Heat-flow properties of systems with alternate masses or alternate on-site potentials

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We address a central issue of phononics: the search of properties or mechanisms to manage the heat flow in reliable materials. We analytically study standard and simple systems modeling the heat flow in solids, namely, the harmonic, self-consistent harmonic and also anharmonic chains of oscillators, and we show an interesting insulating effect: While in the homogeneous models the heat flow decays as the inverse of the particle mass, in the chain with alternate masses it decays as the inverse of the square of the mass difference, that is, it decays essentially as the mass ratio (between the smaller and the larger one) for a large mass difference. A similar effect holds if we alternate on-site potentials instead of particle masses. The existence of such behavior in these different systems, including anharmonic models, indicates that it is a ubiquitous phenomenon with applications in the heat flow control.

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I. INTRODUCTION

The understanding of the macroscopic laws of thermodynamic transport starting from the underlying microscopic models is still a challenge in physics. In particular, the microscopic study of energy transport, which mainly involves conduction of heat or electricity, is of great theoretical and practical interest. In the one hand, the advances in modern electronics (which stands for the study of electric charge currents) are well known, but on the other hand, its thermal counterpart, the phononics, i.e. the study of information processing and control of heat flow by phonons, is much less developed. However, due to several recently proposed devices designed to manage the heat flow, such as thermal rectifiers [1–3], thermal transistors [4], thermal logic gates [5], etc., phononics has attracted increasing attention [6].

One of the most fundamental components of these devices of phononics is the thermal rectifier or diode, a structure in which the heat flows preferably in one direction. The first diode has been proposed by Terraneo *et al.* [1], and since then the phenomenon of thermal rectification has been intensively investigated, mostly by numerical simulations [6–8]. The most common and recurrent design of thermal diode is given by the sequential coupling of two or three different segments with different anharmonic potentials. Although frequently studied, such structure is criticized [3] due to the significant decay of the rectification factor with the system size, and mainly due to the difficulty to be constructed in practice. Thus, the search of a experimentally feasible diode and other devices to manage the heat flow has become an important problem in phononics, with many works dedicated to the theme [9,10]: in particular, the use of graded materials has deserved attention [7,11,12].

The present paper is also devoted to this central issue of phononics: the investigation of the heat flow control by searching for nontrivial thermal properties of reliable systems [11,13,14], i.e., of systems that may be built in practice. We perform here a detailed analysis of some harmonic chains of oscillators, where precise analytic computations are possible, as well as of certain anharmonic chains - where more usual features may be seen, such as the normal conductivity and rectification in asymmetric systems. We recall that, since Debye, the standard microscopic models used to describe the heat conduction in solids are mainly given by lattice systems of oscillators. We show an "insulating" effect due to the presence of alternate masses. That is, for these harmonic and anharmonic chains of oscillators, we show that while in the homogeneous system the heat flow decays as the inverse of the particle mass, in the alternate mass chain it decays as the inverse of the square of the mass difference, i.e., it decays essentially as the mass ratio (between the smaller and the larger one) for a large mass difference. Precisely, if in the alternate mass chain we decrease one of the masses as $m_1 \sim \epsilon$ (ϵ small) and increase the other one as $m_2 \sim 1/\epsilon$, then the heat flow $\mathcal{F}$ decays as $\mathcal{F} \sim \epsilon^2$. But, in the case of a homogeneous system (with identical masses), by increasing the mass as $m \sim 1/\epsilon$, we have $\mathcal{F} \sim \epsilon$. In short, our analytical study indicates that in order to make smaller the heat flow in a system, it is more efficient to take alternate masses, increase one and, at the same rate, decrease the other than simply increase the masses of the particles in a homogeneous chain. Similar effects hold if we fix the particle masses but change the on-site potentials (details ahead).

In order to justify the analytic investigation of simple systems, we quote Ruelle [15]: a "detailed analysis of simple models can introduce a new degree of understanding" in the study of the heat flow. Moreover, properties found in simple (say, naked) models may be ubiquitous, since they do not depend on specific and intricate interactions.

The rest of the paper is organized as follows. In Sec. II, we extend the results of a previous work [16] and derive an exact expression for the heat flow of a harmonic chain with alternate masses. By using such expression, we present the effect and offer an explanation. We also (briefly) review the result for the self-consistent harmonic chain. In Sec. III, we describe a previously developed method aiming to study the heat conduction in some anharmonic models [12], and derive the expression for the thermal conductivity of a self-consistent

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anharmonic chain with alternate masses in order to show the existence of the effect also in these more intricate systems. Section IV is devoted to the final remarks.

