Author: Burak Himmetoglu

Details on the transport code implementation

Scattering rates:

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

where

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

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

$$\delta(F_{n\mathbf{k},\,m\mathbf{k+q}}) = \frac{1}{\sqrt{\pi}\,\sigma}\,\exp\left[-\frac{F^2_{n\mathbf{k},\,m\mathbf{k+q}}}{\sigma^2}\right]$$
$$\sigma = \Delta F_{n\mathbf{k},\,m\mathbf{k+q}} = a\left|\frac{\partial F_{n\mathbf{k},\,m\mathbf{k+q}}}{\partial\mathbf{k}}\right|\Delta\mathbf{k}$$
$$F_{n\mathbf{k},\,m\mathbf{k+q}} = \epsilon_{m,\mathbf{k+q}} - \epsilon_{n\mathbf{k}} \pm \hbar\omega_{L\nu} \tag{3}$$

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

$$D_n\,\tau^{-1}_n(E_F) \equiv \sum_{\mathbf{k}}\delta(E_F - \epsilon_{n\mathbf{k}})\,\tau^{-1}_{n\mathbf{k}}. \tag{4}$$

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

$$|\epsilon_{n\mathbf{k}} - E_F| < c\times kT \tag{5}$$

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 $16\times16\times16$ 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.

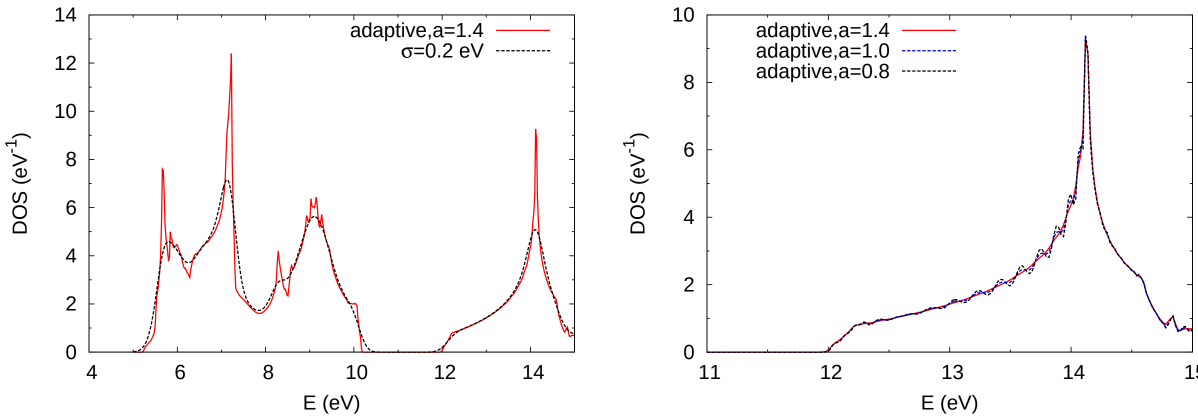

FIG. 1: Left: Comparison of constant smearing (width = 0.2eV) and adaptive smearing with $a = 1.4$. Right: Comparison of different values of the parameter a. Fermi level corresponding to $n = 10^{20} cm^{-3}$ is used.

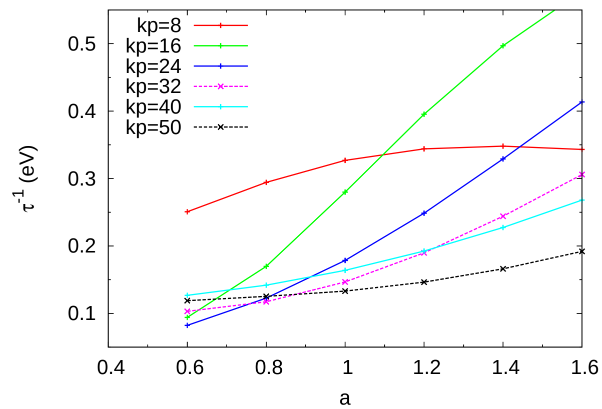

FIG. 2: Calculated $D_n\, \tau_n^{-1}(E_F)$ for $c = 10.0$ for different choices of k-point grid as a function of a. Fermi level corresponding to $n = 10^{20} cm^{-3}$ is used.

