$G_i(\omega, T) = G_i^0(\omega) + G_i^0(\omega)\Sigma_{ii}(\omega, T)G_i(\omega, T)$$

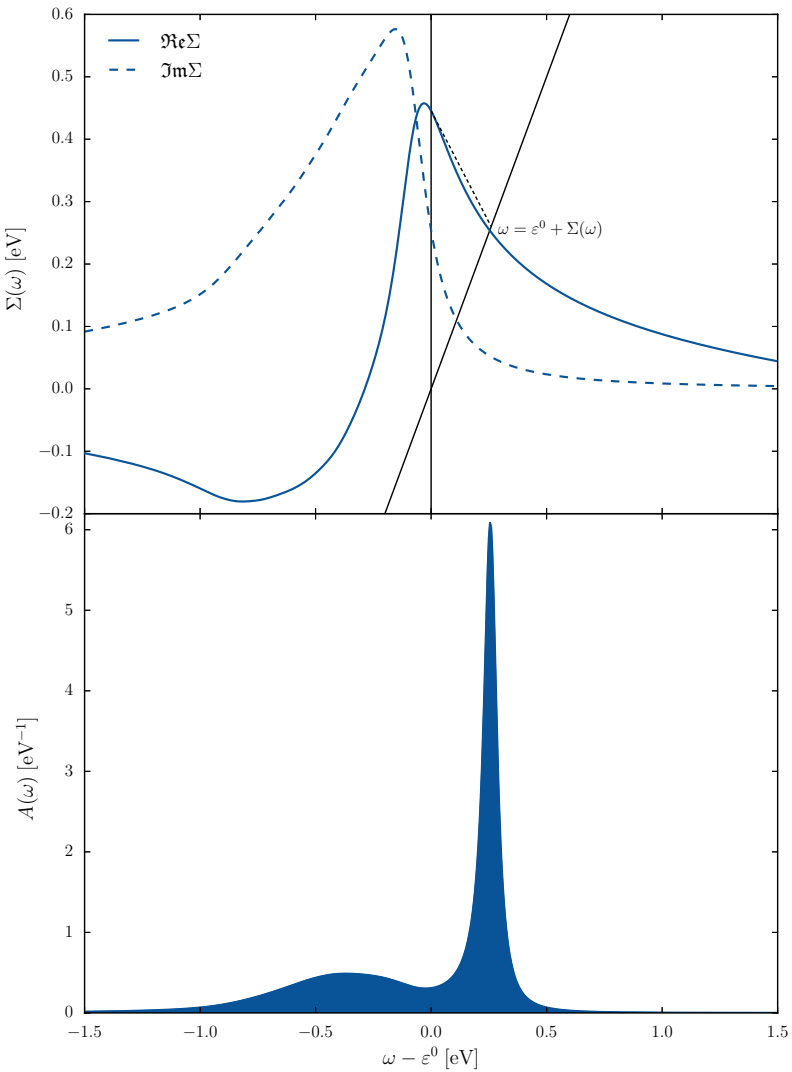
The spectral function is defined as

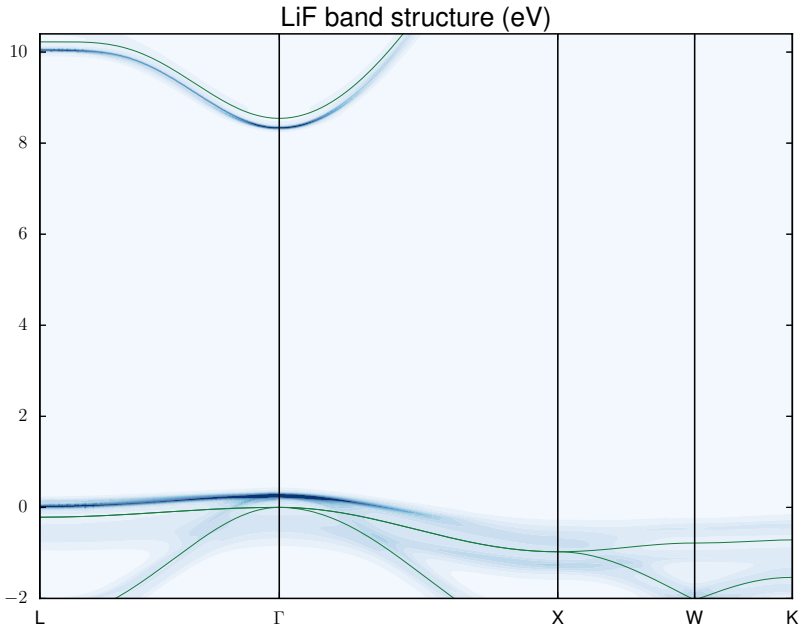
$$\begin{aligned} A_{\mathbf{k}n}(\omega, T) &= \frac{1}{\pi}\Im G_{\mathbf{k}n}(\omega, T) \\ &= \frac{1}{\pi}\frac{|\Im\Sigma^{ep}_{\mathbf{k}n}(\omega, T)|}{[\omega - \varepsilon^0 - \Re\Sigma^{ep}_{\mathbf{k}n}(\omega, T)]^2 + \Im\Sigma^{ep}_{\mathbf{k}n}(\omega, T)^2} \end{aligned}$$

