School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

10-16 June 2024, Austin TX

Mike Johnston, "Spaceman with Floating Pizza"

Hands on Tutorial on QDPT

Sat.7.Tiwari

1. Remove reservation from bash scripts

2. QE_BIN_DIR=/work2/05193/sabyadk/stampede3/EPWSchool2024/q-e_<hint>/bin/
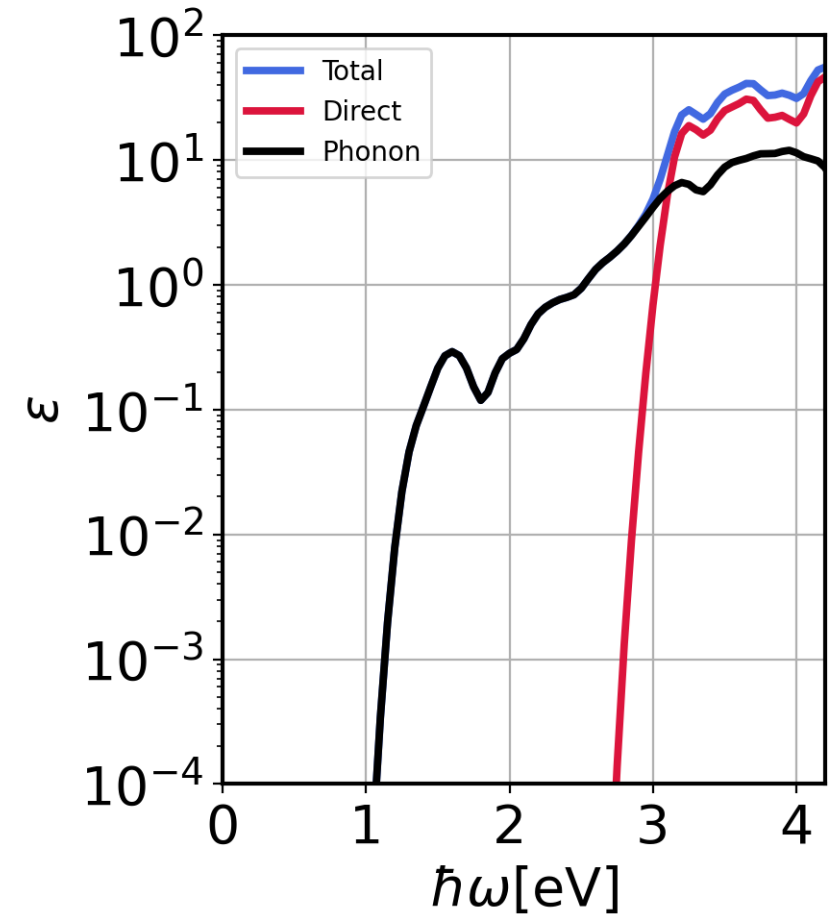   1. Figure out yourself how to use ELPA compilation

1. Silicon scf and phonon calculations (submit1.sh)

2. Silicon wannierization and coarse-grid calculation of (submit2.sh)

3. QDPT calculation (Uncomment second line in submit2.sh)
   1. epsilon2_indabs_300.0K_XX.dat
   2. c_dir300.0K_XX.dat
   3. c_ph300.0K_XX.dat

4. Various plotting codes to plot multiple quantities

$$\varepsilon_2(\omega) = \frac{\pi e^2}{\epsilon_0 \Omega} \frac{1}{\omega^2} \frac{1}{N} \sum_{i_0, p} Z^{-1} \exp\left(-\beta E_{i_0}\right)$$

$$\times \left| \mathbf{e} \cdot \sum_{cvk} \left\{ U^*_{p, i_0 - 1_{vk} + 1_{ck}} \mathbf{V}_{cvk} \right. \right.$$

$$+ N^{-1/2} \sum_{qv\eta} \sqrt{n_{qv} + \frac{1+\eta}{2}} \; U^*_{p, i_0 - 1_{vk} + 1_{ck+q} + \eta 1_{-\eta qv}}$$

