Thermal conductance of one-dimensional materials calculated with typical lattice models

Chunyi Zhang,[1] Wei Kang,[1,*] and Jianxiang Wang[1,2]

[1]*HEDPS, Center for Applied Physics and Technology, College of Engineering, Peking University, Beijing 100871, China*

[2]*State Key Laboratory for Turbulence and Complex Systems, Department of Mechanics and Engineering Science, College of Engineering, Peking University, Beijing 100871, China*

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We show through calculations on typical lattice models that thermal conductance σ can well describe the near-equilibrium thermal transport property of one-dimensional materials of finite length, which presents a situation often met in the application of nanoscale devices. The σ generally contains contributions from the material itself and those from the thermal reservoirs. The intrinsic σ of the material, i.e., the one with the fewest external influences, can be efficiently calculated with the help of the "blackbody"-like nonreflective thermal reservoir, either through the nonequilibrium method or through the Green-Kubo-type formula. σ thus calculated would be helpful to guide the design of thermal management and heat control in nanoscale devices.

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I. INTRODUCTION

With the scale of materials decreasing to the nanoscale, the cooling of nanoscale devices [1–5] becomes a challenge. As a result, the past few decades have witnessed a rapid growth of interest in thermal transport properties of low-dimensional systems [6,7]. Through concerted efforts in theory, experiments, and numerical simulations, it has been gradually accepted that microscopic thermal properties are distinct from their macroscopic counterparts [6,8–13]. In particular, Fourier's law, which governs macroscopic thermal transport phenomena, may not be appropriate on the nanoscale [9–13]. Whether the thermal transport property of a nanoscale material can be well characterized by a set of appropriate material parameters is still an open question. A consistent theoretical understanding of all the experimental findings to guide the design of nanoscale thermal management has not emerged yet.

The thermal transport property of a material is usually described by its thermal conductivity κ. It is defined through a differential form of Fourier's law, $\mathbf{j} = -\kappa \nabla T$, which linearly connects the local heat flux density $\mathbf{j}$ and the gradient of local temperature T. This definition essentially relies on the assumption of local equilibrium [6], i.e., there is a well-defined local temperature that can represent local thermal properties at equilibrium. However, in reduced dimensions, the local equilibrium assumption has not been conclusively justified yet [14–17], which not only raises ambiguities in theoretical discussions, but also causes difficulties in the interpretation of experimental measurements. For example, there is inconsistency between the local equilibrium assumption [14–17] and the length dependency of the measured thermal conductivity of nanotubes or nanowires [9–12,18,19].

Instead, one can treat the material in reduced dimensions as a finite-size open system [7,20]. It has been proposed theoretically [20] that the thermal conductance

$$\sigma = \lim_{\Delta T \to 0} \frac{S}{\Delta T}, \tag{1}$$

instead of the conductivity κ, is a better physical quantity to describe the thermal transport properties of a finite system in reduced dimensions. Here S is the average total thermal flux. With the validity of the steady-state-fluctuation theorem [21,22], or on conditions that the Fokker-Planck equation is sufficient for the description of the system together with the thermal reservoirs connected to it [20], σ can be further expressed with the correlation function of the average total thermal flux $S(t)$ in a Green-Kubo type formula,

$$\sigma_{\mathrm{GK}} = \frac{1}{k_B T^2} \lim_{t \to \infty} \int_0^t d\tau \langle S(\tau) S(0) \rangle, \tag{2}$$

where k_B is the Boltzmann constant and L is the length of the system.

It has been revealed that the value of σ in an open system sensitively depends on the connection between the system and the reservoirs [23]. A major factor that affects the magnitude of σ is the reflection at the interfaces, as displayed by the velocity correlation functions of the system [24]. It suggests that σ is composed of both contributions from the material itself and from the reservoirs. When the intrinsic thermal transport property of the system is involved, as encountered in the design of nanoscale thermal management [3,5,25], or in the control of heat balance for microchips [1,2,4], this situation of including external influences in σ is quite unfavorable.

