Adaptive Smearing Method

WH

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1 The case of three phonon interation

we follow the derivation of the *ShengBTE* paper. [1] To approximate a delta function $\delta(q_1 - q_2 - q_3)\delta(\omega_1 - \omega_2 - \omega_3)$, we first write:

$$W(q_2) = \omega_2 + \omega_3 \tag{1}$$

to linear approximation, we have:

$$W(q_2') \approx W(q_2^0) + \sum_{\mu} \left(\frac{\partial W}{\partial q_2^{\mu}}\right) \left({q'}_2^{\mu} - {q^0}_2^{\mu}\right) \tag{2}$$

where q^0 indicate a q point that we sampled in the BZ. The mean square deviation of $W(q_2')$ in the volume Ω_{BZ}/N_q around q^0 will be given by:

$$\sigma^2_{W,q_2^0} = \sum_{\mu} \left(\frac{\partial W}{\partial q_2^{\mu}}\right)^2 E\left\{\left(q_2'^{\mu} - q_2^{0\mu}\right)^2\right\} \tag{3}$$

using:

$$E\left\{\left(q_2'^{\mu} - q_2^{0\mu}\right)^2\right\} = \left(\frac{\Delta q_2^{\mu}}{\sqrt{12}}\right)^2 \tag{4}$$

so that we have, for the mean square deviation:

$$\sigma_{W,q_2^0} = \frac{1}{\sqrt{12}} \sqrt{\sum_{\mu} \left(\frac{\partial W}{\partial q_2^{\mu}}\right)^2 (\Delta q_2^{\mu})^2} \tag{5}$$

$$= \frac{1}{\sqrt{12}} \sqrt{\sum_{\mu} \left[\sum_{\alpha} \left(\frac{\partial W}{\partial q_2^{\alpha}}\right) \frac{Q_{\alpha}^{\mu}}{N_{\mu}}\right]^2} \tag{6}$$

where we use μ to indicate direction along a reciprocial lattice vector and α for the cartesian direction. The term $\partial W/\partial q_2^{\alpha}$ is given by:

$$\frac{\partial(\omega_2 + \omega_3)}{\partial q_2^{\alpha}} = v_{q_2}^{\alpha} + \sum_{\beta} v_{q_3}^{\beta} \frac{\partial q_3^{\beta}}{\partial q_2^{\alpha}} = v_{q_1}^{\alpha} - v_{q_2}^{\alpha} \tag{7}$$

where the second equal comes from the requirement that $q_1 + q_2 = q$. The final smearing width is given by the group velocity of phonons:

$$\sigma_{W,q_2^0} = \frac{1}{\sqrt{12}} \sqrt{\sum_{\mu} \left[\sum_{\alpha} \left(v_{q_2}^{\alpha} - v_{q_3}^{\alpha}\right) \frac{Q_{\alpha}^{\mu}}{N_{\mu}}\right]^2} \tag{8}$$

The second delta function $\delta(q_1 - q_2 - q_3)\delta(\omega_1 + \omega_2 - \omega_3)$ gives:

$$\frac{\partial(-\omega_2 + \omega_3)}{\partial q_2^{\alpha}} = -v_{q_2}^{\alpha} + \sum_{\beta} v_{q_3}^{\beta} \frac{\partial q_3^{\beta}}{\partial q_2^{\alpha}} = -(v_{q_1}^{\alpha} + v_{q_2}^{\alpha}) \tag{9}$$

so that

$$\sigma_{W,q_2^0} = \frac{1}{\sqrt{12}} \sqrt{\sum_{\mu} \left[\sum_{\alpha} \left(v_{q_2}^{\alpha} + v_{q_3}^{\alpha}\right) \frac{Q_{\alpha}^{\mu}}{N_{\mu}}\right]^2} \tag{10}$$