$$\times \left[\sum_{c'} \frac{g_{cc'v}(\mathbf{k}, \mathbf{q}) \mathbf{V}_{c'vk}}{(\bar{E} - E_{i_0}) - (\varepsilon_{c'k} - \varepsilon_{vk})} \theta_{c'vk} \right.$$

$$+ \sum_{v'} \frac{\mathbf{V}_{cv'k+q} \, g_{v'vv}(\mathbf{k}, \mathbf{q})}{(\bar{E} - E_{i_0}) - (\varepsilon_{ck+q} - \varepsilon_{v'k+q})} \theta_{cv'k+q}$$

$$+ \sum_{c'} \frac{\mathbf{V}_{cc'k+q} \, g_{c'vv}(\mathbf{k}, \mathbf{q})}{\varepsilon_{vk} - \varepsilon_{c'k+q} - \eta \hbar \omega_{-\eta qv}}$$

$$\left. \left. \left. + \sum_{v'} \frac{g_{cv'v}(\mathbf{k}, \mathbf{q}) \mathbf{V}_{v'vk}}{\varepsilon_{v'k} - \varepsilon_{ck+q} - \eta \hbar \omega_{-\eta qv}} \right] \right\} \right|^2$$
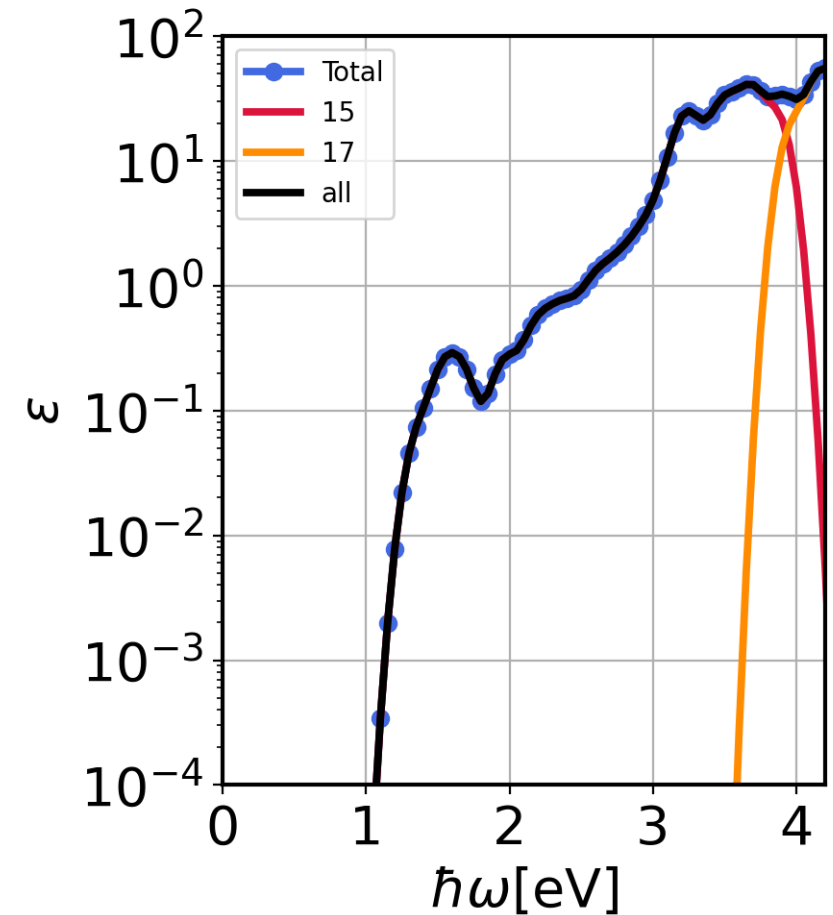
$$\times \; \delta(E_p - E_{i_0} - \hbar \omega) \, . \tag{47}$$

