Requisite ingredients for thermal rectification

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The present work is devoted to an analytical investigation of the thermal rectification mechanism. More specifically, we attempt to find the requisite ingredients for such a phenomenon to occur. Starting from the linearization of the time evolution equations of anharmonic chains of oscillators, we propose some effective harmonic toy models with a potential that is dependent on temperature, and we investigate their steady heat currents. This unusual temperature-dependent potential is the footprint of nonlinearity in the final effective linear model. The approach is not restricted to any particular regime of heat transport. Our results show that thermal rectification holds in a system if it has asymmetric parameters related to its own structure, e.g., a graded particle mass distribution and some other parameters or features dependent on the inner temperatures that change as we invert the baths at the boundaries. The description of rectification in these simplified models, with minimal ingredients, shows that it is a ubiquitous phenomenon, and it may serve as a guide for further research.

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I. INTRODUCTION

One of the central issues of nonequilibrium statistical physics is the derivation of the macroscopic laws of transport from the underlying microscopic models. For the past few decades, a great deal of work has been devoted to this subject, particularly to the study of energy transport, whose predominant mechanisms are conduction by electricity and heat. It is interesting to note that both of these mechanisms are of comparable importance, but they occupy a different status in science. On the one hand, there has been amazing progress in the field of electronics, not only in the form of considerable theoretical and experimental advances, but also with the incredible technological development due to the invention of transistors and other electronic devices. On the other hand, despite decades of research [1], the evolution of the counterpart of electronics that is devoted to the control and manipulation of heat current has been slow. This lack of progress has been due mainly to a lack of efficient and practicable thermal diodes.

A thermal diode, or rectifier, is the basic element in heat manipulation devices. In a thermal rectifier, the magnitude of the heat current changes as we invert the system between two thermal baths; in other words, the current has a preferential direction. The phenomenon of thermal rectification was observed long ago [2], but the first manageable theoretical rectifier was proposed only in 2002 [3]. The most recurrent diode designs are given by the coupling of two or three different anharmonic segments, and they present critical problems: rectification power is small and decays rapidly to zero as the system size increases [4]. Improvements have been made by extending the use of a few asymmetric parts to graded materials, i.e., inhomogeneous systems with a composition that changes gradually in space. The first microscopic solid-state thermal diode was built experimentally with graded nanotubes by Chang *et al.* [5]. Since then, rectification in different graded materials has been investigated numerically [6–10] and analytically [8,11–13]. Another enhancement that was investigated theoretically [13] and numerically [9] was given by the use of systems with long-range interparticle interactions. This enhancement increases the rectification power significantly and prevents its decay with the system size.

In short, some progress has been made in the area of thermal rectification, but we are still waiting for results leading to an irreproachable and reliable diode. To achieve such an end, a much better theoretical comprehension of the ingredients of thermal rectification is highly desirable. However, our scenario is discouraging: since the work of Debye and Peierls, the archetypal models for the study of heat conduction in insulating solids have been given by anharmonic chains of oscillators, and their analytical investigation is extremely difficult [14].

To overcome these technical obstacles, approximations [11] and toy models [8] have been considered in some previous works. Moreover, there are some previous approaches for the description of rectification that start by assuming an expression for the heat current (instead of deriving it) [12,15], thus they skip the nonlinear dynamical analysis of the underlying microscopic models. However, these approaches, starting from established expressions for the heat current, are restricted to the case of normal transport, in which the heat current is given by Fourier's law.

In the present paper, we attempt to find the requisite ingredients for the occurrence of thermal rectification, independent of the transport regime. Here, based on our awareness of the technical imbroglio of anharmonic models, we address two issues: (i) first, we search for effective and treatable models, with linear dynamics but with the footprint of the anharmonic chains, i.e., with some residual anharmonic characteristic related to the rectification; (ii) second, based upon our investigation of these minimal, simplified models, we want to point out the basic ingredients responsible for the occurrence of thermal rectification. We believe that such knowledge will be quite helpful in future research for efficient diodes.