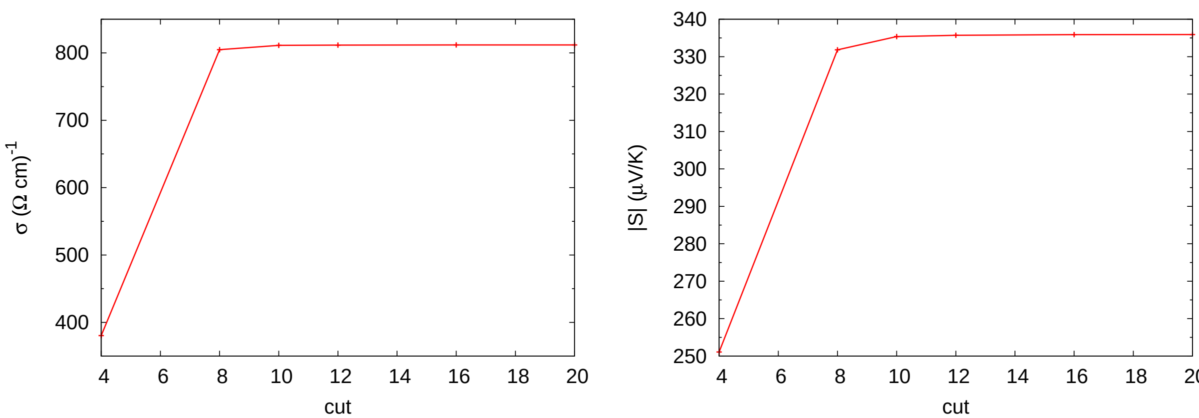

FIG. 3: Calculated transport coefficients for $16 \times 16 \times 16$ grid with varying c, using a constant scattering rate of 0.1 eV at 300 K.

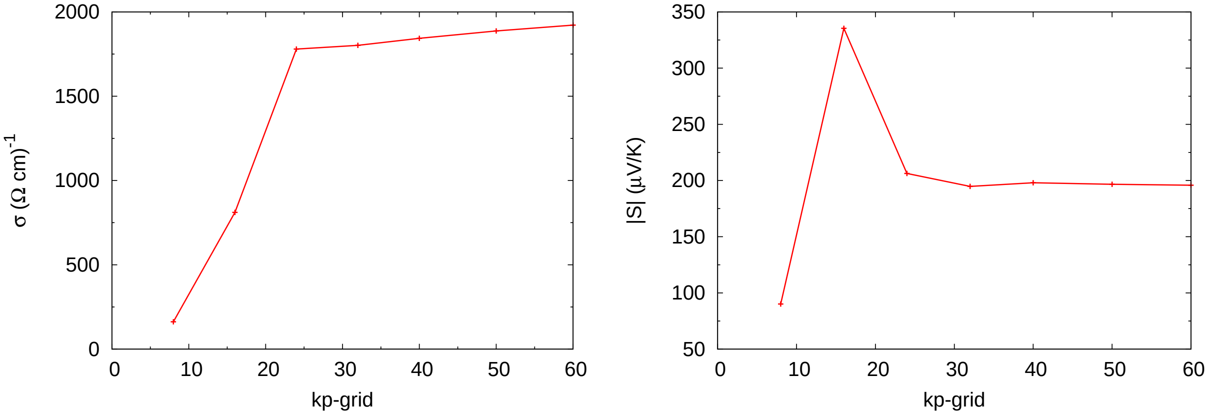

FIG. 4: Calculated transport coefficients for $c = 10.0$, with varying grids, a constant scattering rate of 0.1 eV at 300 K.