Interpolation of phonons

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1 Transformation of phonon green's function

The temperature phonon green's function in terms of phonon creation and annihilation operator can be written as

$$G(qvv',\tau) = \langle \mathcal{T}[A_{qv}(\tau)A^{\dagger}_{qv'}(0)]\rangle \tag{1}$$

where $A_{qv} = a_{qv}+a^{\dagger}_{-qv}$. The atomic displacement operator is connected with the phonon operator by transformation

$$\eta_{lb} = \sum_{qv}\left(\frac{\hbar}{2N\omega_{qv}m_b}\right)^{\frac{1}{2}} e^{b}_{qv}e^{iql}A_{qv} \tag{2}$$

$$A_{qv} = \sum_{lb}\left(\frac{2\omega_{qv}m_b}{N\hbar}\right)^{\frac{1}{2}} e^{b*}_{qv}e^{-iql}\eta_{lb} \tag{3}$$

The phonon green's function in terms of atomic displacement operator is written as:

$$D_{ll'bb'}(\tau) = \langle \mathcal{T}[\eta_{lb}(\tau)\eta_{l'b'}(0)]\rangle \tag{4}$$

substituting Eq.2, we obtain the relationship:

$$\begin{aligned}
D_{ll'bb'}(\tau) &= \sum_{qq'vv'}\langle \mathcal{T}[\left(\frac{\hbar}{2N\omega_{qv}m_b}\right)^{\frac{1}{2}} e^{b}_{qv}e^{iql}A_{qv}(\tau)\left(\frac{\hbar}{2N\omega_{q'v'}m_{b'}}\right)^{\frac{1}{2}} e^{b'*}_{q'v'}e^{-iq'l'}A^{\dagger}_{q'v'}(0)]\rangle &(5)\\
&= \frac{\hbar}{2N}\sum_{qq'vv'}(\omega_{qv}m_b\omega_{q'v'}m_{b'})^{-\frac{1}{2}}\langle \mathcal{T}[e^{b}_{qv}e^{iql}A_{qv}(\tau)e^{b'*}_{q'v'}e^{-iq'l}A^{\dagger}_{q'v'}(0)]\rangle &(6)\\
&= \frac{\hbar}{2}\sum_{qvv'}(\omega_{qv}m_b\omega_{qv'}m_{b'})^{-\frac{1}{2}}e^{iq(l-l')}e^{b}_{qv}e^{b'*}_{qv'}\langle \mathcal{T}[A_{qv}(\tau)A^{\dagger}_{qv'}(0)]\rangle &(7)\\
& &(8)
\end{aligned}$$

where we used the result $\sum_{qq'} e^{i(ql-q'l')} = N\delta_{qq'}e^{iq(l-l')}$. The reverse of the above relationship is:

$$\begin{aligned}
G(qvv',\tau) &= \sum_{ll'bb'}\frac{2}{N\hbar}(\omega_{qv}\omega_{qv'}m_bm_{b'})^{\frac{1}{2}}e^{b*}_{qv}e^{b'}_{qv'}e^{-iq(l-l')}\langle \mathcal{T}[\eta_{lb}(\tau)\eta_{l'b'}(0)]\rangle\\
&= \sum_{ll'bb'}\frac{2}{N\hbar}(\omega_{qv}\omega_{qv'}m_bm_{b'})^{\frac{1}{2}}e^{b*}_{qv}e^{b'}_{qv'}e^{-iq(l-l')}D_{ll'bb'}(\tau) &(9)
\end{aligned}$$