II. HARMONIC MODELS

Now we describe the heat flow in some harmonic models, where rigorous computations are possible and the mechanisms underlying the behavior of the heat flow in the presence of alternate masses are transparent. For clearness, we repeat some results already described in previous works [16,17].

First we consider a chain of oscillators with nearest neighbor interactions and thermal baths on the boundaries. Recall that as the system is fully harmonic, it does not obey the Fourier's law of heat conduction. The exact expression for the heat flow in the case of a homogeneous system (all the particles with the same mass) has been obtained a long time ago, in the seminal paper of Rieder, Lebowitz and Lieb [18]. Now, for the case of alternate masses, we follow the rigorous approach proposed by Casher and Lebowitz [19], and extend the analysis presented in Ref. [16] in order to obtain an exact expression for the heat flow.

Now we introduce the model and derive the results. We take a system of N oscillators (particles) with Hamiltonian

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

where m_j, q_j are the mass and position of the j-th particle; p_j is the associated momentum; J is a self-adjoint matrix describing the interparticle interactions; M_j is the strength of the harmonic on-site potential. The term $M_j q_j^2$ may be written together with $q_l J_{lj} q_j$ by defining $J_{jj} = M_j$ and including the term $j = l$ in the sum above for the interparticle interaction. The dynamics, as usual, is given by

$$\begin{aligned} dq_j &= \frac{\partial H}{\partial p_j} dt = \frac{p_j}{m_j} dt, \\ dp_j &= -\frac{\partial H}{\partial q_j} dt - \zeta_j p_j dt + \gamma_j^{\frac{1}{2}} dB_j, \end{aligned} \quad (2)$$

where B_j are independent Wiener processes (i.e., dB_j/dt are Gaussian white-noises); $\zeta_i = \zeta(\delta_{1j} + \delta_{Nj})$ is the heat bath coupling (the dissipative constant); $\gamma_j = 2m_j\zeta_j T_j$ where T_1 and T_N are the temperatures of the thermal reservoirs. Note that, for this specific model, only ζ_1 and ζ_N are nonzero.

Before carrying out the computations, we remark that changes in the particle masses m_j lead to the same effect of (other properly chosen) changes in the on-site potentials M_j and in the interparticle interaction J: i.e., the system above can be mapped onto a system with equal on-site potentials, i.e. $M_j = M$ for all $j = 1,...,N$ (and vice-versa: a system with different particle masses can be mapped onto another one with equal masses but with different on-site potentials). Precisely, with the change of variables given by

$$Q_j = M_j^{\frac{1}{2}} q_j, \quad P_j = M_j^{-\frac{1}{2}} p_j,$$

we map the equations above onto

$$\begin{aligned} \tilde{H}(\mathbf{Q},\mathbf{P}) &= \sum_{j=1}^{N} \frac{1}{2}\left(\frac{P_j^2}{\tilde{m}_j} + Q_j^2 + \sum_{l\neq j=1}^{N} Q_l \tilde{J}_{lj} Q_j\right), \\ dQ_j &= \frac{\partial \tilde{H}}{\partial P_j} dt = \frac{P_j}{\tilde{m}_j} dt, \\ dP_j &= -\frac{\partial \tilde{H}}{\partial Q_j} dt - \zeta_j P_j dt + \tilde{\gamma}_j^{\frac{1}{2}} dB_j, \end{aligned} \quad (3)$$

with $\tilde{m}_j = m_j/M_j$, $\tilde{J}_{lj} = M_l^{-\frac{1}{2}} J_{lj} M_j^{-\frac{1}{2}}$ and $\tilde{\gamma}_j = 2\tilde{m}_j\zeta_j T_j$.

Thus, for ease of computation, in what follows we will analyze a system with alternate masses and equal on-site potentials, which will be included in the diagonal part of J. Precisely, we take

$$H(\mathbf{q},\mathbf{p}) = \sum_{j=1}^{N} \frac{1}{2}\left(\frac{p_j^2}{m_j} + \sum_{l=1}^{N} q_l J_{lj} q_j\right), \quad (4)$$

$$J_{lj} = 2\delta_{lj} - \delta_{l+1,j} - \delta_{l-1,j}, \quad j,l = 1,\ldots,N, \quad (5)$$

(i.e., J is the negative lattice Laplacian with Dirichlet boundary conditions) and we take the odd sites with particle mass m_1 and the even sites with particle mass m_2.

