Symmetry properties of heat conduction in inhomogeneous materials

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We address the analysis of the energy flow properties of lattice Hamiltonian systems: precisely, we investigate, by using analytical methods, a schematically anharmonic and inhomogeneous model: namely, the chain of oscillators with self-consistent reservoirs. We obtain a symmetric thermal conductivity even for a system with inhomogeneous interparticle interactions or with graded particle masses. Our results show that inhomogeneity in a system obeying Fourier's law does not guarantee an asymmetric heat flow, and they pose the question if only anharmonicity and inhomogeneity are sufficient to assure a significative thermal rectification in a system, as suggested in the recent literature for graded structures.

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I. INTRODUCTION

The derivation of macroscopic phenomenological laws of thermodynamic transport from the underlying microscopic Hamiltonian systems is still a challenge to theoretical physics. In particular, we still ignore the precise conditions in a microscopic dynamical system of interacting particles that lead to Fourier's law of heat conduction, $\mathcal{F}=-\kappa\nabla T$, which relates the heat flow $\mathcal{F}$ to the temperature gradient ∇T. For a long time many works have been devoted to this and other related problems [1], almost all of them by means of computer simulations. Contradictions exist: for example, the authors of Ref. [2] affirm that anharmonicity (soft or hard) of the on-site potential is enough to guarantee Fourier's law, but in Ref. [3] it is presented a counterexample. The difficulty to arrive at precise conclusions from numerical studies in these problems with convergent and divergent thermal conductivity makes evident the importance of more accurate treatments (more comments are presented, e.g., in Ref. [4]). Analytical investigations have appeared, always considering approximations or simplified models due to the huge technical difficulty associated with the nonlinear dynamics—to quote some well-known mathematical physicists [5,6]: a complete analytical treatment of these nonlinear systems "is not even on the horizon," or, according to the authors of Refs. [7,8], "a rigorous treatment of a nonlinear system, even the proof of existence of the conductivity coefficient, is out of reach of current mathematical techniques." As an example of (recurrently revisited) simplified model, we recall the harmonic crystal with self-consistent stochastic reservoirs, which has been recently analytically investigated (the inner reservoirs are a simplified representation of the anharmonic part of the interaction): the classical and quantum versions are analyzed, respectively, in [9,10]. In Ref. [11], to mention another recent work still considering such model, the phenomenon of crossover from ballistic to diffusive thermal transport (as the system size is changed) is treated. Other approximative analytical schemes to study the energy flux are considered, e.g., in [5,12].

On the other hand, besides the interest in the origin of the physical mechanism of energy transport, another very important question has been attracted much attention: applications based on the possibility to control the heat flow. With the advent of nanotechnology, the possibility of constructing thermal (nano)devices such as rectifiers or diodes [13] and thermal transistors [14] becomes of great interest. As well known, a thermal diode is a device in which the heat flow becomes different if the device is inverted between two heat baths. We recall some works which propose to build, again via computer simulations, a thermal diode. In [13], a thermal diode is constructed (for the first time) by coupling three nonlinear chains with different Morse on-site potential lattices; in [15], a higher-gain diode is proposed, whose structure consists of two coupling Frenkel-Kontorova lattices connected by a harmonic string. However, for these two-segment models, in Ref. [16], the authors claim that the asymmetry in the heat conduction critically depends on the properties of the interface and system size, and so, they conclude that it will be a difficulty task to construct a thermal rectifier in practice. But in a recent work [17], Chang *et al.* experimentally build a nanoscale thermal rectifier using a different procedure: they take carbon and boron nitride nanotubes, initially with symmetric axial thermal conductance, and then they mass-load externally and inhomogeneously the nanotubes with heavy molecules. The resulting graded mass systems yield asymmetric axial thermal conductance, with greater heat flow in the direction of decreasing mass density. About graded materials—i.e., inhomogeneous materials whose composition and/or structure change gradually in space—it is worth recalling that they are abundant in nature, can also be manufactured, and have recently attracted great interest in many areas (due to their physical properties): material sciences, engineering, optics, etc. [18]. We also recall that in a recent paper [19], the authors investigate an anharmonic chain (precisely, a system with a quite specific interaction, the Fermi-Pasta-Ulam β potential) and, by means of computer simulations, they conclude that the heat flow is asymmetric in lattices with a mass gradient (and fixed boundary conditions). Moreover, they discuss possible applications in constructing thermal rectifiers and thermal transistors by using graded materials. Again, in [20], Casati claims that it is possible to make a thermal rectifier by coating a nanotube with a molecular layer that is thicker on one end