From the point of view of the property of a nanoscale system, a good question for the theoretical part is whether there is a set of physical quantities of the system that can describe the thermal transport property in reduced dimensions, for example in nanotubes or nanowires. More specifically, can such a physical quantity as σ be derived from the equilibrium properties of the material itself? For an open system, this further requires the separation of the intrinsic thermal transport property of the material from those that were externally induced.

In this work, we show that in typical one-dimensional model lattices, the thermal conductance σ can serve the purpose. By showing that σ defined in Eq. (1) can be readily calculated through the Green-Kubo-type formula Eq. (2) in these lattices, we display that σ is a material parameter, i.e., a constant, that only relies on the equilibrium properties of the

*weikang@pku.edu.cn

material. In addition, the σ with the fewest external influences, i.e., the "intrinsic" σ of the lattice, can be determined with "blackbody"-like nonreflective thermal reservoirs. These results give a clue as to what kind of physical quantities can be meaningfully measured in an experiment, and which would provide a better starting point to the future investigation of thermal transport in low-dimensional materials.

The rest of the work is organized as follows. In Sec. II, the model lattices and thermal reservoirs used in the work are concisely described. Details of the calculation are provided in Sec. III. In Sec. IV, the thermal conductances calculated with various lattices and thermal reservoirs are carefully examined. Finally, we conclude our work with a short summary in Sec. V.

II. MODEL LATTICES AND THERMAL RESERVOIRS

A. Model lattices

Model lattices have been used extensively to illustrate the thermal transport properties of one-dimensional systems [6,7]. In general, they can be divided into three categories according to Ref. [26]. The first is the integrable harmonic chain, where heat conduction is ballistic and the observed thermal conductance σ is a constant independent of the system length L [27]. The second is the nonintegrable momentum-conserved lattices, for example the Fermi-Pasta-Ulam-β (FPU-β) lattice [6,28,29] and the Toda lattice [30], in which σ is proportional to $L^{\alpha-1}$ with $\alpha \in (0,1)$ [9–11]. The third is the nonintegrable momentum-nonconserved lattices, such as the ϕ^4 lattice and the Frenkel-Kontorova (FK) lattice, in which Fourier's law is recovered and κ is displayed as a constant independent of the system length. As has been pointed out by several authors [26,31], the recovery of the Fourier law in the momentum-nonconserved model lattices is attributed to the external potential. The FPU-β lattice is used primarily to illustrate the calculation details of σ in this work. The results of the harmonic lattice and the ϕ^4 lattice are also displayed as representatives of two other types of model lattices.

The harmonic and the FPU-α-β model lattices can be directly derived from a real one-dimensional material in a series expansion of the interaction potential. The FPU-β model is obtained by ignoring the cubic term in the Hamiltonian of the FPU-α-β model. Details of the derivation are described in Ref. [24]. The Hamiltonian of both model lattices can be expressed as

$$H = \sum_i \frac{p_i^2}{2m} + \frac{k}{2}(x_i - x_{i-1} - a)^2 + \frac{B'}{4}(x_i - x_{i-1} - a)^4, \tag{3}$$

where m, x_i, and p_i are the mass, position, and momentum of the particles, respectively, a is the lattice constant, k is the spring constant, and B' is the cubic force constant. When B' is set to zero, Eq. (3) is reduced to the Hamiltonian of the harmonic lattice. Using m, a, and k as units, Eq. (3) can be transformed into a dimensionless form of $H = \sum_i h_i$, where

$$h_i = \frac{p_i^2}{2} + \frac{1}{2}(x_i - x_{i-1} - 1)^2 + \frac{B}{4}(x_i - x_{i-1} - 1)^4. \tag{4}$$

In our calculations, $B = 1$ is assumed throughout. Similarly, the dimensionless h_i for the ϕ^4 lattice is written as

$$h_i = \frac{p_i^2}{2} + \frac{1}{2}(x_i - x_{i-1} - 1)^2 + \frac{1}{4}(x_i - i)^4, \tag{5}$$

where $x_i - i$ denotes the displacement of the ith particle from its equilibrium position.

