Author: Burak Himmetoglu

Details on the transport code implementation

Scattering rates:

$$\tau_{n\mathbf{k}}^{-1} = \frac{2\pi}{\hbar} \sum_{\mathbf{q}\nu,m} |g_{\mathbf{q}\nu}|^2 \, (1 - \hat{v}_{n\mathbf{k}} \cdot \hat{v}_{m\mathbf{k+q}}) \Big\{ (n_{\mathbf{q}\,\nu} + f_{m,\mathbf{k+q}})\, \delta(\epsilon_{m,\mathbf{k+q}} - \epsilon_{n\mathbf{k}} - \hbar\omega_{L\nu}) + (1 + n_{\mathbf{q}\,\nu} - f_{m,\mathbf{k+q}})\, \delta(\epsilon_{m,\mathbf{k+q}} - \epsilon_{n\mathbf{k}} + \hbar\omega_{L\nu}) \Big\} \tag{1}$$

where

$$g_{\mathbf{q}\,\nu} = i \frac{e^2}{\epsilon_0 \, V} \sum_{\mathbf{G}} \sum_{\alpha,\beta,s,\nu} \left(\frac{\hbar}{2\, M_s\, \omega_{\mathbf{q}\,\nu}} \right)^{1/2} \frac{(q+G)_\alpha \, Z_s^{*\,\alpha\beta}}{(\mathbf{q}+\mathbf{G}) \cdot \epsilon_\infty \cdot (\mathbf{q}+\mathbf{G})} \, e_{s\,\beta}(\mathbf{q};\nu) \tag{2}$$

Or, in a simplified approximate form

$$|g_{\mathbf{q}\,\nu}|^2 = \frac{1}{q^2} \left(\frac{e^2\, \hbar\, \omega_{L\nu}}{2\epsilon_0\, V_{\rm cell}\, \epsilon_\infty} \right) \frac{\prod_{j=1}^{N} \left(1 - \frac{\omega_{Tj}^2}{\omega_{L\nu}^2}\right)}{\prod_{j\neq\nu} \left(1 - \frac{\omega_{Lj}^2}{\omega_{L\nu}^2}\right)} \tag{3}$$

In Eq.(1) the delta-function is replaced by a Gaussian smearing with adaptive smearing width:

$$\begin{aligned} \delta(F_{n\mathbf{k},\,m\mathbf{k+q}}) &= \frac{1}{\sqrt{\pi}\,\sigma} \, \exp\left[-\frac{F_{n\mathbf{k},\,m\mathbf{k+q}}^2}{\sigma^2} \right] \\ \sigma = \Delta F_{n\mathbf{k},\,m\mathbf{k+q}} &= a \left| \frac{\partial F_{n\mathbf{k},\,m\mathbf{k+q}}}{\partial \mathbf{k}} \right| \Delta\mathbf{k} \\ F_{n\mathbf{k},\,m\mathbf{k+q}} &= \epsilon_{m,\mathbf{k+q}} - \epsilon_{n\mathbf{k}} \pm \hbar\omega_{L\nu} \end{aligned} \tag{4}$$

where a is a dimensionless parameter that determines the width of the smearing. The natural choice is $a = 1.0$, however larger values of a produces smoother densities of states.

In order to compute the electron-phonon scattering strength at the Fermi level, we define

$$D_n\, \tau_n^{-1}(E_F) \equiv \sum_{\mathbf{k}} \delta(E_F - \epsilon_{n\mathbf{k}})\, \tau_{n\mathbf{k}}^{-1}. \tag{5}$$

The above integral can be carried out in a reduced grid where the **k**-points are restricted to the region where the energy eigenvalues satisfy

$$|\epsilon_{n\mathbf{k}} - E_F| < c \times kT \tag{6}$$

where T is the temperature and c is a dimensionless parameter(we refer to it as "cut"). This results is a band-dependent grid size. This choice is related to the fact that the transport integrals contain the derivative of the Fermi-Dirac distribution, which is peaked around E_F. For example, in case of a $16 \times 16 \times 16$ grid, a choice of $c = 10.0$ reduces the integration grid from a the full 4096 points, to 438 for band 1, 57 for band 2 and 33 for band 3.

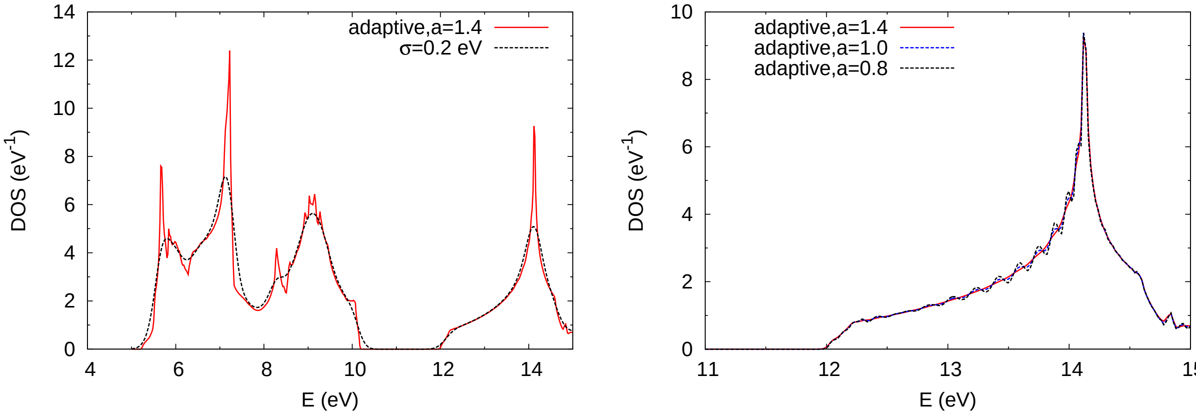

FIG. 1: Left: Comparison of constant smearing (width = 0.2eV) and adaptive smearing with $a = 1.4$. Right: Comparison of different values of the parameter a. Fermi level corresponding to $n = 10^{20} cm^{-3}$ is used.