We follow Casher and Lebowitz (see Eq. (3.12), derived in more detail in Ref. [19]). In the limit of an infinite chain with two alternate masses, say, $m_1 < m_2$, the heat flow is given by

$$\mathcal{F} = \frac{(T_1 - T_N)m_1 m_2 \zeta}{\pi} \times \int \frac{|\omega \sin q|}{|(1 + \zeta^2 m_1 m_2 \omega^2)(m_2 K_{1,1} + m_1 K_{2,2})|} d\omega, \quad (6)$$

the integration being over the region where ω satisfies

$$|K_{1,2} - K_{2,1}| \leqslant 2,$$

that is,

$$-2 \leqslant K_{1,2}(\omega) - K_{2,1}(\omega) = 2\cos q \leqslant 2, \quad (7)$$

where $K_{2,1} = 1$, and $K_{j,l}(\omega)$ is the determinant of the $(l - j) \times (l - j)$ matrix $(\mathcal{J} - w^2\mathcal{M})$ for a particular chain which starts from the jth site and ends with the lth one. $\mathcal{M}$ above is the diagonal matrix whose diagonal entries are the particle masses $(m_j, m_{j+1}, \ldots, m_l)$. $\mathcal{J}$ is the matrix for the interparticle interaction (5) (for a chain that starts from the jth site and ends with the lth one, as already said).

Now we make explicit the region of integration. The extremes of the integration intervals are the roots of $(2 - m_1\omega^2)(2 - m_2\omega^2)$ and $(2 - m_1\omega^2)(2 - m_2\omega^2) - 4$ in Eq. (7). By using that

$$|\sin q| = \sqrt{1 - \cos^2 q},$$

where q is related to ω via Eq. (7)

$$\cos^2 q = [(1 - m_1\omega^2/2)(1 - m_2\omega^2/2) - 1]^2, \quad (8)$$

and noting that the integrand in Eq. (6) depends only on ω^2 (we denote ω^2 by x in what follows), we obtain

$$\mathcal{F} = \frac{(T_1 - T_N)m_1 m_2 \zeta}{2\pi} \times \left\{ \int_0^{\frac{2}{m_2}} f(x)dx - \int_{\frac{2}{m_1}}^{\frac{2(m_1+m_2)}{m_1 m_2}} f(x)dx \right\}, \tag{9}$$

$$f(x) = \frac{\sqrt{1 - \frac{1}{4}[(2-m_1x)(2-m_2x)-2]^2}}{(1+m_1m_2\zeta^2 x)(m_1+m_2-m_1m_2x)}. \tag{10}$$

After several tedious computations (some convenient changes of variables, algebraic manipulations, etc.), we obtained the exact expression for the heat flow

$$\mathcal{F} = \frac{(T_1 - T_N)}{4m_1m_2\zeta^3}\left[1 + \zeta^2(m_1+m_2) - \frac{\zeta^4(m_2^2 - m_1^2)}{1+\zeta^2(m_1+m_2)} - \frac{\sqrt{[1+2\zeta^2(m_1+m_2)](1+2\zeta^2m_1)(1+2\zeta^2m_2)}}{1+\zeta^2(m_1+m_2)}\right], \tag{11}$$

where we recall that $m_1 < m_2$.

As a test, we note that taking the limit $m_1 \to m_2 = m$ (i.e., considering the homogeneous case) we have

$$\mathcal{F} = \frac{T_1 - T_N}{4m^2\zeta^3}(1 + 2m\zeta^2 - \sqrt{1+4m\zeta^2}), \tag{12}$$

which is exactly the same expression obtained by Rieder, Lebowitz, and Lieb [18]. We note that in the homogeneous case the heat flow decays as we increase the particle mass as

$$\mathcal{F} \sim 1/m \quad \text{as } m \to \infty.$$

Turning to the system with alternate masses, if instead of increasing both masses we increase m_2 and decrease m_1, precisely, if we take $m_2 = 1/\epsilon$ and $m_1 = \epsilon$ (for small ϵ), a direct computation yields

$$\mathcal{F} = \frac{(T_1 - T_N)\zeta}{4}\epsilon^2 + \mathcal{O}(\epsilon^3). \tag{13}$$

That is, the heat flow decays as the inverse of the square of the mass difference (i.e., it decays proportionally to the mass ratio). In other words, we note an interesting (and not obvious) property: To decrease the heat flow, it is more effective to take alternate masses for the particles, increase one and decrease the other, than simply increase the particle mass of a homogeneous system. This phenomenon is clear in Fig. 1. We have a slower decay in the diagonal direction, where $m_1 = m_2$.