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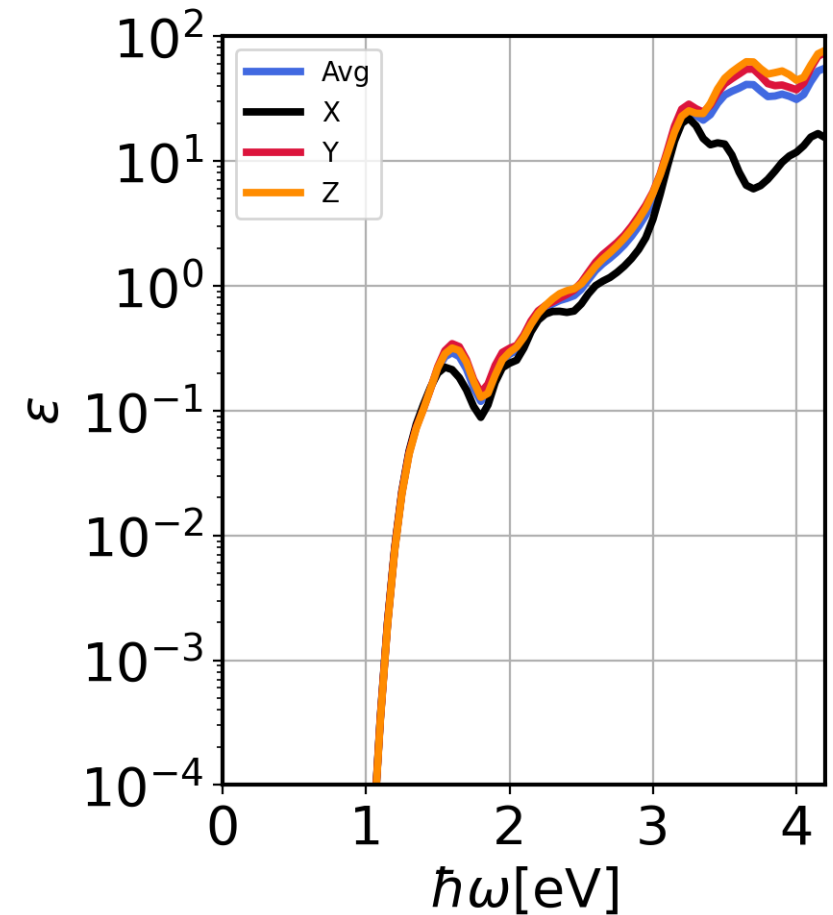4. Various plotting codes to plot multiple quantities

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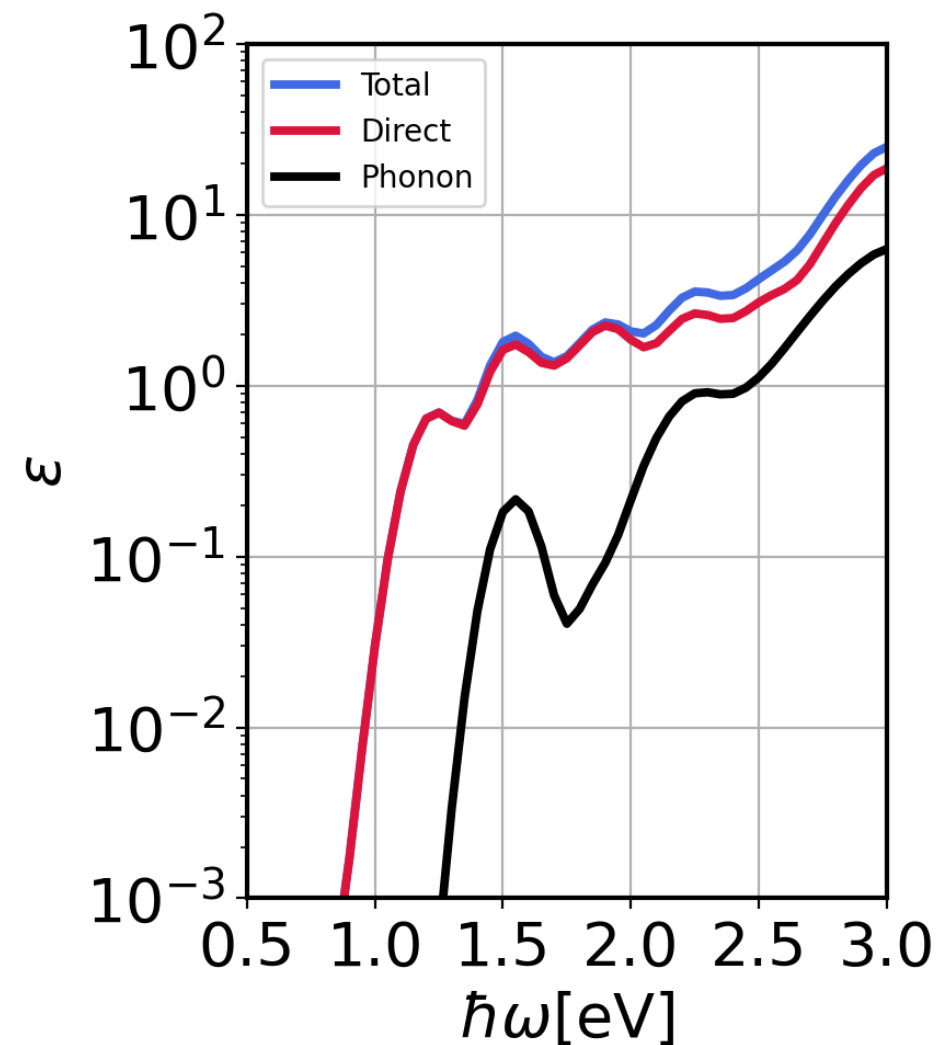4. Various plotting codes to plot multiple quantities

