

# Interpolation of phonons

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## 1 Transformation of phonon green's function

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

$$G(qvv'; t) = \langle i | \mathcal{T}[A_{qv}(t)A_{qv'}^\dagger(0)] | i \rangle \quad (1)$$

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

$$\eta_{lb} = \sum_{qv} \left( \frac{\hbar}{2N\omega_{qv}m_b} \right)^{\frac{1}{2}} e_{qv}^b e^{iq'l} A_{qv} \quad (2)$$

$$A_{qv} = \sum_{lb} \left( \frac{2\omega_{qv}m_b}{N\hbar} \right)^{\frac{1}{2}} e_{qv}^{b*} e^{-iq'l} \eta_{lb} \quad (3)$$

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

$$D_{ll'bb'}(t) = \langle i | \mathcal{T}[\eta_{lb}(t)\eta_{l'b'}^\dagger(0)] | i \rangle \quad (4)$$

substituting Eq.2, we obtain the relationship:

$$D_{ll'bb'}(t) = \sum_{qq'vv'} \langle i | \mathcal{T} \left[ \left( \frac{\hbar}{2N\omega_{qv}m_b} \right)^{\frac{1}{2}} e_{qv}^b e^{iq'l} A_{qv}(t) \left( \frac{\hbar}{2N\omega_{q'v'}m'_b} \right)^{\frac{1}{2}} e_{q'v'}^{b'*} e^{-iq'l'} A_{q'v'}^\dagger(0) \right] | i \rangle \quad (5)$$

$$= \frac{\hbar}{2N} \sum_{qq'vv'} (\omega_{qv}m_b\omega_{q'v'}m'_b)^{-\frac{1}{2}} \langle i | \mathcal{T}[e_{qv}^b e^{iq'l} A_{qv}(t) e_{q'v'}^{b'*} e^{-iq'l'} A_{q'v'}^\dagger(0)] | i \rangle \quad (6)$$

$$= \frac{\hbar}{2} \sum_{qv v'} (\omega_{qv}m_b\omega_{q'v'}m'_b)^{-\frac{1}{2}} e^{iq(l-l')} e_{qv}^b e_{q'v'}^{b'*} \langle i | \mathcal{T}[A_{qv}(t)A_{q'v'}^\dagger(0)] | i \rangle \quad (7)$$

$$(8)$$

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

$$G_{qv v'}(t) = \sum_{ll'bb'} \frac{2}{N\hbar} (\omega_{qv}\omega_{q'v'}m_b m'_b)^{\frac{1}{2}} e_{qv}^{b*} e_{q'v'}^{b'} e^{iq(l-l')} D_{ll'bb'}(t) \quad (9)$$

## 2 Form of the phonon green's function