B. Thermal reservoirs

The influence of thermal reservoirs is investigated with three types of reservoirs, i.e., the Nosé-Hoover deterministic thermal reservoir [32,33], the stochastic Langevin reservoir [34,35], and a "blackbody"-like reservoir without interface reflection [24]. The last one is the major thermal reservoir used throughout the work. It is a series of damping particles attached to the lattice. These damping particles have the same interactions as those in the model lattice, and they are subjected to a gradually increasing frictional force when their position is away from the lattice. With the gradually increasing friction force, the reservoir can absorb as much as possible the incident energy flux without reflection. The equation of motion for the reservoir is

$$\dot{p}_i = -\xi_i p_i + f_{\text{model}} + \varrho_i(t), \tag{6}$$

where the subscript i represents the displacement of reservoir particles from the lattice-reservoir interface. f_{model} is the interacting force between reservoir particles. It keeps the same form as that in the lattice under investigation. For example, with a FPU-β lattice, $f_{\text{model}} = x_{i+1} - 2x_i + x_{i-1} + B(x_{i+1} - x_i - 1)^3 - B(x_i - x_{i-1} - 1)^3$ in the reservoir. ϱ_i is the stochastic force on the reservoir particles. Its time correlation function is determined by the temperature T of the reservoir and the local frictional coefficient ξ_i via the fluctuation-dissipation relation $\langle \varrho_i(0)\varrho_i(t)\rangle = 2T\xi_i\delta(t)$. The Boltzmann constant k_B is set to be 1 in the dimensionless form. This "blackbody"-like thermal reservoir is physically sound, but computationally not the most efficient. For a mathematically rigorous discussion of how to construct efficient thermal reservoirs, the reader is referred to Refs. [36,37].

When the number of particles in this thermal reservoir is reduced to one, it goes back to the stochastic Langevin reservoir [34,35]. In this case, the reservoir particle links to the model lattice on one side, and attaches to a fixed lattice point on the other side. The equation of motion is then

$$\dot{p}_r = -\xi_r p_r + f_{\text{model}} + \varrho_r(t)$$

with $\langle \varrho_r(0)\varrho_r(t)\rangle = 2T\xi_r\delta(t)$. Another thermal reservoir used in the calculation is the deterministic Nosé-Hoover reservoir [32,33]. Its equation of motion is

$$\dot{p}_r = -\xi_r p_r + f_{\text{model}},$$

where ξ_r follows the dynamics of $\dot{\xi}_r = \frac{1}{\Theta^2}(\frac{p_r^2}{T} - 1)$. The Θ here denotes the relaxation time scale of the reservoir. The choice of Θ affects the ergodicity of the reservoir and was set to be 1.0 in most of the literature. We use the same value in our work.

III. NUMERICAL DETAILS OF THE CALCULATION

To show that σ is a material parameter that can be expressed with physical quantities at equilibrium, it is calculated using two different methods. One is the nonequilibrium method, in which the lattice is connected to thermal reservoirs at temperatures $T_H = T_0 + \frac{\Delta}{2}$ and $T_L = T_0 - \frac{\Delta}{2}$, with T_0 denoting the average temperature of the system and Δ the temperature difference. σ is calculated through

$$\sigma_{\rm NE} = \frac{S}{T_H - T_L} = \frac{S}{\Delta}$$

after S reaches its stationary value. The other one is the Green-Kubo-like method formulated in Eq. (2), in which only the fluctuation of S is concerned. If σ indeed characterizes the thermal transport property of the lattice, the values of σ calculated through these two methods should be identical.