To offer an explanation for this phenomenon, namely, for the different behaviors of the heat flows of a homogeneous and an alternate mass chain, we turn to the analysis of the spectra of these systems and their effects in the heat current. First, we note that in the expression for the heat flow (6) [see also Eq. (7)], the region of integration on ω, given by Eq. (7), corresponds to wave vectors q (recall that $2\cos q = e^{iq} + e^{-iq}$) with which waves of one of the frequencies in the band determined by $\omega_j(q)$, $j = 1,2$ will propagate through the lattice. The ω_j^2 are the two roots of the polynomial equation $(K_{1,2} - K_{2,1})(\omega^2) = 2\cos q$, with $(K_{1,2} - K_{2,1})(\omega^2)$ being a polynomial of order 2 in ω^2, and $\omega_j(q)$ are positive for q real (more details in Ref. [19]). That is, in Eq. (6) the integration, as already said, is over $|K_{1,2} - K_{2,1}| \leqslant 2$ [i.e., over the frequency bands of ω^2: $\min\omega_j^2(q) \leqslant \omega^2 \leqslant \max\omega_j^2(q)$, $j = 1,2$, which are the solutions of Eq .(7)]. In a few words, the heat flow is given by an integration over the spectrum of the chain and there is an obvious difference between the expressions involving the spectrum of a single mass chain and those of a binary chain. There is only one interval of integration in the single mass case, but it splits into two parts (considering ω^2 as the variable of integration) for the binary system [see Eq. (9)]; roughly, the prohibited band between $2/m_2$ and $2/m_1$ (which obviously disappears if $m_1 = m_2$) makes the heat flow more difficult.

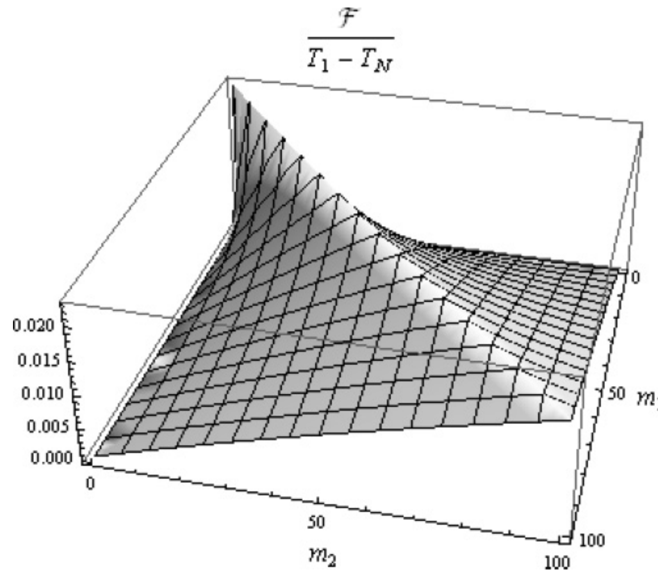

FIG. 1. Heat flow per temperature difference as a function of the masses m_1 and m_2 for $\zeta = 0.046$ [see Eq. (11)]. We note that, of all possible ways to decrease the heat flow, the least efficient is by setting $m_1 = m_2$.

The central question now is the reliability of such property, that is, will we find it in more realistic models? A first step to answering this question may be the analysis of the self-consistent harmonic chain of oscillators. This model, proposed in Ref. [20] and revisited in Ref. [21] (in the latter with homogeneous structures), is a schematic (and analytically treatable) anharmonic system: it consists of a chain of oscillators with harmonic nearest-neighbor interparticle interactions and on-site potentials and stochastic reservoirs coupled to each site. Its mathematical description is given by Eq. (2), now with each γ_j and B_j nonzero. From a physical point of view, the inner reservoirs may be interpreted as a schematic representation of the anharmonic part of the interaction (this model, as proved in Ref. [21] obeys Fourier's law, in opposition to the pure harmonic systems [18]). We stress that the inner reservoirs are not regarded as "real" thermal baths (the real baths are represented by the reservoirs at the boundaries), they describe only some residual mechanism of phonon scattering not present in the Hamiltonian interactions. Such a description is guaranteed by the "self-consistent condition," which means that the temperatures of the inner reservoirs are chosen in such a way that in the average no heat flows between each inner reservoir and its respective site in the steady state.