[1] ShengBTE: a solver for boltzmann transport equation for phonon

2 The case of four phonon

The delta function in the case of four phonon interaction is:

$$\begin{aligned}
&\delta(q_1 - q_2 - q_3 - q_4)\delta(\omega_1 - \omega_2 - \omega_3 - \omega_4) \\
&\delta(q_1 - q_2 - q_3 - q_4)\delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) \\
&\delta(q_1 - q_2 - q_3 - q_4)\delta(\omega_1 - \omega_2 + \omega_3 + \omega_4)
\end{aligned} \tag{11}$$

with now two free paramter, we have, for the first case:

$$W(q_2, q_3) = \omega_2 + \omega_3 + \omega_4 \tag{12}$$

To linear approximation, we can write:

$$W(q_2', q_3') \approx W(q_2^0, q_3^0) + \sum_\mu \left(\frac{\partial W}{\partial q_2^\mu}\right)\left(q_2'^\mu - q_2^{0\mu}\right) + \sum_\nu \left(\frac{\partial W}{\partial q_3^\nu}\right)\left(q_3'^\nu - q_3^{0\nu}\right) \tag{13}$$

The mean square deviation is given by:

$$\sigma^2_{W,q_2^0,q_3^0} = \sum_\mu \left(\frac{\partial W}{\partial q_2^\mu}\right)^2 E\left\{\left(q_2'^\mu - q_2^{0\mu}\right)^2\right\} + \sum_\nu \left(\frac{\partial W}{\partial q_3^\nu}\right)^2 E\left\{\left(q_3'^\nu - q_3^{0\nu}\right)^2\right\} \tag{14}$$

so that sigma is given by:

$$\sigma_{W,q_2^0,q_3^0} = \frac{1}{\sqrt{12}}\sqrt{\sum_\mu \left(\frac{\partial W}{\partial q_2^\mu}\right)^2 (\Delta q_2^\mu)^2 + \sum_\nu \left(\frac{\partial W}{\partial q_3^\nu}\right)^2 (\Delta q_3^\nu)^2} \tag{15}$$

changing the coordinate from reciprocial axis to cartesian axis, we have:

$$\sigma_{W,q_2^0,q_3^0} = \frac{1}{\sqrt{12}}\sqrt{\sum_\mu \left[\sum_\alpha \left(\frac{\partial W}{\partial q_2^\alpha}\right)\frac{Q_\alpha^\mu}{N_\mu}\right]^2 + \sum_\nu \left[\sum_\beta \left(\frac{\partial W}{\partial q_3^\beta}\right)\frac{Q_\beta^\nu}{N_\nu}\right]^2} \tag{16}$$

the linear coefficients are given by:

$$\frac{\partial W}{\partial q_2^\alpha} = \frac{\partial\left[\omega_2 + \omega_3 + \omega_4\right]}{\partial q_2^\alpha} = v_{q_2}^\alpha - v_{q_4}^\alpha \tag{17}$$

$$\frac{\partial W}{\partial q_3^\alpha} = \frac{\partial\left[\omega_2 + \omega_3 + \omega_4\right]}{\partial q_3^\alpha} = v_{q_3}^\alpha - v_{q_4}^\alpha \tag{18}$$

since $\left.\frac{\partial \omega_2(q_2)}{\partial q_1^\alpha}\right|_{q_2^0} = 0$ to first order. The final result is thus:

$$\sigma_{W,q_2^0,q_3^0} = \frac{1}{\sqrt{12}}\sqrt{\sum_\mu \left[\sum_\alpha \left(v_{q_2}^\alpha - v_{q_4}^\alpha\right)\frac{Q_\alpha^\mu}{N_\mu}\right]^2 + \sum_\nu \left[\sum_\beta \left(v_{q_3}^\beta - v_{q_4}^\beta\right)\frac{Q_\beta^\nu}{N_\nu}\right]^2} \tag{19}$$

For the other two delta function, the mean square deviation will be the same, we go through the above step to find:

$$\frac{\partial\left[\omega_2 - \omega_3 - \omega_4\right]}{\partial q_2^\alpha} = v_{q_2}^\alpha + v_{q_4}^\alpha \tag{20}$$

$$\frac{\partial\left[\omega_2 - \omega_3 - \omega_4\right]}{\partial q_3^\alpha} = v_{q_3}^\alpha - v_{q_4}^\alpha \tag{21}$$

and we will have:

$$\sigma_{W,q_2^0,q_3^0} = \frac{1}{\sqrt{12}}\sqrt{\sum_\mu \left[\sum_\alpha \left(v_{q_2}^\alpha + v_{q_4}^\alpha\right)\frac{Q_\alpha^\mu}{N_\mu}\right]^2 + \sum_\nu \left[\sum_\beta \left(v_{q_3}^\beta - v_{q_4}^\beta\right)\frac{Q_\beta^\nu}{N_\nu}\right]^2} \tag{22}$$