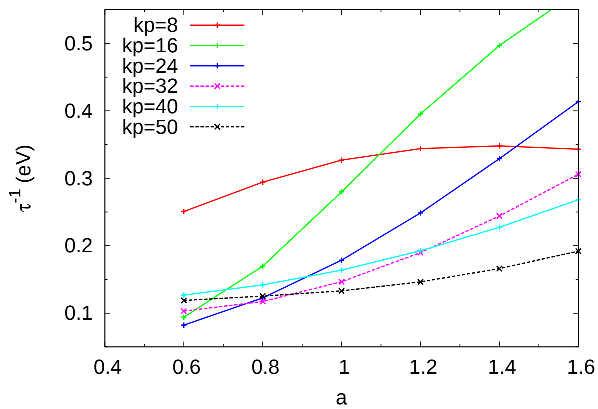

FIG. 2: Calculated $D_n\, \tau_n^{-1}(E_F)$ for $c = 10.0$ for different choices of k-point grid as a function of a. Fermi level corresponding to $n = 10^{20} cm^{-3}$ is used.

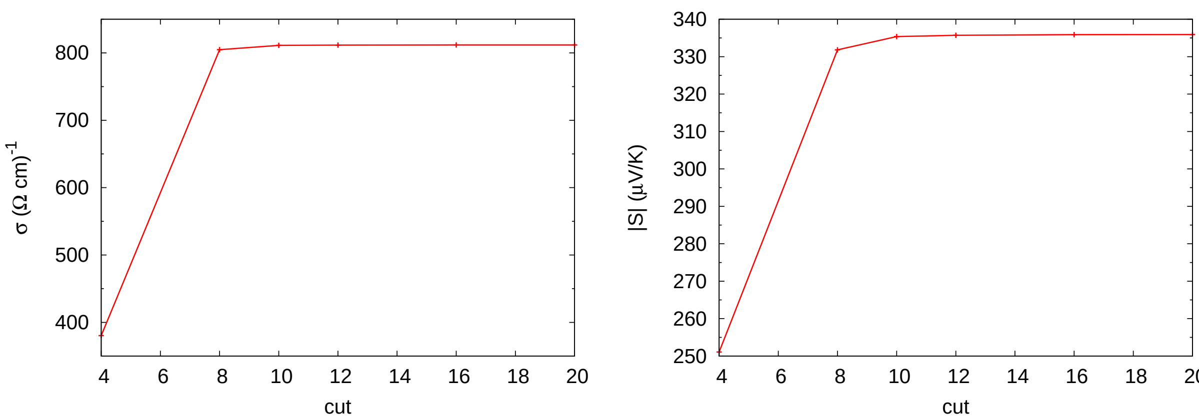

FIG. 3: Calculated transport coefficients for $16 \times 16 \times 16$ grid with varying c, using a constant scattering rate of 0.1 eV at 300 K.

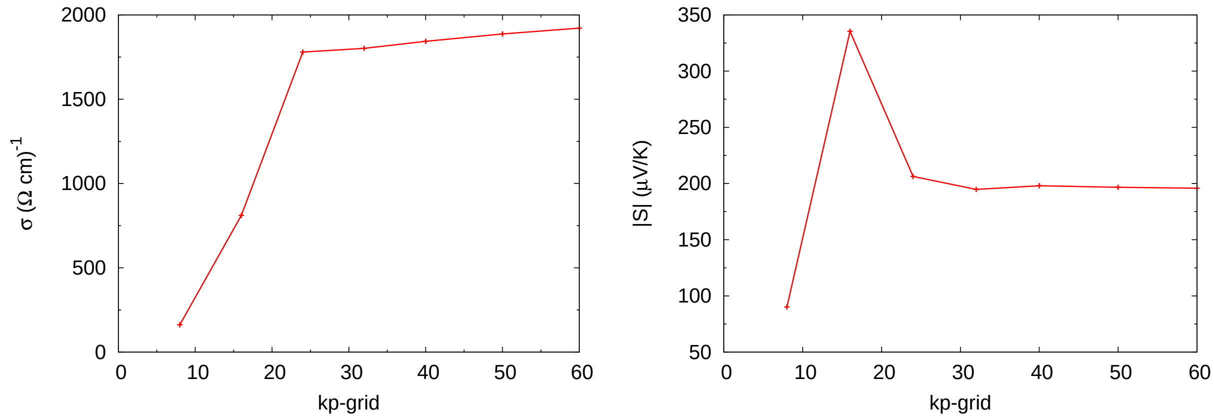

FIG. 4: Calculated transport coefficients for $c = 10.0$, with varying grids, a constant scattering rate of 0.1 eV at 300 K.