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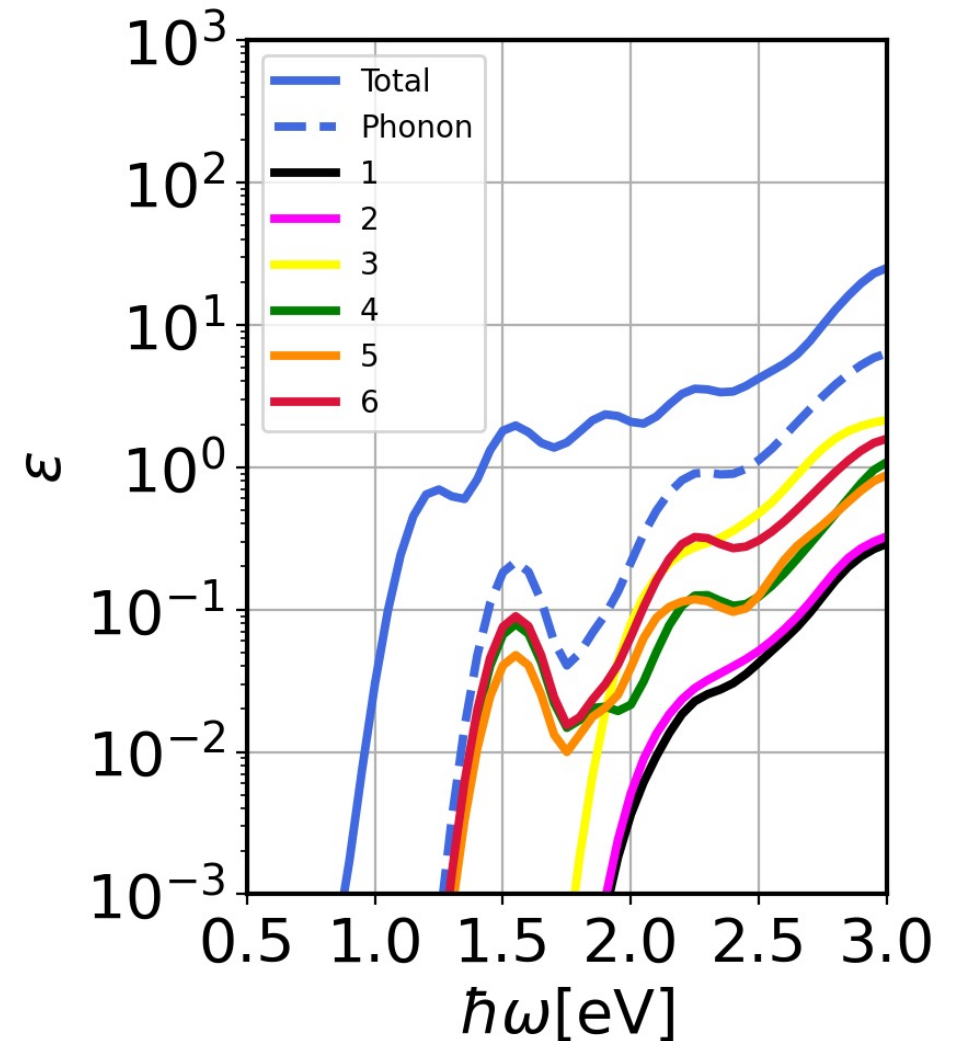4. Various plotting codes to plot multiple quantities