In the calculation, the dynamics of the entire system, including the lattice and the thermal reservoirs, is integrated using the velocity Verlet algorithm [38], which is an energy-conserved symplectic algorithm [39–41]. Other symplectic algorithms such as the symplectic Runge-Kutta-Nystrom (SRKN) algorithm [42] are also tried in the calculation, but they turn out to be far less efficient computationally. The time step used in the calculation is $dt = 0.01$, and the trajectories of lattice particles in the first 2×10^7 dimensionless time units are discarded to ensure the system has arrived at a stationary state. Then, the subsequent trajectories of 2×10^7 time units are used for statistics.

The dimensionless local temperature T_i is calculated as the time average of $\dot{x}_i^2$, i.e., $T_i = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau dt\, \dot{x}_i^2(t)$. S is calculated as the average of the local thermal flux $j_i(t)$ at each lattice point as $S = \sum_i j_i(t)/L$, where $j_i(t)$ is expressed as [6]

$$j_i(t) = \tfrac{1}{2}(x_{i+1} - x_i)(\dot{x}_{i+1} + \dot{x}_i)F(x_{i+1} - x_i) + \dot{x}_i h_i, \quad (7)$$

with h_i defined in Eq. (4) or Eq. (5), depending on the lattice models.

In the nonequilibrium method, the stationary thermal flux presented in the final results is calculated as the time average of $S(t)$ in the 2×10^7 time units after it reaches the stationary state. The instantaneous S in Eq. (2) is calculated as $S(t) = \sum_i j_i(t)/L$. In the calculation of the correlation function $C(t) = L^2\langle S(t)S(0)\rangle$, up to $t = 10\,000$, an ensemble of 120 independent lattices is averaged to get the final results in addition to the time average along the particle trajectories. The convective part, i.e., the contribution of the velocity and the displacement of the center of mass, is subtracted from $S(t)$ when $C(t)$ is calculated [43].

To remove as much as possible the reflection of long-wavelength fluctuations, the length of each "blackbody"-like reservoir is set to be half of the lattice length, i.e., $L/2$ for a lattice of length L. In addition, ξ_i varies linearly from $\xi_i = 0$ at the interface to $\xi_{\rm max} = 20$ at the other end of the reservoir. The effectiveness of this reservoir to reduce reflection is demonstrated in Ref. [24].

IV. RESULTS AND DISCUSSION

With the nonequilibrium method, one can first establish the existence of a linear relation between S and the temperature difference Δ, as Δ approaches zero. Figure 1 displays the σ as a function of Δ in a FPU-β lattice of length $L = 500$ and $T_0 = 0.05$. It suggests that there is a physical quantity, e.g., σ, which can be used to characterize the near-equilibrium thermal transport capability of the system. It should be noted that the σ assessed in this way includes both the contributions from the lattice and those from the interfaces, i.e., the Kapitza effect [44]. Moreover, the existence of such a quantity only means that the thermal flux has a linear response to the small temperature difference imposed at both ends of the system. It does not necessarily imply the validity of Fourier's law inside the lattice.

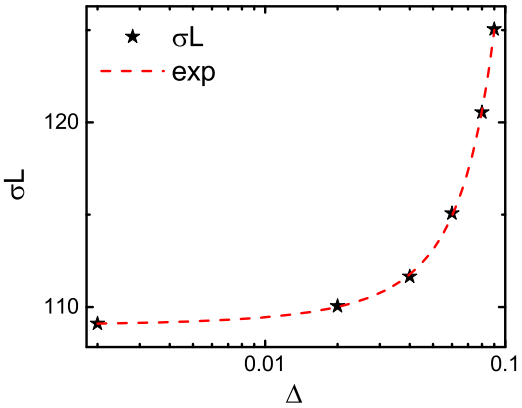

FIG. 1. σL as a function of the temperature difference Δ in a FPU-β lattice connected to the "blackbody"-like nonreflective thermal reservoirs, in which $L = 500$ and $T_0 = 0.05$. The stars represent calculated values, and the dashed line is fitted with an exponential function.

