Physica B 510 (2017) 22–28

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Quantum noise theory for phonon transport through nanostructures

Li Wan[a,*], Yunmi Huang[a], Changcheng Huang[b]

[a] Department of Physics, Wenzhou University, Wenzhou 325035, P.R. China
[b] Department of Computer Science, Wenzhou University, Wenzhou 325035, P.R. China

ARTICLE INFO

Keywords:
Quantum noise
Phonon
Quantum Langevin equation
Thermal conductivity

ABSTRACT

We have developed a quantum noise approach to study the phonon transport through nanostructures. The nanostructures acting as phonon channels are attached to two phonon reservoirs. And the temperature drop between the two reservoirs drives the phonon transport through the channels. We have derived a quantum Langevin equation(QLE) to describe the phonon transport with the quantum noise originated from the thermal fluctuation of the reservoirs. Within the Markov approximation, the QLE is used to get the thermal conductivity κ of the nanostructures and the finite size effect of the κ then is studied. In this study, the advantage of the quantum noise approach lays on the fact that no any local temperature needs to be defined for the nanostructures in its non-equilibrium state.

1. Introduction

The development of nano technologies scales electronic devices down to mesoscopic size. Similar to the electrons showing their peculiar behaviors in the nano-structured devices, thermal transport in the structures has been confirmed to have finite size effects by theories and experiments [1–11]. Especially, the thermal conductivity κ of the structures decreases with the decreasing of the structure size. Nowadays, study of the finite size effects of the thermal transport has became an important issue and has a significant application in the development of nano technologies [6,7]. For these nanostructures fabricated by dielectric or semiconductor materials, the thermal transport is through lattice interaction rather than by electrons. Various methods have been proposed to study the finite size effect of the thermal transport through the lattice interaction [12–18]. Especially, a quantum Langevin equation (QLE) for the lattice vibration in the real space has been obtained, where displacements and momenta of the lattices are used as operators in the equation [6]. In those real space models, local temperatures have to be defined to describe the energy flow through the lattices. In order to make the temperature definition acceptable in the non-equilibrium systems, the assumption of the coarse-grain-equilibrium(CGE) has to be applied [6,7]. However, for structures with their scales down to a few nanometers, the CGE is expected to be invalid. In order to remove the CGE assumption, we converse the study of the thermal transport in the phonon space, and develop a version of the quantum Langevin equation for the phonon transport by using the quantum noise approach. The creation and annihilation operators of phonons are applied and the quantum noise is originated from the thermal leads. In this paper, we will show the details of the development and then study the finite size effects of the κ by using the equation.

Generally, the nanostructures studied for the thermal transport are simplified to be an one-dimensional chain with oscillators distributed uniformly in order [6,7]. Two ends of the nanostructures are attached to two thermal leads, which are set at two different temperatures respectively. The drop of temperature between the two leads drives the thermal flow through the chain by the interactions between the oscillators. In order to describe the energy of each oscillator for the thermal flow, local temperatures have to be defined for the oscillators in such non-equilibrium system. It is well known that the temperature actually is a thermodynamical concept for equilibrium systems. Thus, in various models which treat the thermal transport in the real space, the system is assumed to consist of a large number of coarse grains with each grain in its own thermodynamic equilibrium even though the total system is still kept in the non-equilibrium state [6,7]. Such assumption is called as the coarse-grain-equilibrium (CGE), which is invalid for the nanostructures due to the non-equilibrium nature of the coarse grains. However, the CGE assumption can be removed if we convert the study of the thermal transport into the phonon space.

Phonons have been well accepted as quasi-particles to describe the lattice vibrations in solids [19]. When the system is in equilibrium state, phonons are stimulated by the temperature and the Bose-Einstein distribution can bridge the phonon density and the temperature. However, in the non-equilibrium cases, it is wrong to define the phonon density at any particular space position due to the fact that phonons are extension lattice waves in the whole system. Therefore, it

* Corresponding author.
E-mail address: lwan@wzu.edu.cn (L. Wan).

http://dx.doi.org/10.1016/j.physb.2017.01.016
Received 15 August 2016; Received in revised form 5 January 2017; Accepted 13 January 2017
Available online 15 January 2017

is meaningless to define the local temperatures in the non-equilibrium system when the phonon space is used for the study of the thermal transport. And then the CGE assumption is removed naturally.