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than the other. In short, these last results may suggest us that now we have a precise mechanism to build thermal rectifiers; that is, by taking any anharmonic system and changing its structure gradually in space (e.g., increasing the particle masses), we obtain materials with asymmetric heat properties.

In this article, considering the context of possible applications of the heat flow control, we study the thermal conductivity of a inhomogeneous chain. In this scenario of, say, more accurate study, we perform an analytical (and rigorous) investigation of the harmonic crystal with self-consistent reservoirs and arbitrary structures, including the graded one. This model was proposed by Bolsterli, Rich, and Visscher awhile ago [21] (there with homogeneous structures), and its quantum version was presented in [22]. As already said, it has been revisited many times (e.g., in [9–11]); it is a schematic (and analytically treatable) anharmonic system. Roughly, it consists of a chain of oscillators with harmonic nearest-neighbor interparticle interactions and on-site potentials, and stochastic reservoirs coupled to each site. From a physical point of view, the inner reservoirs are interpreted as a schematic representation of anharmonic on-site potentials: the self-consistent condition means that the inner reservoirs exchange no energy with the system in the steady state; i.e., the inner reservoirs represent only a mechanism of phonon scattering (given by the on-site anharmonic interactions in more complicated models). This model, as proved in [9], obeys the Fourier's law, in opposition to the pure harmonic systems [23]. Moreover, it is rich enough to describe other interesting phenomena: e.g., its quantum version presents a crossover from ballistic to diffusive thermal transport [11], as reminded above.

We derive an expression for the thermal conductivity of the system by means of a perturbative computation. We emphasize that the analysis is rigorous: the perturbative series is convergent [24]. Our results show that inhomogeneity in a system obeying Fourier's law does not guarantee an asymmetric heat flow, and they pose the question of what ingredients in an inhomogeneous material are sufficient to lead to a significant thermal rectification.

The rest of the paper is organized as follows. In Sec. II we present the model in detail and introduce our approach developed to study the heat flow. In Sec. III we describe the perturbative computation up to second order in the coupling interaction, and we argue about the structure of the remaining terms. We also present the expression for the thermal conductivity. Section IV is devoted to final remarks.

II. MODEL AND FORMALISM

Let us introduce the mathematical expressions describing the model. We take a chain of oscillators (we will be restricted to the one-dimensional case, but the analysis follows for any d) with Hamiltonian

$$H(p,q)=\sum_{j=1}^{N}\frac{1}{2}\left[\frac{p_j^2}{m_j}+M_j q_j^2\right]+\frac{1}{2}\sum_{j,l=1}^{N} q_l J_{lj} q_j, \tag{1}$$

where J is Hermitian ($J_{lj}=J_{jl}$) and m_j is the jth particle mass; we will assume nearest-neighbor interactions later. The dynamics (time evolution) we consider are given by the stochastic differential equations, with $j=1,\ldots,N$,

$$dq_j=\frac{\partial H}{\partial p_j}dt=\frac{p_j}{m_j}dt, \tag{2}$$

$$dp_j=-\frac{\partial H}{\partial q_j}dt-\zeta_j p_j dt+\gamma_j^{1/2}dB_j, \tag{3}$$

where B_j are independent Wiener processes, describing the heat baths at $j=1$ and $j=N$, and schematically representing the anharmonic degrees of freedom for the inner sites $j=2,\ldots,N-1$; ζ_j is the stochastic reservoir coupling for the jth site (we take $\zeta_j=\zeta$ for all j); and $\gamma_j=2m_j\zeta_j T_j$, where T_j is the (kinetic) temperature of the jth reservoir. We note that a change of variables allows us to reduce the analysis of any structure (i.e., with different distributions of the particle masses and on-site potentials) to the investigation of the model with $m_j=1$ and $M_j=M$ (i.e., constant for any site j). Indeed, we write (2) as $\sqrt{m_j}q_j=p_j/\sqrt{m_j}$, and define $Q_j\equiv\sqrt{m_j}q_j$, $P_j\equiv p_j/\sqrt{m_j}$ to get