The heat flow for the self-consistent harmonic chain with alternate particle masses and harmonic on-site potentials has been studied in detail in a previous work [17]. For the regime of small (and nearest-neighbor) interparticle interaction J, up to $\mathcal{O}(J^2)$, we have

$$\mathcal{F} = \frac{2J^2\zeta m_1^{-1}m_2^{-1}}{\left(\frac{M_1}{m_1}-\frac{M_2}{m_2}\right)^2+2\zeta^2\left(\frac{M_1}{m_1}+\frac{M_2}{m_2}\right)} \times \left(\frac{T_N-T_1}{N-1}\right). \tag{14}$$

We note that for the homogeneous case $\mathcal{F} \sim 1/m$. For $M_1 = M_2 = 1$ (as already said, M_j denotes the on-site harmonic coefficient and J the interparticle coefficient), $m_1 = \epsilon$ and $m_2 = 1/\epsilon$, we get, when $\epsilon \ll 1$,

$$\kappa = \frac{2J^2\zeta}{(1/\epsilon - \epsilon)^2 + 2\zeta^2(1/\epsilon+\epsilon)} \approx 2J^2\zeta\epsilon^2. \tag{15}$$

That is, the phenomenon also holds in this model with normal conductivity. In short, the presence of this phonon scattering mechanism (i.e., noise in each site) does not destroy it.

III. ANHARMONIC CHAINS

Now we turn to self-consistent anharmonic chains of oscillators, that is, we introduce on-site anharmonic potentials in the previous self-consistent system. It makes the model more realistic since explicit anharmonic terms are found everywhere in interacting models. We keep the "extra" stochastic variables for technical reasons (as is well known, the analytic study of these nonlinear models is very difficult: "a rigorous treatment of a nonlinear system, even the proof of the existence of the conductivity coefficient, is out of reach of current mathematical techniques" [22]). However, we emphasize that they are not determinant for many properties of the heat flow. The inhomogeneous classical harmonic chain, for instance, even with inner reservoirs, does not present rectification, that is, there is rectification only in the model with real anharmonic on-site potentials. In other words, the presence of real anharmonicity may introduce considerable changes in the system behavior, and in that way, it could (in principle) destroy the effect that appears in harmonic chains due to the presence of alternate large and small masses. The use of these hybrid models (i.e., intricate anharmonic Hamiltonian systems still with inner noises) is recurrent [23].

To be precise, we take N oscillators with the Hamiltonian

$$H(q,p)=\sum_{j=1}^{N}\left[\frac{1}{2}\left(\frac{p_j^2}{m_j}+M_jq_j^2+\sum_{l\neq j}q_lJ_{lj}q_j\right)+\lambda_j\mathcal{P}(q_j)\right],$$

where $M_j > 0$, $J_{jl} = J_{lj}$, $\mathcal{P}$ is the anharmonic on-site potential: $\mathcal{P}(q_j) = q_j^4/4$; with the usual time evolution

$$dq_j=(p_j/m_j)dt, dp_j=-(\partial H/\partial q_j)dt-\zeta_j p_j dt+\gamma_j^{1/2}dB_j, \tag{16}$$

where, as in the harmonic case, B_j are independent Wiener processes, ζ_j is the coupling between site j and its reservoir, and $\gamma_j = 2\zeta_j m_j T_j$, where T_j is the temperature of the jth bath. We recall that here we consider only nearest-neighbor interactions.

As usual, the energy current inside the system is given by $\langle\mathcal{F}_{j\rightarrow}\rangle$, where $\langle\cdot\rangle$ means the expectation with respect to the noise distribution, and where

$$\mathcal{F}_{j\rightarrow} = J_{j,j+1}(q_j-q_{j+1})\left(\frac{p_j}{2m_j}+\frac{p_{j+1}}{2m_{j+1}}\right), \tag{17}$$

that is, $\mathcal{F}_{j\rightarrow}$ describes the heat flow from the jth to the $(j+1)$th site.

To ease the computation (i.e., the manipulation with indices, etc.) we map our system onto another with $m_j = 1$, for all j. It only means that we make the change of variables $Q_j = \sqrt{m_j}q_j$, $P_j = p_j/\sqrt{m_j}$, and so, J, M and λ are replaced by $\tilde{J}_{jk} = (m_j)^{-1/2}J_{jk}(m_k)^{-1/2}$, $\tilde{\lambda}_j = \lambda_j/m_j^2$, $\tilde{M}_j = M_j/m_j$. For simplicity, we drop out the tilde notation in the system below with unit masses, but, of course, we will rescale it later to recover the original system with different masses.

