Coherent Heat Transport in Nanostructures by Numerical Solution of Quantum Kinetic Equation of Phonons

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The phonon Boltzmann equation has been widely used in explaining heat transport through nanostructures. However, it becomes no longer valid when the characteristic size of system becomes comparable to or even smaller than the dominant wavelength of phonons, which often happens at very low temperature or in very small nanostructures. In this work, we will propose a methodology to describe the coherent heat transport in nanostructures based on the more fundamental quantum kinetic equation for single-phonon density matrix (Eq. (3) in Page 2) [1]. We also develop a finite difference method for numerical solution of the quantum kinetic equation. The macroscopic field variables including the energy density and heat flux are related to the diagonal components of the density matrix (Eq. (4) and Eq. (5) in Page 2) [2]. The new methodology is demonstrated through modeling heat transport in silicon thin film with a thickness less than 10nm at different temperatures. The results indicate correlation behaviors between different phonon modes at very low temperature, and are reduced to the solution of classical phonon Boltzmann equation around room temperature. With the help of Wigner function (Eq. (6) in Page 2), it is also shown that the phonon Boltzmann equation is recovered from the quantum kinetic equation in the absence of correlations. The present work will promote the understanding and modeling of coherent phonon heat transport in crystals.

[1] F.T. Vasko and O.E. Raichev, Quantum kinetic theory and applications: electrons, photons, phonons. Springer, New York, 2005.
[2] R.J. Hardy, Energy-flux operator for a lattice. Physical Review, 132(1): 168(1963).

The equation of density matrix is the fundamental equation in quantum statistical mechanics [1]:

$$i\hbar\frac{\partial\hat{\eta}_t}{\partial t}=\left[\hat{H},\hat{\eta}_t\right], \tag{1}$$

where $\hat{\eta}_t$ is the many-body density matrix and $\hat{H}$ is the Hamiltonian operator of the system. The solution of Eq. (1) is not easy even for very simple cases. Therefore the one-phonon density matrix is introduced as [1]:

$$N_t\left(\mathbf{k}'j',\mathbf{k}j\right)=\mathrm{Tr}\left(\hat{a}^+_{\mathbf{k}j}\hat{a}_{\mathbf{k}'j'}\hat{\eta}_t\right), \tag{2}$$

where '$\mathbf{k}j$' denotes a phonon mode, $\hat{a}^+_{\mathbf{k}j}$ and $\hat{a}_{\mathbf{k}j}$ being the phonon creation operator and destruction operator respectively. As a first step, we consider the harmonic approximation such that $\hat{H}=\sum_{\mathbf{k}j}\hbar\omega_j\left(\mathbf{k}\right)\left(\hat{a}^+_{\mathbf{k}j}\hat{a}_{\mathbf{k}j}+\frac{1}{2}\right)$. Combining Eq. (1) and Eq. (2), we obtain the quantum kinetic equation of phonons [1]:

$$\left[i\hbar\frac{\partial}{\partial t}-\hbar\left(\omega_{j'}\left(\mathbf{k}'\right)-\omega_j\left(\mathbf{k}\right)\right)\right]N_t\left(\mathbf{k}'j',\mathbf{k}j\right)=0. \tag{3}$$

A finite difference scheme is then devised for numerical solution of Eq. (3). In the harmonic approximation, the calculation of energy density and heat flux is mainly contributed by the diagonal component of the one-phonon density matrix [2]:

$$e=\frac{1}{V}\sum_{\mathbf{k}j}\sum_{\mathbf{k}'j'}\hbar\omega_j\left(\mathbf{k}\right)\delta_{jj'}\delta_{\mathbf{k}\mathbf{k}'}N_t\left(\mathbf{k}'j',\mathbf{k}j\right), \tag{4}$$

$$\mathbf{q}=\frac{1}{V}\sum_{\mathbf{k}j}\sum_{\mathbf{k}'j'}\hbar\omega_j\left(\mathbf{k}\right)\mathbf{v}_{\mathrm{g}}\left(\mathbf{k}j\right)\delta_{jj'}\delta_{\mathbf{k}\mathbf{k}'}N_t\left(\mathbf{k}'j',\mathbf{k}j\right). \tag{5}$$

To obtain the local energy density and heat flux in Eq. (4) and Eq. (5), we have to use the wave packet representation of phonons through a superposition of normal modes with a small spread of wave vectors.

The phonon Wigner function can be defined as [1]:

$$N\left(\mathbf{r},t,\mathbf{k}j\right)=\sum_{\mathbf{g}}\exp\left(i\mathbf{g}\cdot\mathbf{r}\right)N_t^j\left(\mathbf{k}+\frac{\mathbf{g}}{2},\mathbf{k}-\frac{\mathbf{g}}{2}\right), \tag{6}$$

where $N_t\left(\mathbf{k}j,\mathbf{k}'j'\right)=N_t^j\left(\mathbf{k}',\mathbf{k}\right)\delta_{jj'}$ in the absence of correlation between different phonon polarizations. With the help of Eq. (6), one can derive from Eq. (3) the phonon Boltzmann equation without collision term:

$$\frac{\partial N\left(\mathbf{r},t,\mathbf{k}j\right)}{\partial t}+\mathbf{v}_{\mathrm{g}}\left(\mathbf{k}j\right)\cdot\frac{\partial N\left(\mathbf{r},t,\mathbf{k}j\right)}{\partial\mathbf{r}}=0, \tag{7}$$

where the phonon group velocity is: $\mathbf{v}_{\mathrm{g}}\left(\mathbf{k}j\right)=\partial\omega_j\left(\mathbf{k}\right)/\partial\mathbf{k}$. The phonon collision term will be recovered when the anharmonic terms are considered in the Hamiltonian operator.