$$\dot{Q}_j=P_j. \tag{4}$$

Then we write (3) as

$$\frac{\dot{p}_j}{\sqrt{m_j}}=-\frac{J_{jl}+M_j\delta_{jl}}{\sqrt{m_j m_l}}\sqrt{m_l}q_l-\zeta_j\frac{p_j}{\sqrt{m_j}}+\sqrt{2\zeta_j T_j}\eta_j,$$

where $\eta_j=dB_j/dt$. And so, we get

$$\dot{P}_j=-D_{jl}Q_l-\zeta_j P_j+\sqrt{2\zeta_j T_j}\eta_j. \tag{5}$$

Equation (5) describes, together with (4), the dynamics of a particle system with masses $m_j=1$. From DQ we extract the on-site potential term MQ_j; i.e., we write $\Sigma_l D_{jl}Q_l=\Sigma_l(D_{jl}-M\delta_{jl})Q_l+MQ_j$. Hence, without loss of generality, in what follows we consider a system with unitary particle masses and constant on-site potentials (as shown, a graded mass model, for example, may be mapped on such a system).

As usual, we take the energy of the jth oscillator as

$$H_j=\frac{P_j^2}{2}+\frac{M}{2}Q_j^2+\frac{1}{2}\sum_l Q_l D_{lj}Q_j$$

$$=\frac{P_j^2}{2}+U_1(Q_j)+\frac{1}{2}\sum_{l\neq j}U_2(Q_j-Q_l), \tag{6}$$

where U_1 and U_2 come from (1) and $\Sigma_j H_j=H$ [of course, in (1) we make the replacements: $p_j\to P_j$, $q_j\to Q_j$, $m_j=1$, $M_j=M$, $J_{lj}\to D_{lj}$]. Hence, it follows that

$$\left\langle\frac{dH_j(t)}{dt}\right\rangle=\langle R_j(t)\rangle-\langle\mathcal{F}_{j\to}-\mathcal{F}_{\to j}\rangle, \tag{7}$$

where $\langle\cdot\rangle$ means the expectation with respect to the noise distribution and

$$\langle R_j(t)\rangle=\zeta(T_j-\langle P_j^2\rangle) \tag{8}$$

gives the energy flow from the jth reservoir to the jth site. Later, we will analyze the steady state in the self-consistent condition, which means $\langle R_j\rangle=0$ for $j=2,\ldots,N-1$. That is,

the inner reservoirs do not inject energy into the system: as said, we do not take them as real thermal reservoirs, but only as a representation of the anharmonic degrees of freedom not present in the potential. The other term in (7) gives the energy current inside the system:

$$\mathcal{F}_{j\rightarrow} = \sum_{l>j} \nabla U_2(Q_j - Q_l)\frac{P_j + P_l}{2}, \tag{9}$$

where $\mathcal{F}_{j\rightarrow}$ describes the heat flow from the jth site to the lth sites ($l>j$) and $\mathcal{F}_{\rightarrow j}$ the flow from the previous sites to j (its expression is given by changing l with j in $\mathcal{F}_{j\rightarrow}$). We still remark that, if we write the energy current inside the system in terms of the original variables q and p from the Hamiltonian (1), we obtain the same expression of Eq. (9) above.

We are interested in the symmetry properties of the heat flow in the steady state for a generic interaction (which also englobes, as said via a change of variables, generic particle mass distribution, etc.). To analyze the stationary state, we follow our approach proposed in some previous works [25,26]. For clearness, we repeat expressions already described in these papers (of course some expressions change accordingly to the problem).

In a few words, our strategy is to start from a simplified system without the interparticle interactions. This initial dynamical system involves only isolated sites, and it has an easy solution. Then we use a tool of stochastic differential equations, the Girsanov theorem, which gives the solution of the complete problem with the interparticle potential in terms of the simplified problem. We present details ahead.