We also introduce the notation of the phase-space vector $\varphi = (Q,P)$, with $2N$ coordinates. Then, the dynamics (16) becomes

$$\dot{\varphi} = -A\varphi - \lambda\mathcal{P}'(\varphi) + \sigma\eta,$$

where $A = (A^0 + \mathcal{J})$ and σ are $2N \times 2N$ matrices

$$A^0 = \begin{pmatrix} 0 & -I \\ \tilde{\mathcal{M}} & \Gamma \end{pmatrix}, \quad \mathcal{J} = \begin{pmatrix} 0 & 0 \\ J & 0 \end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2\Gamma\mathcal{T}} \end{pmatrix}.$$

I above is the unit $N \times N$ matrix, J is the $N \times N$ matrix describing the interparticle interaction J_{lj}. $\tilde{\mathcal{M}}$,Γ,$\mathcal{T}$ are diagonal $N \times N$ matrices: $\tilde{\mathcal{M}}_{jl} = M_j\delta_{jl}$, $\Gamma_{jl} = \zeta_j\delta_{jl}$, $\mathcal{T}_{jl} = T_j\delta_{jl}$. η are independent white noises, $\mathcal{P}'(\varphi)$ is a $2N \times 1$ matrix with $\mathcal{P}'(\varphi)_j = 0$ for $j = 1,\ldots,N$ and $\mathcal{P}'(\varphi)_i = d\mathcal{P}(\varphi_{i-N})/d\varphi_{i-N}$ for $i = N+1,\ldots,2N$. It is useful to adopt the following index notation: i for index values in the set $[N+1,N+2,\ldots,2N]$, j for values in the set $[1,2,\ldots,N]$, and k for values in $[1,2,\ldots,2N]$.

In an approximative scheme, we establish an integral representation for the correlation functions, and so, for the heat current, of systems with the stochastic dynamics considered here. We emphasize that such an approach turns out to give the same result as the rigorous treatment for the simpler harmonic case [12]. Now we describe our approach. First, we consider the time evolution equations including the anharmonic on-site potential, but without the interparticle interaction J. A strong solution, even for the decoupled anharmonic problem, is unknown, but we may find the steady distribution: We follow Boltzmann, that is, we note that our system with $J = 0$ involves only noninteracting particles, each one connected to a thermal bath, and so we have, in the Q,P notation

$$d\mu_*(Q,P) = \exp\left(-\sum_{j=1}^{N}H_j^{(J=0)}/T_j\right)\prod_j dQ_jdP_j/\text{norm.},$$

$$H_j^{(J=0)} = \left(\frac{1}{2}M_jQ_j^2+\lambda_j\mathcal{P}(Q_j)+\frac{1}{2}P_j^2\right).$$

Now we use the Girsanov theorem (Cameron-Martin formula) [24] to introduce the interparticle interaction J. Such a theorem relates the solution of the complete process φ (including

J, the interparticle interaction) to the previous one ϕ (with $J = 0$): for $t_1, \ldots, t_k \leqslant t$, it states that $\langle \varphi_{r_1}(t_1), \ldots, \varphi_{r_k}(t_k) \rangle = \int \phi_{r_1}(t_1), \ldots, \phi_{r_k}(t_k) Z(t) d\mu$, where $\langle \cdot \rangle$ is the expectation for the complete process φ, while $d\mu$ is the distribution associated with the expectations of the decoupled process ϕ. After some stochastic calculus [12], the factor $Z(t)$ is given by

$$\begin{aligned} Z(t) = \exp\left[-\gamma_i^{-1}\phi_i(t)\mathcal{J}_{ij}\phi_j(t) + \gamma_i^{-1}\phi_i(0)\mathcal{J}_{ij}\phi_j(0)\right] \\ \times \exp\left(\int_0^t ds\gamma_i^{-1}\phi_i(s)\mathcal{J}_{ij}\phi_{j+N}(s) + - \int_0^t ds\phi_j(s)\right. \\ \times \mathcal{J}_{ji}^{\dagger}\gamma_i^{-1}A_{ik}^0\phi_k(s) - \int_0^t ds\phi_j(s)\mathcal{J}_{ji}^{\dagger}\gamma_i^{-1}\lambda\mathcal{P}'(\phi)_i(s) \\ \left. - \frac{1}{2}\int_0^t ds\phi_j(s)\mathcal{J}_{ji}^{\dagger}\gamma_i^{-1}\mathcal{J}_{ij'}\phi_{j'}(s)\right). \end{aligned} \tag{18}$$

The boundary condition $\phi(0) = 0$ is assumed here, for simplicity. As is well known, the heat flow (17) in the steady state involves the expression $\lim_{t\to\infty}\langle \varphi_u(t)\varphi_v(t) - \varphi_{u-N}(t)\varphi_{v+N}(t)\rangle$, $u > N, v \leqslant N$ [i.e., $\int \phi_u(t)\phi_v(t)Z(t)d\mu$, etc]. Note that, by writing $Z(t) = \exp[-\int W(\phi(s)]ds$, and by applying a perturbative analysis we obtain terms such as $\int \{\phi_u(t)\phi_v(t)W[\phi(s)]\} ds d\mu$. However, it is very difficult to calculate the distribution $d\mu$: For the nonlinear process we know only the steady distribution $d\mu_*$. Then, we have to introduce an approximative scheme on which to follow.