In this study, the two thermal leads are in their own equilibrium states and are considered as two phonon reservoirs. The Hamiltonian of the nanostructures can be written in the terms of phonon. The phonon modes of the nanostructures are discrete and determined by the structure size of the system [20]. In this way, the finite size effect then is involved by the discrete phonon modes. By coupling phonons of the system and phonons of the reservoirs, the temperature drop between the two reservoirs drives the phonon transport through the nanostructures. The thermal fluctuation of the reservoirs acts as quantum noise, which is used to derive the QLE. The QLE has been developed for electron transport, but it is still lack for the phonon transport [21–24]. In this work, the phonon version of the QLE is obtained.

2. Quantum langevin equation

2.1. Hamiltonian

The total Hamiltonian H of the full model consists of two parts $H = H_0 + H_I$. Here, H_0 is the Hamiltonian of the full model without the coupling between the reservoirs and the system. And H_I is the interaction Hamiltonian for the coupling in the model. The H_0 and H_I read

$$H_0 = \sum_p \hbar\omega_p^L a_p^+ a_p + \sum_k \hbar\omega_k b_k^+ b_k + \sum_q \hbar\omega_q^R c_q^+ c_q,$$
$$H_I = i\hbar \sum_{p,k} \xi_{p,k} a_p^+ b_k + i\hbar \sum_{q,k} \eta_{q,k} c_q^+ b_k - i\hbar \sum_{p,k} \xi_{p,k} b_k^+ a_p - i\hbar \sum_{q,k} \eta_{q,k} b_k^+ c_q. \tag{1}$$

On the right hand side of the H_0, the first and the third terms are the Hamiltonians of the left and right reservoirs respectively, which can be identified by the superscripts L or R of the phonon frequency ω. The second term is the Hamiltonian of the system. The annihilation operators of phonons have been denoted by a, b and c for the left reservoir, the system and the right reservoir, respectively. The corresponding create operators are then denoted by a^+, b^+ and c^+. The subscripts in the Hamiltonians represent the phonon modes. On the right hand side of the H_I, ξ is the damping parameter coupling the left reservoir and the system, and $\xi_{p,k}$ is for the coupling between the pth phonon mode and the k^{th} mode. η is the coupling between the right reservoir and the system, which has a similar notation of ξ. It should be noted that the phonon modes of the system are selected by the finite size effect and take the values of $\Lambda = \frac{2\pi l}{MD}$ with M the oscillator number and D the lattice parameter of the system [20]. The l takes only the integers in the range from $-\frac{M}{2}$ to $\frac{M}{2}$. The finite size effects on the κ then can be realized through the number M. For the reservoirs, the sizes are regarded to be infinitely long and the temperatures of the reservoirs are not influenced by the system during the phonon transport.

2.2. Equation of motion

By using the Heisenberg equation, we get the following equations of motion directly from the Hamiltonians in eq. (1).

$$\dot{a}_p = -i\omega_p^L a_p + \sum_k \xi_{p,k} b_k,$$
$$\dot{b}_k = -i\omega_k b_k - \sum_p \xi_{p,k} a_p - \sum_q \eta_{q,k} c_q$$
$$\dot{c}_q = -i\omega_q^R c_q + \sum_k \eta_{q,k} b_k. \tag{2}$$

The dot on the top of the annihilation operators means the time derivative of the operators. The formal solutions of a_p and c_q read

$$a_p = e^{-i\omega_p^L t} a_p(0) + \sum_k \xi_{p,k} \int_0^t dt' e^{-i\omega_p^L (t-t')} b_k(t'),$$
$$c_q = e^{-i\omega_p^R t} c_q(0) + \sum_k \eta_{q,k} \int_0^t dt' e^{-i\omega_q^R (t-t')} b_k(t'). \tag{3}$$

Here, $a_p(0)$ and $c_q(0)$ are referred to as the operators at the instant when the coupling between the system and the reservoirs was just switched on. Multiplying both sides of the equations in eq. (3) by the damping parameters, we obtain

$$\sum_p \xi_{p,k} a_p = \sum_p \xi_{p,k} e^{-i\omega_p^L t} a_p(0) + \sum_{p,k'} \xi_{p,k} \xi_{p,k'} \int_0^t dt' e^{-i\omega_p^L (t-t')} b_{k'}(t'),$$
$$\sum_q \eta_{q,k} c_q = \sum_q \eta_{q,k} e^{-i\omega_q^R t} c_q(0) + \sum_{q,k'} \eta_{q,k} \eta_{q,k'} \int_0^t dt' e^{-i\omega_q^R (t-t')} b_{k'}(t'). \tag{4}$$