For convenience, let us introduce the phase-space vector $\phi=(Q,P)$, with $2N$ coordinates. Now the time evolution equation becomes

$$\dot{\phi} = -A\phi - U_2' - \sigma\eta, \tag{10}$$

where $U_2'=\mathcal{D}\phi$; A, σ, and $\mathcal{D}$ are the $2N\times 2N$ matrices given by

$$A = \begin{pmatrix} 0 & -I \\ MI & \zeta I \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & 0 \\ 0 & 2\zeta\mathcal{T} \end{pmatrix}, \quad \mathcal{D} = \begin{pmatrix} 0 & 0 \\ D & 0 \end{pmatrix}, \tag{11}$$

with the $N\times N$ matrices: I (the identity), $\mathcal{T}_{jl}=\delta_{jl}T_j$, and D is the interparticle potential; η are independent white noises. The solution of the dynamical equation (10) is the Ornstein-Uhlenbeck process

$$\phi(t) = e^{-tA}\phi(0) + \int_0^t ds e^{-(t-s)A}\sigma\eta(s). \tag{12}$$

For simplicity, we take as initial condition $\phi(0)=0$. Hence, the covariance of this Gaussian process becomes

$$\langle \phi(t)\phi^T(s)\rangle \equiv \mathcal{C}(t,s) = \begin{cases} e^{-(t-s)A}\mathcal{C}(s,s), & t \geqslant s, \\ \mathcal{C}(t,t)e^{-(s-t)A^T}, & t \leqslant s, \end{cases} \tag{13}$$

$$\mathcal{C}(t,t) = \int_0^t ds e^{-sA}\sigma^2 e^{-sA^T}. \tag{14}$$

A useful expression, obtained by, e.g., diagonalizing A, is the following

$$\exp(-tA) = e^{-t\zeta/2}\left\{\cosh(t\rho)\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} + \frac{\sinh(t\rho)}{\rho}\begin{pmatrix} (\zeta/2)I & I \\ -MI & -(\zeta/2)I \end{pmatrix}\right\},$$

where $\rho=[(\zeta/2)^2-M]^{1/2}$. It is also useful to note that $\mathcal{C}(t,s)$ above may be written as, for $t\geqslant s$,

$$\mathcal{C}(t,t) = \exp[-(t-s)A]C + O(\exp[-(t+s)\zeta/2]),$$

and the effects of the second term disappear in some computations ahead as $t\rightarrow\infty$. In short, in many computations ahead we have that, in the expression for $\mathcal{C}(t,s)$, Eq. (13), the terms $\mathcal{C}(s,s)$ and $\mathcal{C}(t,t)$ may be replaced by C, which makes the analysis easier. For this case—i.e., without the interparticle interaction—each (isolated) site is connected to one stochastic reservoir, and so, each one converges to equilibrium as $t\rightarrow\infty$. The final Gaussian stationary distribution, related to Boltzmann-Gibbs states, has mean zero and covariance

$$C = \int_0^\infty ds e^{-sA}\sigma^2 e^{-sA^T} = \begin{pmatrix} M^{-1}\mathcal{T} & 0 \\ 0 & \mathcal{T} \end{pmatrix}. \tag{15}$$

Thus, for the computations in the next section, we write the covariance of the Gaussian measure above (13) as

$$\mathcal{C}(t,s) = \begin{pmatrix} \mathcal{C}_{JJ}(t,s) & \mathcal{C}_{JI}(t,s) \\ \mathcal{C}_{IJ}(t,s) & \mathcal{C}_{II}(t,s) \end{pmatrix}, \tag{16}$$

where each one of the four $N\times N$ matrices $\mathcal{C}_{KK'}$ above are diagonal and their elements are

$$\mathcal{C}_{jj}(t,s) = e^{-|t-s|\zeta/2}\left[\cosh(\rho|t-s|) + \frac{\zeta}{2\rho}\sinh(\rho|t-s|)\right]\frac{T_j}{M},$$

$$\mathcal{C}_{ji}(t,s) = e^{-|t-s|\zeta/2}\frac{1}{\rho}\sinh[\rho(t-s)]T_i,$$

$$\mathcal{C}_{ij}(t,s) = -e^{-|t-s|\zeta/2}\frac{1}{\rho}\sinh[\rho(t-s)]T_j,$$

$$\mathcal{C}_{ii}(t,s) = e^{-|t-s|\zeta/2}\left[\cosh(\rho|t-s|) - \frac{\zeta}{2\rho}\sinh(\rho|t-s|)\right]T_i.$$