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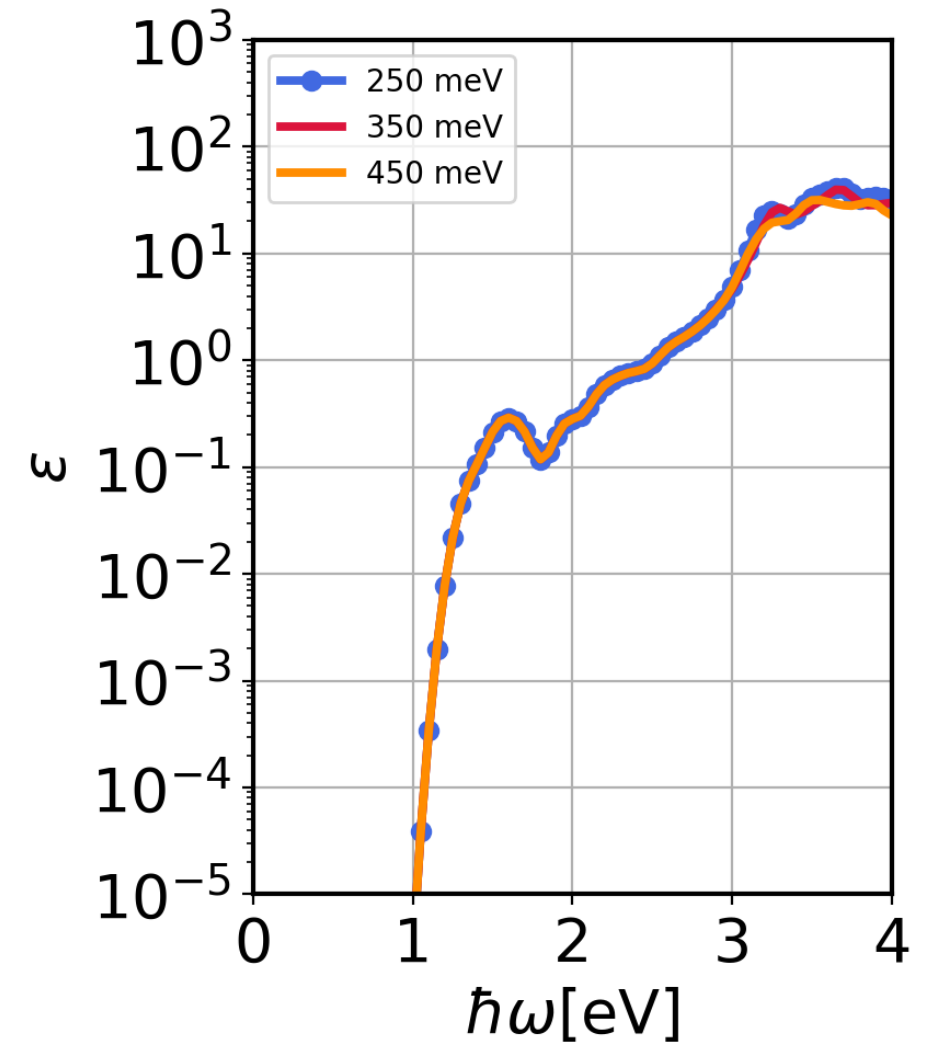4. Various plotting codes to plot multiple quantities

- Test convergence of QDPT with QD bin size
- $\Delta E \to \infty$ Check convergence

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The Hands-On document is self-explanatory