Here, we show that, within a simple, linear toy model with an effective potential that is dependent on temperature, it is possible to guarantee the occurrence of thermal rectification. Our results, obtained without the necessity of normal transport, indicate that thermal rectification shall appear in a system de-

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scribed by more intricate interactions if it presents asymmetric parameters associated with its own structure, such as a graded particle mass distribution and some other inner parameters or related features that are dependent on the temperatures in the bulk, which are determined by the baths at the boundaries; that is, parameters that are dependent on inner temperatures, which modify as we invert the baths. In short, we point out a few ingredients that guarantee the occurrence of thermal rectification.

The rest of the paper is organized as follows. In Sec. II we present the harmonic toy model related to the linearization in the dynamics of an anharmonic model, without normal transport. Then, we show the existence of thermal rectification in such linear, effective model. In Sec. III we extend our approach, i.e., we build a toy model based on the linear approximation for the case of a chain with inner stochastic baths and on-site potentials. Our aim is to show that, also for an asymmetric system with normal transport, an effective linear potential that is dependent on temperature is sufficient to guarantee the occurrence of rectification. Section IV is devoted to the final remarks.

II. RECTIFICATION IN A CHAIN WITH TRANSLATIONALLY INVARIANT POTENTIAL

In our search to find the minimal requirements for the occurrence of thermal rectification in solid-state materials, we aim to find a streamlined, unadorned, effective model, but with sufficient ingredients. Moreover, we want to describe the onset of rectification in models that do not require the local heat flow expression $\mathcal{F} = -\kappa(T,x)dT/dx$ (or its discrete version), i.e., Fourier's law, which is related to normal transport, and which was used in some previous works devoted to the study of rectification [12,15]. Hence, in this section we present an analytical investigation of systems with translationally invariant potentials in which an expression for the local heat current (such as that given above) does not hold.

It is worthwhile to emphasize the following point: When pursuing the basic ingredients of a given phenomenon, it may be helpful to use simplified and even toy models, as such models may serve to distinguish intricate but unimportant details from the minimal ingredients. Along those lines, i.e., as an example of previous research using that strategy, we recall the description of thermal rectification in the bare, straightforward model of bars and balls [8]. The results of that study clarified the ubiquitous occurrence of rectification in more intricate graded models with normal transport.

One more comment is in order in the context of effective models for the study of heat conduction: It is also interesting to recall the harmonic chain of oscillators with inner stochastic baths in a self-consistent condition (i.e., a condition in which the temperatures of the inner baths are chosen such that there is no net heat flow from the inner baths to the chain in the steady state). It is an old and recurrently studied (harmonic) version of an "effective anharmonic chain" [16–18]. The inner baths represent a mechanism of phonon scattering, i.e., this simplified model takes traces of a system with anharmonic on-site potentials. Indeed, the Fourier law holds in such a model, but it does not hold in the purely harmonic chain without the inner baths [19]. However, this model does not contain the ingredients necessary for the occurrence of thermal rectification: in Ref. [20], it is rigorously proved that no asymmetric version of the model results in thermal rectification (i.e., versions with interactions that are not dependent on temperature). See also Ref. [21]. It is very important to stress that the existence of asymmetry in a system is absolutely not a guarantee of thermal rectification. More comments and a simple example are found in the introduction of Ref. [22]. However, in Sec. III, we address these self-consistent chains of oscillators, and we show that an extended harmonic version, in which we add an extra potential that is dependent on temperature, becomes suitable to describe thermal rectification.

To construct an effective system, we first analyze some more complete, reliable models. For the sake of generality, we consider the most basic models for the study of the heat conduction mechanism in insulating solids, namely chains of anharmonic oscillators. As was already mentioned, these prototype models have been recurrently investigated since the work of Debye and Peierls [23]. More specifically, we consider asymmetric chains with translationally invariant potentials and thermal baths at the boundaries.

We recall that the occurrence of thermal rectification in some asymmetric anharmonic chains of oscillators has already been observed, with most of the results achieved by means of computer simulations. Some examples include the case of anharmonic on-site potentials [11], in which Fourier's law holds, and even graded Fermi-Pasta-Ulam models [6] with abnormal transport. However, the question regarding the requisite ingredients for thermal rectification is still open.