Usage: spectral function

```
import ElectronPhononCoupling as epc

analyzer = epc.compute(
    self_energy = True,         # Compute frequency-dependent self-energy
    spectral_function = True,   # Compute the spectral function as well
    temperature = True,         # Compute at several temperatures

    smearing_eV = 0.01,           # Imaginary broadening parameter
    temp_range = [0, 1000, 250],  # Temperatures (min, max, step)

    nqpt = 3,                    # Number of q-points
    wtq = [0.125, 0.5, 0.375],   # Weights of the q-points.

    eigk_fname    = EIG_nc_at_k,           # All the netcdf files
    eigq_fnames   = list_of_EIG_nc_at_kq,  # produced by Abinit.
    ddb_fnames    = list_of_DDB_nc,        #
    eigr2d_fnames = list_of_EIGR2D_nc,     #
    gkk_fnames    = list_of_GKK_nc,        #
    )
```

Spectral function

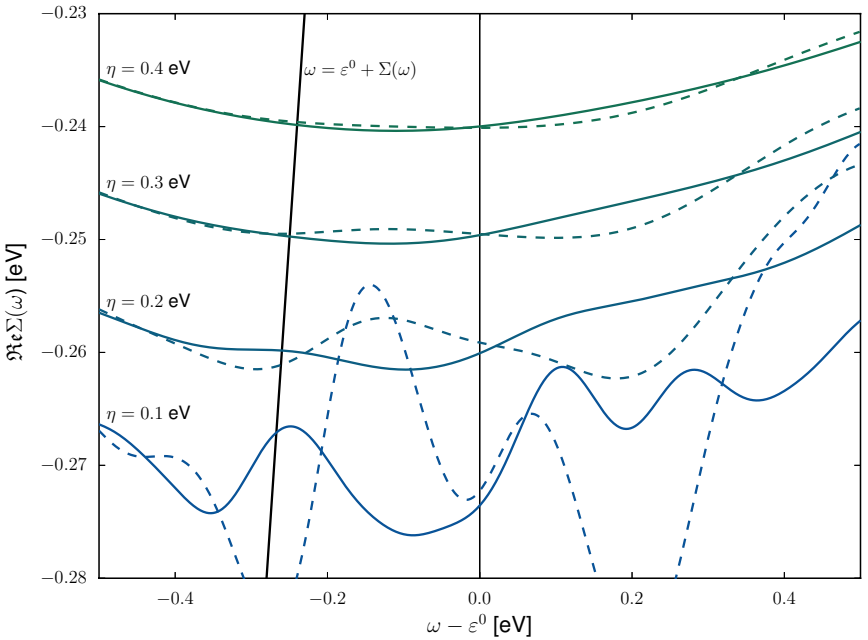




- Important renormalization factor: $Z \approx 0.6$
- Satellite band
- Future work: cumulant expansion

G. Antonius et al. (2015). *Physical Review B* 92.8, p. 085137

Choosing the imaginary parameter η



- Depends on the q-point grid
- η should be as small as possible
- $\Sigma(\omega)$ should remain smooth