First, we note that, from the Itô calculus, we have $\langle f[\phi(t)]\rangle = e^{-t\mathcal{H}} f[\phi(0)]$, $\mathcal{H} = -\frac{1}{2}\gamma_i\nabla_i^2 + [A^0\phi + \lambda\mathcal{P}'(\phi)]\nabla$, where ∇ means the derivative with respect to ϕ (the index i, as is well known, takes values in $[N+1, \ldots, 2N]$). Thus, to relate $\phi(t)$ and $\phi(s)$, we replace $\phi(\cdot)$ by its average value. Moreover, we also replace $\mathcal{P}'(\phi)/\phi$ by its average value in the exponential relaxation of ϕ (more details ahead). In short, we propose the changes: $\phi(t) \to e^{-(t-s)\mathcal{H}}\phi(s) = e^{-(t-s)\mathcal{A}}\phi(s)$, where $\mathcal{A}$ is given by A^0 with M replaced by $\mathcal{M} \equiv M + \langle \lambda\mathcal{P}'(\phi)/\phi\rangle$. But recall that the computation of $\int \phi(s)\phi(s)d\mu$ is not possible since we do not know the distribution $d\mu$, as said before. As we have a fast (exponential) convergence to the steady state (i.e., the main contribution in our computations comes from the terms with s close to t) , we propose to replace $d\mu$ by $d\mu_*$, the well-known steady distribution.

In summary, our approximative scheme essentially means the replacement of $\phi(t)$ by $\langle \phi(t)\rangle$ and of $d\mu$ by $d\mu_*$.

Now, we may carry out the computations in an anharmonic model. Thus, up to the first order in J, after using a suitable representation [24] for $e^{-\tau\mathcal{A}}$ and performing the integration in τ, we obtain, for $u > N, v \leqslant N$

$$\begin{aligned} \langle \varphi_u\varphi_v\rangle = -(2\zeta_u T_u)^{-1}\mathcal{J}_{uv}\langle \phi_u^2\phi_v^2\rangle + (\mathcal{M}_v - \mathcal{M}_u)(D_{uv})^{-1}\left(\gamma_u^{-1} + \gamma_v^{-1}\right)\mathcal{J}_{uv}\langle \phi_u^2\phi_{v+N}^2\rangle \\ + \frac{\zeta_u + \zeta_v}{D_{uv}}\left[\mathcal{M}_u\zeta_v\gamma_v^{-1}\langle \phi_{u-N}^2\phi_{v+N}^2\rangle - \mathcal{M}_v\zeta_u\gamma_u^{-1}\langle \phi_u^2\phi_v^2\rangle\right]\mathcal{J}_{vu}^{\dagger} + \frac{\mathcal{M}_u}{D_{uv}}\left[(\mathcal{M}_u - \mathcal{M}_v) + \zeta_v(\zeta_u + \zeta_v)\right] \\ \times \left\{\left(M_u\gamma_u^{-1} + M_v\gamma_v^{-1}\right)\langle \phi_{u-N}^2\phi_v^2\rangle\mathcal{J}_{uv}^{\dagger} + \left[\lambda_{u-N}\langle \phi_{u-N}\mathcal{P}'(\phi_{u-N})\phi_v^2\rangle\gamma_u^{-1} + \lambda_v\langle \phi_{u-N}^2\mathcal{P}'(\phi_v)\phi_v^2\rangle\gamma_v^{-1}\right]\mathcal{J}_{vu}^{\dagger}\right\}, \end{aligned} \tag{19}$$