Here, our departure point is the one-dimensional chain of N oscillators with translationally invariant potentials (such as in the Fermi-Pasta-Ulam case), i.e., a system with the Hamiltonian

$$\mathcal{H}(q,p) = \sum_{j=1}^{N} \frac{p_j^2}{2m_j} + \sum_{j=1}^{N-1} \left[\frac{J}{2}(q_{j+1}-q_j)^2 + \frac{\lambda}{4}(q_{j+1}-q_j)^4 \right],$$

where (as we want to study thermal rectification) we take an asymmetric, graded mass version, e.g., $m_1 < m_2 < \cdots < m_N$. For concreteness, we write a quartic anharmonic potential in the above Hamiltonian, but the specific power is unimportant in our forthcoming analysis. To describe the contact with two thermal baths at different temperatures, we assume the usual Langevin dynamics,

$$\begin{aligned} dq_j &= \frac{\partial \mathcal{H}}{\partial p_j} dt = \frac{p_j}{m_j} dt, \\ dp_j &= -\frac{\partial \mathcal{H}}{\partial q_j} dt - \zeta_j p_j dt + \gamma_j^{1/2} dB_j, \\ &= -\sum_{|j-\ell|\leqslant 1} [\mathcal{J}_{j,\ell} q_\ell + \lambda(q_j - q_\ell)^3] dt \\ &\quad - \zeta_j p_j dt + \gamma_j^{1/2} dB_j, \end{aligned} \tag{1}$$

where the harmonic interaction is written by means of the matrix $\mathcal{J}_{j,\ell} = \frac{J}{2}(-\Delta)_{j,\ell}$, with Δ denoting the lattice Laplacian; ζ is a dissipative constant: $\zeta_j = \zeta(\delta_{j,1} + \delta_{j,N})$; $\gamma_j = 2\zeta_j m_j T_j$ represents the dissipation to the temperatures of the baths T_1 and T_N; and the baths are described by Brownian motions B_1 and B_N, with

$$\langle B_j(t)\rangle = 0; \quad \langle B_j(t)B_\ell(s)\rangle = \delta_{j,\ell}(\delta_{j,1}+\delta_{j,N})\min\{t,s\}$$

(i.e., dB_j/dt are independent white noises).

It is convenient to introduce the phase-space vector ϕ with $2N$ coordinates, $\phi=(q,p)$, and to rewrite the dynamical equations above as

$$d\phi_k = -(A\phi)_k dt - \lambda\mathcal{P}'(\phi)_k dt + (\sigma dB)_k, \tag{2}$$

where A and σ are $2N\times 2N$ matrices,

$$A = \begin{pmatrix} 0 & -M^{-1} \\ \mathcal{J} & L\end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\Gamma}\end{pmatrix},$$

where $\mathcal{J}$ is the $N\times N$ matrix for the interparticle interaction $\mathcal{J}_{lj}$; M, L, and Γ are diagonal $N\times N$ matrices: $M^{-1}_{jj}=1/m_j$, $L_{jj}=\zeta(\delta_{j,1}+\delta_{j,N})$, and $\Gamma_{jj}=\gamma_j$; and

$$\begin{aligned}\mathcal{P}'(\phi)_k &= 0 \quad \text{if } k>N,\\ &= \lambda[(\phi_k-\phi_{k+1})^3+(\phi_k-\phi_{k-1})^3] \quad \text{if } 1<k<N,\\ &= \lambda(\phi_k-\phi_{k+1})^3 \quad \text{if } k=1,\\ &= \lambda(\phi_k-\phi_{k-1})^3 \quad \text{if } k=N.\end{aligned}$$

To investigate the heat flow into the system, we define, as usual, the energy $\mathcal{H}_j$ of a single site j from $\mathcal{H}=\sum_j\mathcal{H}_j$ (we split the terms in $\mathcal{H}$ that involve two sites into two equal parts, one for $\mathcal{H}_j$ and the other for $\mathcal{H}_{j-1}$ or $\mathcal{H}_{j+1}$). Then we study $d\mathcal{H}_j/dt$, and from the continuity equation (for the inner sites),

$$\frac{d\mathcal{H}_j}{dt} = \mathcal{F}_{j-1,j} - \mathcal{F}_{j,j+1},$$

we determine the heat current $\mathcal{F}_{j-1,j}$ from the previous site to j, and $\mathcal{F}_{j,j+1}$ from j to the following site. Of course, in the steady state we have $\langle d\mathcal{H}_j/dt\rangle = 0$, and so $\langle\mathcal{F}_{j-1,j}\rangle = \langle\mathcal{F}_{j,j+1}\rangle \equiv \mathcal{F}$.