The fitted curve, displayed as a red dashed line in Fig. 1, shows that σ increases exponentially when Δ is on the same order of T_0. The region in which σ is nearly a constant, i.e., where the deviation of σ is less than 1.0%, lies in the range of Δ less than 0.01, which is around 20% of T_0. This 20% condition can be met by most of the experiments [45–47] conducted near room temperature, i.e., ~300 K, where Δ is usually smaller than 60 K.

The convergence of the correlation function $C(t)$ and σ in a FPU-β lattice of length $L = 100$ connected to the "blackbody"-like nonreflective thermal reservoirs is displayed in Fig. 2. The results calculated with various trajectory lengths are presented with different symbols. Note that the solid and dashed lines closely match each other. It unambiguously displays that the convergence of $C(t)$ and σ has been reached. A typical unconverged calculation is displayed by the dash-dotted lines. They show clearly that the time integration of $C(t)$ keeps increasing with t. In a converged calculation, as displayed by the solid and dashed lines, $C(t)$ decreases to nearly zero at $t \sim 100$, which is the time that the influence of a thermal fluctuation travels through the system at the sound speed ($v_s \sim 1$ here). This observation also gives an estimation as to the length of trajectory necessary to converge the calculation of $C(t)$. For the lattice of $L = 100$, the length of the trajectory to converge $C(t)$ up to $t \sim 100$ is $\sim 1 \times 10^5$, and for $L = 5000$, the longest lattice length investigated in our work, the trajectory length necessary for convergence is

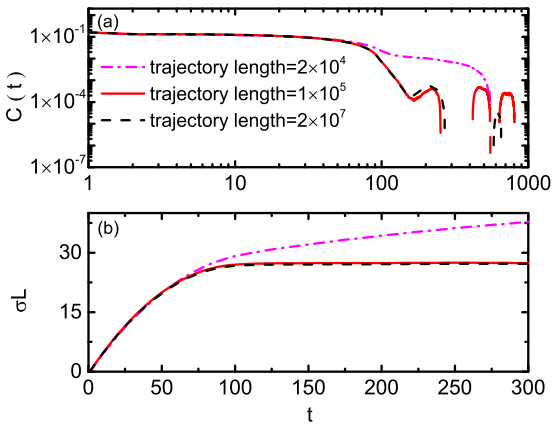

FIG. 2. (a) Heat current correlation function $C(t)$ in a FPU-β lattice connected to the nonreflective thermal reservoirs, with $T_0 = 0.05$ and $L = 100$. Various trajectory lengths were used to examine the convergence of $C(t)$. (b) Corresponding σL integrated from $C(t)$ with various trajectory lengths.

$\sim 5 \times 10^6$. Note that this estimation is based on the ensemble average of 120 samples in each calculation.

The $C(t)$ thus calculated displays a distinct behavior from those reported in previous works, as displayed in Fig. 3. In most of the works [48–52], $C(t)$ is calculated as follows: First, the system is put into a canonical distribution of the desired temperature. Then, the system is allowed to evolve with a periodic boundary condition. The $C(t)$ is calculated in the second step. This procedure is useful for systems approaching the thermodynamic limit, however it would be problematic for a lattice of finite length. The recurrence of the system [28,51] in this procedure causes a fundamental problem, i.e., $C(t)$ thus calculated does not decay to zero with increasing t, as displayed by the dash-dotted curve in Fig. 3. This makes the integration of $C(t)$ in the calculation of σ unbounded [43,48]. Putting an artificial cutoff time $t_c = L/v_s$ in the integration, as practically employed in the literature, does not solve the problem completely. The σ calculated in this way is essentially overestimated compared to those calculated using the nonequilibrium method [23,50]. The nonundulated decaying behavior in a system with periodic boundaries itself is