This equation gives the interpolation of the green's function from the correlation function of atomic displacement. If we assume function $G(qvv',\tau)$ is diagonal in terms of phonon branches v, then, we have:

$$\begin{aligned}
G(q'v',\tau) &= \sum_{ll'bb'}\frac{2}{N\hbar}\omega_{q'v'}(m_bm_{b'})^{\frac{1}{2}}e^{b*}_{q'v'}e^{b'}_{q'v'}e^{-iq'(l-l')}\left(\frac{\hbar}{2}\sum_{qv}\omega^{-1}_{qv}(m_bm_{b'})^{-\frac{1}{2}}e^{iq(l-l')}e^{b}_{qv}e^{b'*}_{qv}G(qv,\tau)\right) &(10)\\
&= \frac{1}{N}\sum_{ll'bb'qv}\frac{\omega_{q'v'}}{\omega_{qv}}e^{b*}_{q'v'}e^{b'}_{q'v'}e^{b}_{qv}e^{b'*}_{qv}e^{-i(q-q')(l-l')}G(qv,\tau) &(11)
\end{aligned}$$

In frequency space, we have:

$$G(q'v', i\omega_n) = \frac{1}{N} \sum_{ll'bb'qv} \frac{\omega_{q'v'}}{\omega_{qv}} e^{b*}_{q'v'} e^{b'}_{q'v'} e^{b}_{qv} e^{b'*}_{qv} e^{-i(q-q')(l-l')} G(qv, i\omega_n) \tag{12}$$

which can be analytically continued to real frequency and coinicide with the retarded function.

$$G_0^R(qv,\omega) = \frac{1}{\omega + \omega_{qv}} - \frac{1}{\omega - \omega_{qv}} \tag{13}$$

which has pole at frequency ω_{qv} and $-\omega_{qv}$. The interacting phonon greens function can be written with self-energy:

$$\begin{aligned} G^R(qv,\omega)^{-1} &= G_0^R(qv,\omega)^{-1} - \Sigma_{qv}(\omega) && (14)\\ &= \frac{\omega^2 - \omega_{qv}^2}{2\omega_{qv}} - \Sigma_{qv}(\omega) && (15) \end{aligned}$$

taking the self-energy to be $\mathrm{Re}\Sigma_{qv}(\omega_{qv}) + i\mathrm{Im}\Sigma_{qv}(\omega_{qv})$, we can find the pole of the interacting phonon greens function by $G^R(qv,\omega)^{-1} = 0$. The result can be approximated as:

$$G^R(qv,\omega) = \frac{1}{\omega + \omega_{qv} + i\Gamma_{qv}} - \frac{1}{\omega - \omega_{qv} - i\Gamma_{qv}} \tag{16}$$

So that the interpolated function can be written as:

$$G^R(q'v',\omega) = \frac{1}{N} \sum_{ll'bb'qv} \frac{\omega_{q'v'}}{\omega_{qv}} e^{b*}_{q'v'} e^{b'}_{q'v'} e^{b}_{qv} e^{b'*}_{qv} e^{-i(q-q')(l-l')} \left[\frac{1}{\omega + \omega_{qv} + i\Gamma_{qv}} - \frac{1}{\omega - \omega_{qv} - i\Gamma_{qv}}\right] \tag{17}$$

Finally, we find the pole of the function

2 Phonon green's function

We write the phonon Green's function as:

$$G(qvv';t) = -i\langle \mathcal{T}[A_{qv}(t)A^\dagger_{qv'}(0)]\rangle \tag{18}$$

The time dependence of the operator is:

$$A(t) = e^{i\frac{t}{\hbar}H} A e^{-i\frac{t}{\hbar}H} \tag{19}$$

$\mathcal{T}$ is the Wick's time ordering operator and average is taken at a finite temperature:

$$iG(qvv';t) = \begin{cases} \frac{1}{Z}\mathrm{Tr}\sum_n \langle n|e^{-\beta H} e^{i\frac{t}{\hbar}H}(a_{qv} + a^\dagger_{-qv})e^{-i\frac{t}{\hbar}H}(a^\dagger_{qv'} + a_{-qv'})|n\rangle & t > 0 \\ \frac{1}{Z}\mathrm{Tr}\sum_n \langle n|e^{-\beta H}(a^\dagger_{qv'} + a_{-qv'})e^{i\frac{t}{\hbar}H}(a_{qv} + a^\dagger_{-qv})e^{-i\frac{t}{\hbar}H}|n\rangle & t < 0 \end{cases} \tag{20}$$