To proceed, we first perform a general analysis of the stochastic dynamics. From the Itô formula [24], for the function $f=(f_1,f_2,\dots,f_r)$ of the phase-space vector ϕ (which is an Itô process) and t, i.e., $f_j(t,\phi)$, we have

$$df_j = \frac{\partial f_j}{\partial t}dt + \frac{\partial f_j}{\partial\phi_k}d\phi_k + \frac{1}{2}\frac{\partial^2 f_j}{\partial\phi_r\partial\phi_\ell}d\phi_r d\phi_\ell$$

(the sum over repeated indices is assumed). And so, for the case of ϕ given by Eq. (2) above and f not an explicit function of t, i.e., $f_j\equiv f_j(\phi)$, we obtain

$$\begin{aligned} f_j(\phi(t)) &= f_j(\phi(0)) + \int_0^t \frac{\partial f_j}{\partial\phi_i}(\phi(s))\gamma_i^{1/2}dB_i(s)\\ &\quad + \int_0^t\left[\frac{1}{2}\gamma_i\frac{\partial^2 f_j}{\partial\phi_i^2}(\phi(s)) - [A\phi+\lambda\mathcal{P}'(\phi)]_k\frac{\partial f_j}{\partial\phi_k}(\phi(s))\right]ds.\end{aligned}$$

With the notation $Q_t f \equiv \langle f(\phi(t))\rangle$, the Itô formula gives, for the dynamics,

$$Q_t(f_j) = f_j(\phi(0)) - \int_0^t (Q_s H f_j)(\phi(s))ds,$$
$$H = -\frac{1}{2}\gamma_i\frac{\partial^2}{\partial\phi_i^2} + [A\phi+\lambda\mathcal{P}'(\phi)]_k\frac{\partial}{\partial\phi_k}. \tag{3}$$

The index i above runs in $\{N+1,N+2,\dots,2N\}$ (i.e., ϕ_i above represents only the variable p), and the index k runs in $\{1,2,\dots,2N\}$.

As is well known and mentioned repeatedly, the analytical investigation of these nonlinear stochastic dynamical systems is an extremely arduous task. In addition to the technical difficulties of an intricate study with numerous expressions, certain relations and details may camouflage the ingredients of rectification. Consequently, in order to make the problem treatable and also more transparent, we pursue an effective simplification involving harmonic interactions. That is, we aim now to build an effective, toy model with a modified linear dynamics with traces of nonlinearity, and one that will be beneficial for the investigation of rectification. It is important to point out that this strategy of finding amendments in the linear dynamics part of the model, in some way representing nonlinear effects, is used recurrently in the study of heat conduction. For example, we recall the "effective phonon theory" proposed in Ref. [25], in which the starting point is a modification in the spectrum of the harmonic lattice in order to obtain the frequencies of the "effective phonon," which describe the heat in the anharmonic lattice (see also Refs. [26,27]). As another example of a related approach that uses corrections in the harmonic theory in order to describe some aspect of anharmonicity, we recall Ref. [28], in which the authors propose an effective anharmonic phonon wave number as a function of temperature. Of course, with such approaches we hope only to describe qualitative aspects of the complete problem.