Solid lines: $32 \times 32 \times 32$ q-point grid

Dashed lines: $24 \times 24 \times 24$ q-point grid

G. Antonius et al. (2015). *Physical Review B* 92.8, p. 085137

Interpolation of the active space

We can use different q-point grids for the active space and the Sternheimer contributions

$$\Sigma_{\mathbf{k}n}(T,\omega) = \sum_{\mathbf{q}\lambda}^{\text{fine}} \Sigma^{\text{Active}}_{\mathbf{k}n,\mathbf{q}\lambda}(T,\omega) + \sum_{\mathbf{q}\lambda}^{\text{coarse}} \Sigma^{\text{Sternheimer}}_{\mathbf{k}n,\mathbf{q}\lambda}(T,\varepsilon^0_{\mathbf{k}n})$$

We want to interpolate the dynamical matrices and the electron-phonon coupling potentials onto a fine q-point grid.

Interatomic force constants:

$$\Phi_{\kappa j,\kappa' j'}(\mathbf{R}_l) = \sum_{\mathbf{q}} \Phi_{\kappa j,\kappa' j'}(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}_l}$$

Interpolated dynamical matrix:

$$\Phi_{\kappa j,\kappa' j'}(\tilde{\mathbf{q}}) = \sum_{l} \Phi_{\kappa j,\kappa' j'}(\mathbf{R}_l) e^{-i\tilde{\mathbf{q}}\cdot\mathbf{R}_l}$$

Interpolation of the coupling potential

Fourier interpolation of the potential[3]

$$W_{\kappa j}(\mathbf{r}-\mathbf{R}_l) = \sum_{\mathbf{q}} V^{(1)}_{\mathbf{q}\kappa j}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{R}_l}$$

Represents the potential induced by the displacement of a single atom along a Cartesian direction.

Allows to interpolate

$$V^{(1)}_{\tilde{\mathbf{q}}\kappa j}(\mathbf{r}) \approx \sum_{l} W_{\kappa j}(\mathbf{r}-\mathbf{R}_l) e^{-i\tilde{\mathbf{q}}\cdot\mathbf{R}_l}$$

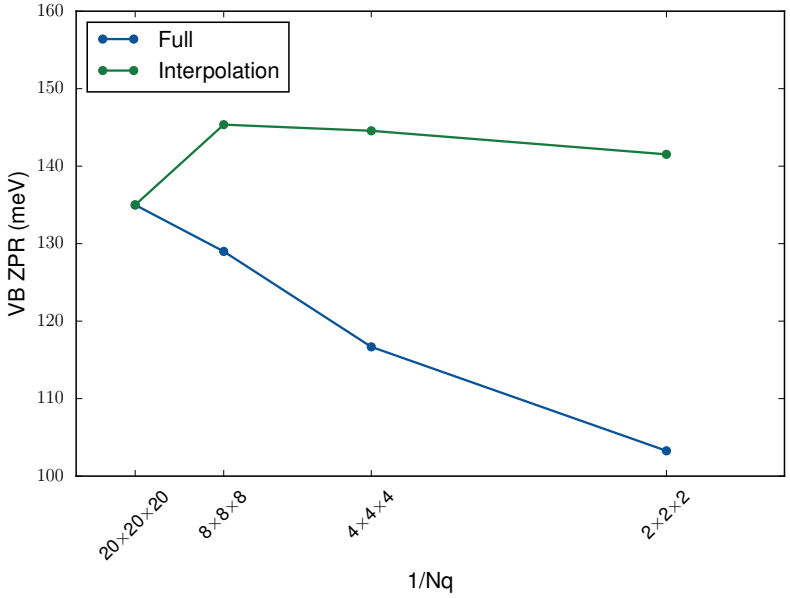
Where the real-space summation is truncated.