We can obtain the result:

$$\begin{aligned} G(qvv';t>0) &= -i\delta_{vv'}(e^{i\omega_{qv}t}\langle n_{qv}\rangle + e^{-i\omega_{qv}t}\langle n_{qv}+1\rangle) && (21)\\ G(qvv';t<0) &= -i\delta_{vv'}(e^{-i\omega_{qv}t}\langle n_{qv}\rangle + e^{i\omega_{qv}t}\langle n_{qv}+1\rangle) && (22) \end{aligned}$$

Define the fourier transformation into frequency space:

$$\begin{aligned} G(qvv';\omega) &= \int_{-\infty}^{\infty} G(qvv';t)e^{-i\omega t}dt && (23)\\ &= \int_{-\infty}^{0} G(qvv';t<0)e^{-i\omega t}dt + \int_{0}^{\infty} G(qvv';t>0)e^{-i\omega t}dt && (24)\\ & && (25) \end{aligned}$$

and we have:

$$\int_0^\infty G(qv;t>0)e^{-i\omega t}dt = -i\int_0^\infty \left(e^{i(\omega_{qv}-\omega)t}\langle n_{qv}\rangle + e^{-i(\omega_{qv}+\omega)t}\langle n_{qv}+1\rangle\right)dt$$
$$= -i\lim_{\eta\to 0^+}\left(\frac{\langle n_{qv}\rangle}{i(\omega-\omega_{qv})+\eta} + \frac{\langle n_{qv}+1\rangle}{i(\omega+\omega_{qv})+\eta}\right)$$
$$= -\lim_{\eta\to 0^+}\left(\frac{\langle n_{qv}\rangle}{\omega-\omega_{qv}-i\eta} + \frac{\langle n_{qv}+1\rangle}{\omega+\omega_{qv}-i\eta}\right) \tag{26}$$

Similarly, for the second term in the integral, we have:

$$\int_{-\infty}^0 G(qvv';t<0)e^{-i\omega t}dt = -i\int_{-\infty}^0 \left(e^{-i(\omega_{qv}+\omega)t}\langle n_{qv}\rangle + e^{i(\omega_{qv}-\omega)t}\langle n_{qv}+1\rangle\right)dt$$
$$= i\int_0^\infty \left(e^{i(\omega_{qv}+\omega)t}\langle n_{qv}\rangle + e^{-i(\omega_{qv}-\omega)t}\langle n_{qv}+1\rangle\right)dt$$
$$= i\lim_{\eta\to 0^+}\left(\frac{\langle n_{qv}\rangle}{-i(\omega+\omega_{qv})+\eta} + \frac{\langle n_{qv}+1\rangle}{i(\omega_{qv}-\omega)+\eta}\right)$$
$$= \lim_{\eta\to 0^+}\left(-\frac{\langle n_{qv}\rangle}{\omega+\omega_{qv}-i\eta} + \frac{\langle n_{qv}+1\rangle}{\omega_{qv}-\omega-i\eta}\right) \tag{27}$$

So that the complete green's function is then:

$$G(qvv';\omega) = \delta_{vv'}\lim_{\eta\to 0^+}\left(-\frac{\langle n_{qv}\rangle}{\omega+\omega_{qv}-i\eta} + \frac{\langle n_{qv}+1\rangle}{\omega_{qv}-\omega-i\eta} - \frac{\langle n_{qv}\rangle}{\omega-\omega_{qv}-i\eta} - \frac{\langle n_{qv}+1\rangle}{\omega+\omega_{qv}-i\eta}\right) \tag{28}$$

Appendix

This section summarized the formulation of paper *Review of Modern Physics, 89 Electron-phonon from first principle*. In that work, the displacement-displacement correlation function of atomic motion is given by the function:

$$D_{k\alpha p,k'\alpha' p'}(t) = -\frac{i}{\hbar}\langle \mathcal{T}[\tau_{k\alpha p}(t)\tau_{k'\alpha' p'}(0)]\rangle \tag{29}$$