Notice that $\mathcal{C}_{ji}(t,s)$ and $\mathcal{C}_{ij}(t,s)$ depend on $(t-s)$, and so they change sign if $t>s$ or $t<s$. To obtain the solution for the process φ with the interparticle potential U_2, we use the Girsanov theorem [27], which gives the solution of the new process φ in terms of the previous one ϕ. In particular, for the two-point correlation function, which gives the heat flow, this theorem states that (details in [25,26])

$$\langle \varphi_u(t_1)\varphi_v(t_2)\rangle = \mathcal{N}^{-1}\int \phi_u(t_1)\phi_v(t_2)Z(t)d\mu_{\mathcal{C}}, \quad (17)$$

where $\mathcal{N}$ is a normalization factor, $d\mu_{\mathcal{C}}$ is the Gaussian measure with zero mean and covariance given by (13), and $t_1, t_2 < t$. The corrective factor $Z(t)$ is related to the coupling potential, and it is given by (we omit obvious sum in the notation below and everywhere in this article)

$$Z(t) = \exp\left(\int_0^t u dB - \frac{1}{2}\int_0^t u^2 ds\right), \quad (18)$$

where $\gamma_i^{1/2}u_i = -\mathcal{D}_{ik}\phi_k$. In the expression above and in what follows, we use the index notation: i for index values in the set $\{N+1,\ldots,2N\}$, j for values in $\{1,\ldots,N\}$, and k in $\{1,\ldots,2N\}$. The first term above we write as

$$u_i dB_i = \gamma_i^{-1/2}u_i\gamma_i^{1/2}dB_i = -\gamma_i^{-1}\mathcal{D}_{ij}\phi_j(d\phi_i + A_{ik}\phi_k dt).$$

Using the Itô formula [27], we obtain

$$-\gamma_i^{-1}\mathcal{D}_{ij}\phi_j d\phi_i = -dF - \gamma_i^{-1}\phi_i\mathcal{D}_{ij}A_{jk}\phi_k dt$$

$$F(\phi) = \gamma_i^{-1}\phi_i\mathcal{D}_{ij}\phi_j.$$

Hence, the expression for $Z(t)$ becomes

$$Z(t) = \exp\left(-F(\phi(t)) + F(\phi(0)) - \int_0^t ds W(\phi(s))\right), \quad (19)$$

$$W(\phi(s)) = \gamma_i^{-1}\phi_i(s)\mathcal{D}_{ij}A_{jk}\phi_k(s) + \phi_k(s)A_{ki}^T\gamma_i^{-1}\mathcal{D}_{ij}\phi_j(s) + \frac{1}{2}\phi_{j'}(s)\mathcal{D}_{j'i}^T\gamma_i^{-1}\mathcal{D}_{ij}\phi_j(s). \quad (20)$$

The heat current in the steady state, $\lim_{t\to\infty}\mathcal{F}_{j\to}(t)$, Eq. (9), for U_2 quadratic, is given in terms of two-point correlation functions such as

$$\lim_{t\to\infty}\langle \varphi_u(t)\varphi_v(t)\rangle = \mathcal{N}^{-1}\lim_{t\to\infty}\int \phi_u(t)\phi_v(t)Z(t)d\mu_{\mathcal{C}}, \quad (21)$$

for $u \in \{N+1,\ldots,2N\}$ and $v \in \{1,\ldots,N\}$.

