Green Kubo formula for thermal conductivity

WH

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1 formulation

With the harmonic hamiltonian and periodic condition not assumed:

$$H = \sum_i \frac{1}{2m_b} p_i p_i + \frac{1}{2}\sum_{ij} G_{ij} u_i u_j + V_0 \tag{1}$$

G is the harmonic force constants. i is the index of the atom in the whole sample that we concern. p_i and u_i are the momentum and displacement of atom i. Summation of cartesian direction is implied. The heat flux can be written as:

$$J = \frac{1}{2}\sum_{ij}(R_i - R_j) G_{ij} u_i \dot{u}_j \tag{2}$$

using the standard form of phonon creation and annihiliation operator (taking summation of q to consist of only Γ, then $N = 1$):

$$u_i = \sum_m \sqrt{\frac{\hbar}{2\omega_m m_i}} e_m^i (a_m + a_m^\dagger) \tag{3}$$

$$p_i = -i\sum_m \sqrt{\frac{\hbar\omega_m m_i}{2}} e_m^i (a_m - a_m^\dagger) \tag{4}$$

The current flux operator is then:

$$\begin{aligned} J &= -\frac{i}{2}\sum_{ij}(R_i - R_j) G_{ij} \sum_m \sqrt{\frac{\hbar}{2\omega_m m_i}} e_m^i (a_m + a_m^\dagger) \sum_n \sqrt{\frac{\hbar\omega_m}{2m_j}} e_n^j (a_n - a_n^\dagger) \\ &= -\frac{i\hbar}{2}\sum_{mn}\left(\frac{1}{2}\sum_{ij}\frac{R_i - R_j}{\sqrt{m_i m_j}} G_{ij} e_m^i e_n^j\right)\left(\frac{\omega_n}{\omega_m}\right)^{1/2} (a_m + a_m^\dagger)(a_n - a_n^\dagger) \\ &= -\frac{i\hbar}{2} V_{mn}\omega_n (a_m + a_m^\dagger)(a_n - a_n^\dagger) \end{aligned} \tag{5}$$

with the term V_{mn} given by:

$$V_{mn} = \frac{1}{2\sqrt{\omega_m \omega_n}} \sum_{ij} \frac{R_i - R_j}{\sqrt{m_i m_j}} G_{ij} e_m^i e_n^j \tag{6}$$

The green kubo formula of thermal conductivity is given by:

$$\kappa_{\alpha\beta} = \frac{1}{VT}\int_0^\beta d\tau \int_0^{+\infty} \langle J_\alpha(t + i\hbar\tau) J_\beta(0)\rangle \tag{7}$$