Here, a possible attempt is to consider some sort of mean-field approximation for the nonlinear part of Eq. (3) above in order to conceive a modification leading to a linear term. Hence, we may write λx^3 in $\lambda\mathcal{P}'$ [$x=(\phi_j-\phi_{j-1})$] as $\lambda\langle x^2\rangle x$, where $\langle\cdot\rangle$ is, e.g., the average in the steady state. Of course, we do not know the stationary distribution for these nonlinear stochastic dynamics, but we may consider the case of a system subjected to a small temperature gradient, and, assuming local thermal equilibrium, we may use the local Boltzmann-Gibbs distribution. Roughly, for the case of large λ,

$$\begin{aligned}\langle x^2\rangle &\approx \int_{-\infty}^{\infty} x^2\exp\left[-\left(\frac{Jx^2}{2}+\frac{\lambda x^4}{4}\right)\frac{1}{T}\right]dx/\text{norm}\\ &= \frac{2\int_0^\infty 2\left(\frac{T}{\lambda}\right)^{1/2}u^{1/2}u^{-3/4}\exp\left[-\frac{J}{T}\left(\frac{T}{\lambda}\right)^{1/2}u^{1/2}-u\right]du}{2\int_0^\infty u^{-3/4}\exp\left[-\frac{J}{T}\left(\frac{T}{\lambda}\right)^{1/2}u^{1/2}-u\right]du}\\ &= c_0\left(\frac{T}{\lambda}\right)^{1/2} + O(\lambda^{-1}),\end{aligned} \tag{4}$$

where c_0 is the coefficient of the leading term in the λ expansion above: it does not depend on λ, and it comes from the integration; T is the local temperature (as was already mentioned, the expression is valid for a large anharmonic term; in the opposite, purely harmonic case with $\lambda=0$, which does not interest us, we obviously have $\langle x^2\rangle = T/J$). For the case of sharp anharmonicity, i.e., λx^α with α large, we expect $\langle x^{\alpha-1}\rangle$ proportional to T: more specifically, $\lambda\langle x^{\alpha-1}\rangle\approx c(\lambda)T^{1-1/\alpha}$ for $c(\lambda)$ some function of λ.

Hence, considering these previous arguments and manipulations, we propose to investigate a toy model in our search for the basic ingredients needed for thermal rectification. This toy model is given by a modified linear dynamical system that is related, in some way, to simplifications in the anharmonic chain of oscillators. In the simplified model, an effective anharmonicity, i.e., some vestige of anharmonic interactions, is represented by the addition (in the linear interaction $\mathcal{J}\phi$) of another linear term that is dependent on temperature. We investigate the chain with dynamics,

$$d\phi_k = -(\tilde{A}\phi)_k dt + (\sigma dB)_k, \tag{5}$$

where

$$\tilde{A} = \begin{pmatrix} 0 & -M^{-1} \\ \tilde{\mathcal{J}} & L \end{pmatrix},$$

and $\tilde{\mathcal{J}} = \mathcal{J} + \Lambda$; for example, $\tilde{\mathcal{J}}_{j,j+1} = \mathcal{J}_{j,j+1}\{1 + c(\lambda)[T_j + T_{j+1}]/2\}$, where $c(\lambda)$ is some properly chosen parameter. That is, $\tilde{\mathcal{J}}$ is the previous, usual harmonic interaction $\mathcal{J}$ plus an extra term that depends on temperature. For ease of computation, instead of taking Λ as $\mathcal{J}$, with off-diagonal elements, we assume it is a diagonal matrix, with elements changing linearly with temperature,

$$\Lambda_{j,j} \equiv a_j = c(\lambda)\left[T_1 + \frac{j-1}{N-1}(T_N - T_1)\right]. \tag{6}$$

T_1 and T_N are the temperatures of the sites at the boundaries, linked to the baths. We emphasize that the detailed expression for Λ assumed above (as a diagonal matrix and linear function of T) is not important to establish the occurrence of thermal rectification: the key fact, as we will see, is the bulk of the chain with some dependence on temperature, which will change as we invert the baths at the boundaries.

Now, with a linear model, the problem becomes more accessible: the analytical study of the classical harmonic chain of oscillators is an old problem. Precise approaches and some rigorous, exact results are well known for the case of a homogeneous (or essentially homogeneous) system. For example, the exact expression for the heat current in a homogeneous chain is presented in the seminal work of Rieder, Lebowitz, and Lieb [19]. A different approach, as well as properties for the steady state of periodic harmonic chains, is obtained by Casher and Lebowitz [29]. Detailed results for chains of oscillators with alternated masses are presented in Ref. [30]. However, the precise analytical study of a complete inhomogeneous chain seems more complicated.