III. PERTURBATIVE COMPUTATION FOR THE THERMAL CONDUCTIVITY

We will perform a detailed computation up to second order in the coupling interaction $\mathcal{D}$, and we will argue about the structure of the remaining orders. From Eqs. (19) and (20), writing $Z=\exp(-V)$, we have (up to second order) the truncated expansion

$$\langle \varphi_u\varphi_v\rangle = \langle \phi_u\phi_v\rangle - \langle \phi_u\phi_v; V\rangle + \frac{1}{2}\langle \phi_u\phi_v; V; V\rangle, \quad (22)$$

where

$$V = \gamma_i^{-1}\phi_i(t)\mathcal{D}_{ij}\phi_j(t) + \int_0^t ds\left[\gamma_i^{-1}\phi_i(s)\mathcal{D}_{ij}A_{jk}\phi_k(s) + \phi_k(s)A_{ki}^T\gamma_i^{-1}\mathcal{D}_{ij}\phi_j(s) + \frac{1}{2}\phi_{j'}(s)A_{j'i}^T\gamma_i^{-1}\mathcal{D}_{ij}\phi_j(s)\right] \equiv A_1 + A_2 + A_3 + A_4. \quad (23)$$

The term corresponding to $F(\phi(0))$ in (19) is not considered above, since it disappears in the computation as $t\to\infty$. Performing the huge, but straightforward computations of the Gaussian integrals (and taking the limit $t\to\infty$), we obtain up to order $\mathcal{D}^2$

$$-\langle \phi_u\phi_v; A_4\rangle = \frac{1}{4\zeta M^2}D_{j,u-N}D_{j,v}\frac{T_{u-N}T_v}{T_j},$$

$$\langle \phi_u\phi_v; A_1; A_2\rangle = -\frac{1}{8\zeta^3 M}D_{u-N,j}D_{j,v}\left(T_j + 2T_v + \frac{T_{u-N}T_v}{T_j}\right),$$

$$\langle \phi_u\phi_v; A_1; A_3\rangle = \frac{1}{8\zeta^3 M}D_{u-N,j}D_{j,v}\left[\left(\frac{2\zeta^2}{M}+1\right)T_j + 2\left(\frac{\zeta^2}{M}+1\right)T_v + \frac{T_{u-N}T_v}{T_j}\right],$$

$$\langle \phi_u\phi_v; A_2; A_3\rangle = \frac{1}{8\zeta^3 M}D_{u-N,j}D_{j,v}\left(T_j - T_v + 3T_{u-N} + \frac{T_{u-N}T_v}{T_j}\right),$$

$$\frac{1}{2}\langle \phi_u\phi_v; A_3; A_3\rangle = D_{u-N,j}D_{j,v}\left[-\left(\frac{1}{4\zeta M^2}+\frac{1}{8\zeta^3 M}\right)T_j + \frac{1}{8\zeta^3 M}T_v - \left(\frac{1}{4\zeta M^2}+\frac{3}{8\zeta^3 M}\right)T_{u-N} - \left(\frac{1}{4\zeta M^2}+\frac{1}{8\zeta^3 M}\right)\frac{T_{u-N}T_v}{T_j}\right].$$

We also have $\langle \phi_u\phi_v; A_1; A_1\rangle = 0 = \langle \phi_u\phi_v; A_2; A_2\rangle$. And so

$$\lim_{t\to\infty}\langle \varphi_u(t)\varphi_v(t)\rangle \equiv \mathcal{G}_{u,v}(T_{u-N} - T_v) = \left[\frac{\mathcal{D}_{u,v}}{2\zeta M} - \frac{1}{4\zeta M^2}\mathcal{D}_{u,l}\mathcal{D}_{l+N,v}\right](T_{u-N} - T_v). \quad (24)$$

The sum over l above is assumed. For simplicity, we consider nearest-neighbor interparticle interaction only. From (9), the heat current $\mathcal{F}_{j\to j+1}$ is

$$\langle \mathcal{F}_{j\to j+1}\rangle = \frac{D_{j,j+1}}{2}\langle (\varphi_{j+1} - \varphi_j)(\varphi_{j+N} + \varphi_{j+1+N})\rangle. \quad (25)$$

Using that in the steady state $\langle dH_j/dt\rangle = 0$ and the self-consistent condition $\lim_{t\to\infty}\langle R_j(t)\rangle = 0$, which is given by $\lim_{t\to\infty}\langle \varphi_j^2(t)\rangle = T_j$, we obtain

$$\mathcal{F}_{1\to 2} = \mathcal{F}_{2\to 3} = \cdots = \mathcal{F}_{N-1\to N} \equiv \mathcal{F}.$$