where $\mathcal{M}_u \equiv \mathcal{M}_{u-N}$, $D_{uv} = (\mathcal{M}_u - \mathcal{M}_v)^2 + (\mathcal{M}_u\zeta_v + \mathcal{M}_v\zeta_u)(\zeta_u + \zeta_v)$. For $u > N$, $\langle \phi_u^2\rangle = T_u$. However, the computation of $\langle \phi_v^2\rangle$, $v \leqslant N$ is not straightforward (note that $d\mu_*$ is a single spin distribution, so that $\langle \phi_u^k\phi_v^m\rangle = \langle \phi_u^k\rangle\langle \phi_v^m\rangle$). To continue the analysis, we assume the system in a high anharmonic regime (i.e., λ large and M small). Thus, we take $\langle \phi_v^2\rangle = 2c_1 T_v^{1/2}/\lambda_v^{1/2}$, $\langle \phi_v^4\rangle = 4c_2 T_v/\lambda_v$. If $M = 0$, we would have $c_1 \simeq \Gamma(3/4)/\Gamma(1/4) \simeq 1/3$, $c_2 \simeq \Gamma(5/4)/\Gamma(1/4) = 1/4$. We may determine the values of c_1 and c_2 by turning to the expression of the heat current $\mathcal{F}_{j\to} = \mathcal{J}_{uv}(\langle \varphi_u\varphi_v\rangle - \langle \varphi_{u-N}\varphi_{v+N}\rangle)/2$, with $u - N = j$, $v = j+1$: namely, we take all sites at the same temperature T and find the values such that $\mathcal{F}_{j\to} = 0$. We obtain $c_2 = 1/4$ and $c_1 = 1/2$. Now we can carry out all the further computations. In the case of high anharmonicity, after rescaling back to the system with general mass values (i.e., $\lambda_j \to \lambda_j/m_j^2$, etc.), we get, up to $\mathcal{O}(J^2)$,

$$\begin{aligned} \mathcal{F}_{j,j+1} = \frac{J^2 2\zeta}{m_j m_{j+1}}\left\{\left[\left(\frac{\lambda_j^{1/2}T_j^{1/2}}{m_j}\right) - \left(\frac{\lambda_{j+1}^{1/2}T_{j+1}^{1/2}}{m_{j+1}}\right)\right]^2 + 2\zeta^2\right. \\ \left. \times \left[\left(\frac{\lambda_j^{1/2}T_j^{1/2}}{m_j}\right) + \left(\frac{\lambda_{j+1}^{1/2}T_{j+1}^{1/2}}{m_{j+1}}\right)\right]\right\}^{-1}(T_j - T_{j+1}). \end{aligned} \tag{20}$$

From $\mathcal{F}_{j,j+1}$ above and the self-consistent condition $\mathcal{F} = \mathcal{F}_{1,2} = \mathcal{F}_{3,4} = \cdots = \mathcal{F}_{N-1,N}$, which essentially means that the heat current comes from the first reservoir, travels through the chain, and goes out by the last reservoir, we derive the temperature profile and the expression for the thermal conductivity. For simplicity, we take only alternate masses, that is, we make the other parameters homogeneous ($\lambda_j = \lambda$, etc.). For a system under a small gradient of temperature, precisely, for $T_1 = T + a_1\delta$ and $T_N = T + a_N\delta$, δ small, we have (up to first order in δ) $T_j = T + a_j\delta$, with a_j determined by the self-consistent condition (i.e., $\mathcal{F}_{1,2} = \mathcal{F}_{2,3} = \cdots = \mathcal{F}_{N-1,N}$), and so we obtain, after some algebraic manipulations

$$\mathcal{F} = \frac{2J^2\zeta/(\lambda^{1/2}T^{1/2})}{\left[\lambda^{1/2}T^{1/2}\frac{(m_1-m_2)^2}{m_1 m_2} + 2\zeta^2(m_1+m_2)\right]} \times \frac{(a_1 - a_N)\delta}{(N-1)}. \tag{21}$$

That is, the heat flow obeys Fourier's law [the term $(a_1 - a_N)\delta/(N-1)$ is the temperature gradient in the chain], with the thermal conductivity

$$\mathcal{K} = \frac{2J^2\zeta}{\lambda^{1/2}T^{1/2}}\left[\lambda^{1/2}T^{1/2}\frac{(m_1-m_2)^2}{m_1 m_2} + 2\zeta^2(m_1+m_2)\right]^{-1}. \tag{22}$$

Hence, we see that the same effect as the one previously described for the harmonic systems due to the presence of alternate masses also holds in the anharmonic chain. In summary, it seems to be a ubiquitous phenomenon. We remark that similar effects appear if we consider alternate on-site potentials instead of alternate masses (it is clear from the previous expressions).

IV. FINAL REMARKS

In the present work, searching for properties or mechanisms to manipulate the heat flow in general materials, we analytically study harmonic and anharmonic chains of oscillators with nearest-neighbor interactions, and show a kind of insulating effect obtained with the use of alternate large and small masses or on-site potentials.

We stress that the existence of similar behaviors in standard systems with different features modeling the heat conduction in solids, such as the harmonic, self-consistent harmonic and anharmonic chains, indicates the ubiquity of the phenomenon. Moreover, the simplicity of the conditions for the existence of the effect (namely, no intricate interaction or specific potential is required, only the presence of alternate masses or on-site potentials) also shows that it may be used in practical devices.

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