Here, we will follow the approach developed by Casher and Lebowitz [29] to obtain an integral representation for the heat current in the chain. The asymmetry in the system complicates the work of solving such integrals to get an exact expression for the current. Thus we take small systems, with few sites, and we use numerical methods to integrate the expression for the heat current. We compare the results for a given chain between two thermal baths and the same chain with inverted baths in order to confirm the occurrence of thermal rectification. The existence of such a phenomenon in larger chains will be made clear by the algebraic expressions in the integral representation, as we will argue later.

According to Ref. [29], for the chain of oscillators with dynamics given by Eq. (5), in a steady state, the heat current from the first bath to the first site, and thus the heat current into the chain, is given by

$$\mathcal{F}_1 = \frac{(T_1 - T_N)\zeta^2 m_1 m_N}{\pi}\int_{-\infty}^{\infty} d\omega\, \omega^2 \left|Z_{1,N}^{-1}(\omega)\right|^2, \tag{7}$$

where $Z_{1,N}^{-1} = C_{1,N}/\det Z$, $C_{1,N}$ is the cofactor of $Z_{1,N}$, and $Z_{1,N}$ is the matrix involving sites $1,2,\ldots,N$ with

$$Z(\omega) = \tilde{\mathcal{J}} - i\omega ML - \omega^2 M. \tag{8}$$

After some algebraic manipulation, it is still possible to rewrite the above equation for $\mathcal{F}_1$ as

$$\mathcal{F}_1 = \frac{(T_1 - T_N)\zeta^2 m_1 m_N}{\pi}\int_{-\infty}^{\infty} d\omega \frac{\omega^2 |C_{1,N}(\omega)|^2}{(K_{1,N} - \zeta^2\omega^2 m_1 m_N K_{2,N-1})^2 + \zeta^2\omega^2(m_1 K_{2,N} + m_N K_{1,N-1})^2} \tag{9}$$

[see Eq. (2.20) in Ref. [29]], where $K_{j,k}$ is the determinant of the matrix $(\tilde{\mathcal{J}} - \omega^2 M)$ for a chain that starts from the jth site and ends with the kth one.

As was mentioned, for our case of asymmetric interactions it is still difficult to find the exact final expression for the heat current given above (i.e., to perform the integral in ω). However, it is not necessary to observe the occurrence of thermal rectification. Indeed, according to the formulas, the heat current is given by the integration of $\det Z$ (or equivalently, by the integration of some $K_{j,\ell}$). In addition, Z involves the sum of Λ, which is the effective anharmonicity represented here by a function of temperature changing linearly as we go along the chain, and of M, which is the particle mass distribution. As we invert the two thermal baths, M does not change since it is determined only by the masses of the particles in the chain, but Λ does change. In our approximation, it is given by the linear function determined by the temperatures of the baths at the boundaries; in any case, even for other functions of T in Λ, it will be related to the baths and it will change as we invert them. In short, we expect to have a different $\det Z$ with the inversion of the baths, and thus a different heat current. That is, we expect the occurrence of thermal rectification. Note that it does not hold for the purely harmonic chain, i.e., in the absence of Λ: in such a case, $|\det Z|$ does not involve the temperatures, and thus $\mathcal{F}_1$ only changes sign upon the inversion of the baths due to the term in front of the integral in Eqs. (7) and (9).