Substitute eq. (4) into the equation of $\dot{b}_k$ in the eq (2) to get the equation of motion

$$\dot{b}_k = -i\omega_k b_k - \sum_p \xi_{p,k} e^{-i\omega_p^L t} a_p(0) - \sum_{p,k'} \xi_{p,k} \xi_{p,k'} \int_0^t dt' e^{-i\omega_p^L (t-t')} b_{k'}(t')$$
$$- \sum_q \eta_{q,k} e^{-i\omega_q^R t} c_q(0) - \sum_{q,k'} \eta_{q,k} \eta_{q,k'} \int_0^t dt' e^{-i\omega_q^R (t-t')} b_{k'}(t'). \tag{5}$$

2.3. Markov approximation

For simplicity, we note

$$\mathcal{L}_k = -\sum_p \xi_{p,k} e^{-i\omega_p^L t} a_p(0); \quad \mathcal{R}_k = -\sum_q \eta_{q,k} e^{-i\omega_q^R t} c_q(0). \tag{6}$$

The $\mathcal{L}_k$ and $\mathcal{R}_k$ are the quantum noise induced by the left and right reservoirs respectively, and act on the k^{th} phonon mode of the system. The temperatures of the left and the right reservoirs are denoted by T^L and T^R respectively. The Bose-Einstein distribution bridges the phonon densities and the temperatures of the reservoirs by

$$< a_k^+(0) a_{k'}(0) > = \frac{\delta_{k,k'}}{e^{\hbar\omega_k^L/k_B T^L} - 1}, \quad < a_k(0) a_{k'}^+(0) > = \frac{\delta_{k,k'}}{1 - e^{-\hbar\omega_k^L/k_B T^L}},$$
$$< c_k^+(0) c_{k'}(0) > = \frac{\delta_{k,k'}}{e^{\hbar\omega_k^R/k_B T^R} - 1}, \quad < c_k(0) c_{k'}^+(0) > = \frac{\delta_{k,k'}}{1 - e^{-\hbar\omega_k^R/k_B T^R}}. \tag{7}$$

For convenience, we use $\overline{N}(\omega_k, T)$ to denote the distribution $\overline{N}(\omega_k, T) = \frac{1}{e^{\hbar\omega_k/k_B T} - 1}$ in the following derivation. The correlation of the $\mathcal{L}_k$ then reads

$$< \mathcal{L}_k^+(t) \mathcal{L}_{k'}(t') > = \sum_p \xi_{p,k} \xi_{p,k'} e^{-i(\omega_p^L t' - \omega_p^L t)} \overline{N}(\omega_p^L, T^L). \tag{8}$$

Since the phonon frequencies of the reservoirs are continuous, the sum of the frequencies in eq. (8) can be transformed in integral, reading

$$< \mathcal{L}_k^+(t) \mathcal{L}_{k'}(t') > = \int d\omega_p^L \frac{dD(\omega_p^L)}{d\omega_p^L} \xi_{p,k} \xi_{p,k'} e^{-i(\omega_p^L t' - \omega_p^L t)} \overline{N}(\omega_p^L, T^L). \tag{9}$$

The factor of $\frac{dD(\omega_p^L)}{d\omega_p^L}$ in the above equation is the density of state of phonons. Now we suggest the Markov Approximation by

$$\frac{dD(\omega_p^L)}{d\omega_p^L} \xi_{p,k} \xi_{p,k'} = \frac{\omega_p^L \gamma_{k,k'}^L}{2\pi}. \tag{10}$$

Here, $\gamma_{k,k'}^L$ is the coupling strength between the k^{th} and the k'^{th} phonon modes of the nanostructures. Physically, the $\gamma_{k,k'}^L$ is realized through the coupling of the system and the left reservoir by $\xi_{p,k}$ and $\xi_{p,k'}$. Substituting the eq. (10) into the eq. (9), we get the correlation of $\mathcal{L}$ as

$$< \mathcal{L}_k^+(t) \mathcal{L}_{k'}(t') > = \int d\omega_p^L \frac{\omega_p^L \gamma_{k,k'}^L}{2\pi} e^{-i(\omega_p^L t' - \omega_p^L t)} \overline{N}(\omega_p^L, T^L) = \gamma_{k,k'}^L f_L(t - t'), \tag{11}$$

with