Hence, we get $\mathcal{F}=\mathcal{G}_1(T_1-T_2)=\cdots=\mathcal{G}_{N-1}(T_{N-1}-T_N)$, where we use the notation $\mathcal{G}_j \equiv \mathcal{D}_{j+N,j+1}\mathcal{G}_{j+N,j+1}$. And so it follows that

$$\mathcal{F} = \kappa(T_1 - T_N)/(N-1),$$

which is Fourier's law with thermal conductivity κ:

$$\kappa(N-1)^{-1} = ({\mathcal{G}_1}^{-1} + {\mathcal{G}_2}^{-1} + \cdots + {\mathcal{G}_{N-1}}^{-1})^{-1}. \quad (26)$$

For $\mathcal{G}_j$ we have

$$\mathcal{G}_j = \mathcal{D}_{j+N,j+1}\left\{\frac{\mathcal{D}_{j+N,j+1}}{2\zeta M} - \frac{\mathcal{D}_{j+N,j+1}}{4\zeta M^2}\frac{\mathcal{D}_{j+N,j}+\mathcal{D}_{j+1+N,j+1}}{2}\right\}. \quad (27)$$

And so, from the expressions above, the symmetry in the thermal conductivity is clear: nothing changes if the chain is inverted (i.e., if we replace particle 1 by N, 2 by $N-1$, etc.)—recall that $\mathcal{D}_{j+N,j+1}=D_{j,j+1}$, and D is Hermitian. Hence, for our system with weak interparticle interaction D, or any interaction J and heavy-particle masses (graded or not—see details ahead), the effect of thermal rectification does not exist or, at least, in the case of asymmetric upper order corrections, it is very small: $O(D^4)$. This connection between a system with heavy-particle masses and another with weak interaction D and same particle masses is clear from the expression before Eq. (5): note the relation $D=\mathfrak{M}^{-1/2}J\mathfrak{M}^{-1/2}$, where $\mathfrak{M}$ is the diagonal matrix for the heavy (graded or not) particle masses.

Now we briefly comment on the possible symmetric contribution of the upper terms in the perturbative series. From the structure of the representation for the two-point correlation, and so, for the heat flow—i.e., from (21) and remaining terms in (22)—e.g., $\langle \phi_u \phi_v; V; V; V\rangle$, the next terms in the perturbation expansion shall introduce expressions with $\mathcal{D}_{u,l}\mathcal{D}_{l+N,j}\mathcal{D}_{j+N,v}$, etc. [see (24)], corrections which do not break the symmetry of the thermal conductivity κ, as we shall see by following the derivation of κ, Eq. (26).

IV. FINAL REMARKS

We first remark that our perturbative treatment is a rigorous analysis: the convergence of the perturbative series for any harmonic chain with self-consistent stochastic reservoirs (and small interparticle potential D) is rigorously proved in [24], which shows the trustworthiness of our computations. Moreover, we recall that in Ref. [25], for the completely homogeneous case (the system with same particle masses and interparticle potentials), we show that our first-order perturbative result for the heat conductivity and the exact one obtained in Ref. [9] (and valid even for large D) are the same one, which indicates that the perturbative expansion shall be valid for any value of D.

In this article, we investigate the thermal conductivity of graded materials, represented by a schematically anharmonic model (which obeys Fourier's law) with inhomogeneous interparticle interaction. In some previous numerical or experimental works, as recalled in the Introduction, thermal rectification is found for some quite specific anharmonic and inhomogeneous models or materials, and it is claimed to be a general phenomenon. Our analytical results show that a significative thermal rectification is absent in the inhomogeneous self-consistent harmonic chain, an effective anharmonic model, proposed awhile ago and used by several other researches. If we believe that such a model is indeed efficient to describe some properties of the thermal conductivity of realistic systems, then our results indicate that only anharmonicity and inhomogeneity, such as structures with graded masses, may not be sufficient to guarantee a significative effect of thermal rectification: some other ingredient is necessary.

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