For the sake of transparency, we compute the heat current for different chains with $N = 3,4,5,6$ sites subjected to different temperatures; we repeat the computation as we invert the baths in order to confirm the occurrence of thermal rectification. We list the results below, computed by using free boundary conditions, which means the end terms in the diagonal of $\mathcal{J}$ are $\mathcal{J}_{1,1} = \mathcal{J}_{N,N} = 1$. We repeated the computations for the case of fixed boundary conditions, $\mathcal{J}_{1,1} = \mathcal{J}_{N,N} = 2$, and we obtained similar results (not described here). We define the rectification factor as the difference between the energy flow in a given situation and the related flow as we invert the baths, divided by the smallest of the flows:

$$\mathcal{R} \equiv \frac{||\mathcal{F}| - |\mathcal{F}_I||}{\min\{|\mathcal{F}|,|\mathcal{F}_I|\}}. \tag{10}$$

Such a definition is usual in the related study of rectification in classical anharmonic chains of oscillators, and its meaning is clear: if, for instance, the flow in a given direction is twice the flow in the inverted chain, we obtain $\mathcal{R} = 1$, which means a difference of 100%.

In all situations, we take $\zeta^2 = 1/1000$; $a_1 = T_1$, $a_N = T_N$, and of course $a'_1 = T_N$, $a'_N = T_1$, and $a'_j = a_{N-j+1}$. a_j is the element of Λ, the "effective anharmonicity"; see Eq. (6).

First, we analyze some systems subjected to different temperatures at the boundaries, with different numbers of sites but with the same mass difference: $m_N = 2$ and $m_1 = 1$. The results are as follows:

N	m_1	δm_j	a_1	δa_j	$\mathcal{R}$
3	1	0.5	0.1	0.1	0.18
3	1	0.5	0.1	0.2	0.42
3	1	0.5	1	1	2.70
3	1	0.5	1	2	5.56
4	1	*	0.1	0.1	0.31
4	1	*	0.1	0.2	0.63
4	1	*	1	1	9.75
4	1	*	1	2	36.07
5	1	0.25	0.1	0.1	0.43
5	1	0.25	0.1	0.2	0.61
5	1	0.25	1	1	23.16
5	1	0.25	1	2	53.07
6	1	0.2	0.1	0.1	0.43
6	1	0.2	0.1	0.2	0.77
6	1	0.2	1	1	231.01
6	1	0.2	1	2	762.52

An asterisk indicates that we take a nonlinear mass distribution: as in the other cases, $m_1 = 1$ and $m_4 = 2$, but $m_2 = 1.5$ and $m_3 = 1.8$.

The effect of increasing the mass gradient for a fixed difference of temperature in the system is as follows:

N	m_1	δm_j	a_1	δa_j	$\mathcal{R}$
6	1	0.2	0.1	0.2	0.77
6	1	0.6	0.1	0.2	3.68
6	1	1	0.1	0.2	7.97
6	1	**	0.1	0.2	26.15

Two asterisks indicate that we consider a geometric mass distribution: $m_1 = 0.1$, $m_2 = 0.2$, $m_3 = 0.4$, $m_4 = 0.8$, $m_5 = 1.6$, and $m_6 = 3.2$.

It is clear that the simplified linear toy model, in addition to being suited to describe the occurrence of thermal rectification, can also show other properties already observed in related anharmonic models by means of computer simulations [6]. For example, the rectification factor increases with the increment of the temperature gradient in the system, as well as with the rise of asymmetry (mass gradient).

III. THE EFFECTIVE LINEAR MODEL RELATED TO A SYSTEM WITH ON-SITE ANHARMONIC POTENTIAL AND INNER RESERVOIRS

To confirm that harmonic chains of oscillators with effective, temperature-dependent potentials contain features that are sufficient to describe the intricate properties of anharmonic chains, specifically thermal rectification, we proceed with a rapid investigation starting from the model with self-consistent inner stochastic baths. As was previously recalled, in this old and recurrently studied model, an effective anharmonicity (or at least some mechanism of phonon scattering) is already represented by the inner baths: even in the harmonic version, Fourier's law of heat conduction holds [17,18], and it disappears if we turn off the inner reservoirs. However, these inner baths, which lead to Fourier's law, are not sufficient to guarantee thermal rectification, which is indeed absent in any asymmetric version of the model (as was proven in Ref. [20]). An important comment is in order: in these models with self-consistent inner baths, the average energy is conserved in the steady state, thus the models are suitable for the investigation of heat conduction.

In this section, we show that if we add a temperature-dependent interaction in the harmonic model with inner reservoirs while maintaining the linear dynamics, i.e., following the strategy described in the previous section, then thermal rectification emerges.