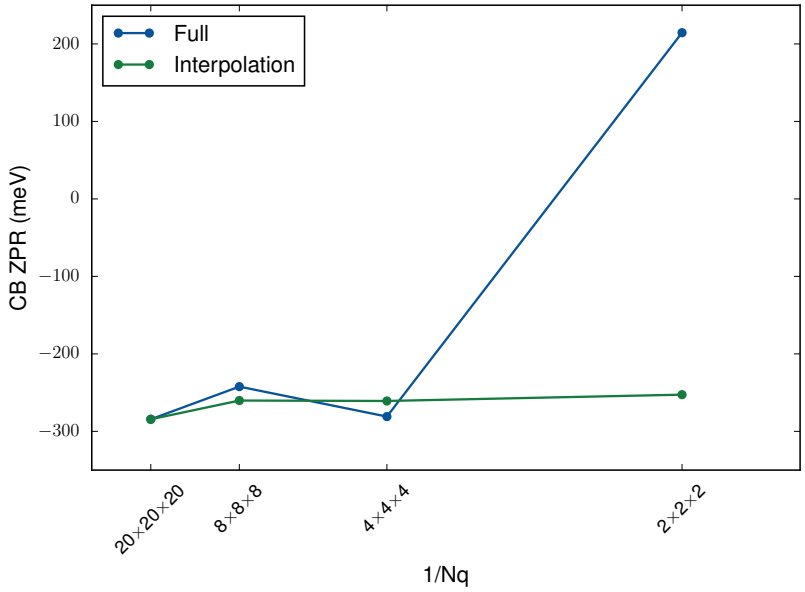
Asier Eiguren and Claudia Ambrosch-Draxl (2008). *Physical Review B* 78.4, p. 045124

Usage: double grid

```
import ElectronPhononCoupling as epc

analyzer = epc.compute(
    renormalization = True,  # Compute the eigenvalues renormalization
    broadening = True,       # Compute broadening
    temperature = True,      # Compute at several temperatures
    double_grid = True,      # Use double grid technique

    smearing_eV = 0.01,           # Imaginary broadening parameter
    temp_range = [0, 1000, 250],  # Temperatures (min, max, step)

    # Q-points on the coarse grid
    nqpt = 8,
    wtq = list_of_weights_coarse,

    # Q-points on the fine grid
    nqpt_fine = 256,
    wtq_fine = list_of_weights_fine,

    # Files on the coarse grid
    eigk_fname    = EIG_nc_at_k,
    eigq_fnames   = list_of_EIG_nc_at_kq,
    ddb_fnames    = list_of_DDB_nc,
    eigr2d_fnames = list_of_EIGR2D_nc,
    gkk_fnames    = list_of_GKK_nc,

    # Files on the fine grid
    eigq_fine_fnames = list_of_EIG_nc_at_kq_fine_grid,
    ddb_fine_fnames  = list_of_DDB_nc_kq_fine_grid,
    gkk_fine_fnames  = list_of_GKK_nc_kq_fine_grid,
    )
```

Tests on diamond





Future work: polar materials

The long-ranged Fröhlich interaction needs to be treated separately.

We can model this interaction as

$$V_{\mathbf{q}\kappa j}^{\text{Frolich}}(\mathbf{r}) = \sum_{\mathbf{G}\neq-\mathbf{q}} \frac{(\mathbf{q}+\mathbf{G})\cdot\mathbf{Z}_{\kappa j}^{*}}{(\mathbf{q}+\mathbf{G})\cdot\varepsilon^{\infty}\cdot(\mathbf{q}+\mathbf{G})} e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}$$

Where $\mathbf{Z}_{\kappa j}^{*}$ are the Born effective charges and ε^{∞} is the macroscopic dielectric tensor.

This anlytic potential must be removed from the el-ph coupling potential before interpolation, then added after.

S. Poncé et al. (2016). *Computer Physics Communications* 209, pp. 116–133

Distribution

Maintained on github

`https://github.com/GkAntonius/ElectronPhononCoupling`

Distributed in abinit

`~abinit/scripts/post_processing/ElectronPhononCoupling`

Documentation

- Extensive doc strings
- Examples directory for users
  - Abinit calculations
  - EPC examples
  - Plotting examples
- Doc directory for developers
  - How to add a test
  - How to add an example

Test suite

- nosetests
- Comparison with reference NetCDF data
- Self-generation of reference data
- Files produced by Abinit stored in the package ($<$ 5 Mb)
- **Not** integrated the Abinit test suite yet

Acknowledgments

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- Xavier Gonze

Thank you for your attention!