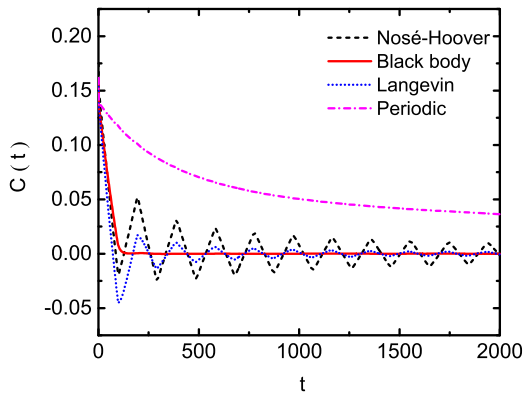

FIG. 3. $C(t)$ calculated with three different kinds of reservoirs as well as that calculated with periodic boundary conditions in a FPU-β lattice, with $T_0 = 0.05$ and $L = 100$.

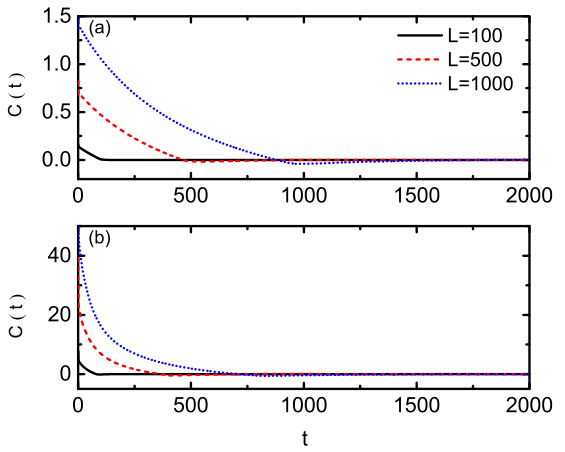

FIG. 4. $C(t)$ for various system lengths of $L = 100, 500, 1000$ in a FPU-β lattice connected to the nonreflective thermal reservoirs. (a) $T_0 = 0.05$ and (b) $T_0 = 0.25$.

of interest. It was attributed by Chen *et al.* [51] to the vanishing correlation of the local current to either the position or the momentum.

Alternatively, Kundu *et al.* [20] proposed to calculate $C(t)$ using Eq. (2) with thermal reservoirs attached. Recently, Das *et al.* showed [23] in a FPU-α-β lattice attached to stochastic Langevin thermal reservoirs that the $C(t)$ thus calculated indeed decayed to zero, and the calculated σ agreed with those estimated with the nonequilibrium method. However, it was also observed [23] that $C(t)$ decayed slowly with strong oscillations, which makes the calculation of σ via Eq. (2) converge extremely slowly and the method practically less attractive. The oscillatory behavior is also reproduced in Fig. 3 with a FPU-β lattice connected to Nosé-Hoover deterministic or stochastic Langevin thermal reservoirs, displayed as a dashed curve and a dotted curve, respectively. The oscillatory behavior, which repeats with a period of $2L/v_s$, is quite similar to that in the velocity correlation functions revealed in Ref. [24]. It is attributed to the reflection at the interfaces between the lattice and the thermal reservoirs, and it can be eliminated using nonreflective "blackbody"-like thermal reservoirs. The solid curve in Fig. 3 shows the $C(t)$ calculated with the nonreflective thermal reservoirs, where the oscillatory behavior duly disappears.

Figure 4 shows the dependency of $C(t)$ on the system size after the interfacial reflection is removed. Two temperatures of T_0, i.e., $T_0 = 0.05$ and 0.25, are displayed to represent low- and high-temperature conditions, respectively. It shows that $C(t)$ does not have a long-time tail that slowly decayed with the power law at large t. Instead, there is a natural time scale proportional to the length of the lattice, on which the correlation decays to a value close to zero. Noticing that the time scale in which a thermal fluctuation travels through the lattice is around L/v_s, where $v_s \sim 1$, these results suggest that $C(t)$ thus calculated may well reflect the intrinsic property of the lattice itself. The σ integrated from the $C(t)$ is thus also a physical property associated with the lattice itself, without or with the fewest external influences. This should be the very thermal transport property looked for by the nanoscale heat management or thermal control design [53,54].

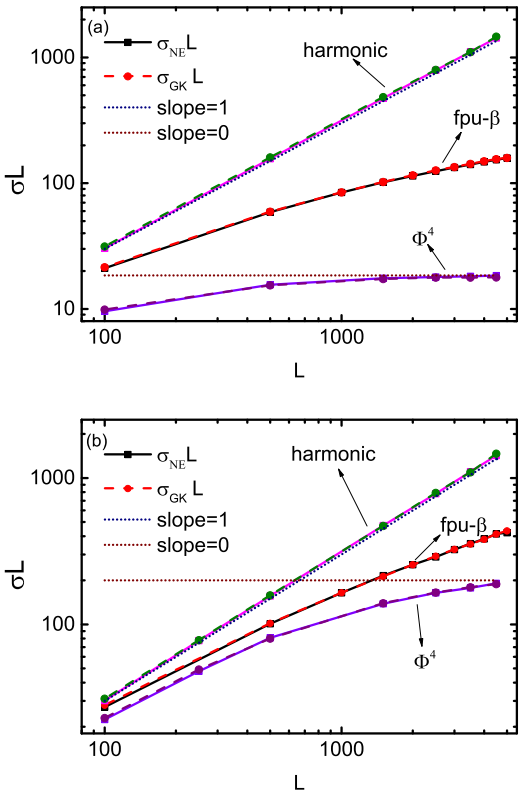

FIG. 5. Comparison of σL calculated using the nonequilibrium method and the Green-Kubo-type formula in various model lattices up to $L = 5000$. (a) $T_0 = 0.25$ and (b) $T_0 = 0.05$.

Figure 5 presents a systematic investigation of the σ in three typical lattices, i.e., the FPU-β, ϕ^4, and harmonic lattices, The σ's calculated using the $C(t)$ with nonreflective thermal reservoirs, denoted as σ_{GK}, are displayed as dots and dashed lines in the figure. To compare with the results of other studies [23,50], σ is multiplied by the length of the system as σL, which can be regarded as the effective thermal conductivity of the system [7,47,55]. σ calculated using the nonequilibrium method, denoted as σ_{NE}, are also displayed as dots and solid lines for comparison. The σ's calculated using these two methods are almost identical to each other in all cases independent of the model lattice and system size, as illustrated by the figure.

At high temperature, as displayed in Fig. 5(a) for $T_0 = 0.25$, σL is proportional to L for the harmonic lattice, and it approaches a constant for the ϕ^4 lattice. These agree well with previous findings [26,27,31]. For the FPU-β lattice, our calculation shows that σL approaches L^{α}, with α between 0.3 and 0.4, as the system size increases. It should be noted that, as pointed out by Refs. [50,56], the scaling may change with the transition of the transport region when the length increases further. However, that discussion is beyond the scope of the current work. At low temperature, as displayed in Fig. 5(b) for $T_0 = 0.05$, the power law of the ϕ^4 model is less evident up to the system size of $L = 4500$, which may be caused by the decreasing phonon scattering frequency at lower temperature [57]. Nevertheless, our calculation shows that σ's calculated with the two methods agree with each other. This suggests it a well-behaved physical quantity in various conditions regardless of whether the thermal transport behavior itself is normal or abnormal.

V. SUMMARY

In summary, we show through calculations on typical models that the thermal conductance σ can be used to characterize the thermal transport of one-dimensional materials of finite length, e.g., nanotubes and nanowires. The σ generally contains the contribution of the material itself and that from the thermal reservoirs. The value of σ with the fewest external influences can be efficiently calculated by employing nonreflective thermal reservoirs, either through the nonequilibrium method or through the Green-Kubo-type formula.

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