Let us present some technical details. In order to derive the effective linear toy model, we start from N oscillators with the Hamiltonian

$$H(q,p) = \sum_{j=1}^{N}\left[\left(\frac{p_j^2}{2m_j} + \frac{\mu_j q_j^2}{2} + \sum_{l\neq j} q_l \mathcal{J}_{lj} q_j\right) + \lambda_j \mathcal{P}(q_j)\right], \tag{11}$$

where $\mathcal{J}$ is symmetric, $\mathcal{J}_{jl} = \mathcal{J}_{lj}$ (a nearest-neighbor interaction, as in the previous section), $\mu_j > 0$, and $\mathcal{P}$ is the anharmonic on-site potential, e.g., $\mathcal{P}(q_j) = q_j^4/4$. In addition, for the dynamics,

$$\begin{aligned} dq_j &= (p_j/m_j)dt, \\ dp_j &= -(\partial H/\partial q_j)dt - \zeta_j p_j dt + \gamma_j^{1/2} dB_j, \end{aligned} \tag{12}$$

where $\gamma_j = 2\zeta_j m_j T_j$, ζ_j is the coupling between site j and its reservoir, and T_j is the temperature of the jth bath; B_j are independent Wiener processes. With the phase-space notation $\phi = (q,p)$, we have

$$\dot{\phi} = -A\phi - \lambda\mathcal{P}'(\phi) + \sigma\eta, \tag{13}$$

where $\eta_j = dB_j/dt$ are independent white noises; A and σ are $2N \times 2N$ matrices,

$$A = \begin{pmatrix} 0 & -M^{-1} \\ \mathcal{J} + \mathcal{M} & L \end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\Gamma} \end{pmatrix}, \tag{14}$$

where M, L, $\mathcal{M}$, and Γ are the diagonal matrices with $M_{jj} = m_j$, $L_{jj} = \zeta_j$, $\mathcal{M}_{j,j} = \mu_j$, and $\Gamma_{jj} = \gamma_j$. $\mathcal{P}'$ is the derivative of $\mathcal{P}$.

Hence, from Itô's formula,

$$Q_t(f) \equiv \langle f(\phi(t))\rangle = f(\phi(0)) - \int_0^t (Q_s H f)(\phi(s))ds,$$
$$H = -\frac{1}{2}\gamma_i \nabla_i^2 + [A\phi + \lambda \mathcal{P}'(\phi)] \cdot \nabla,$$

where ∇ means the derivation with respect to ϕ (i takes values in $[N+1,\ldots,2N]$). Again, a possible linearization is obtained with the replacement

$$A\phi + \lambda \mathcal{P}'(\phi) \longrightarrow [A + \lambda\langle\phi^2\rangle]\phi,$$

where, for the case of weak interparticle interaction $\mathcal{J}$ and large anharmonicity λ, the average is essentially given by [see Eq. (4)]

$$\langle\phi_j\rangle \approx \int_{-\infty}^{\infty} q^2 \exp\left[-\frac{1}{T_j}\left(\frac{\mu q^2}{2} + \frac{\lambda q^4}{4}\right)\right] dq/\text{norm}$$
$$\approx c\left(\frac{T_j}{\lambda}\right)^{1/2},$$

where T_j is the temperature of the jth bath.

That is, a toy model related to this anharmonic problem is given by the stochastic dynamics

$$\dot{\phi} = -\tilde{A}\phi + \sigma\eta, \tag{15}$$

where now

$$\tilde{A} = \begin{pmatrix} 0 & -M^{-1} \\ \mathcal{J} + \mathcal{M} + c_\lambda \mathcal{T}^\alpha & L \end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\Gamma} \end{pmatrix},$$

c_λ is some function of λ (and gives the "anharmonicity" strength), $\mathcal{T}$ is the diagonal matrix $\mathcal{T}_{j,k} = \delta_{j,k} T_j$, and α is some parameter also related to the anharmonicity. It is important to stress that, for the occurrence of thermal rectification, as we show below, it is only necessary to have $\alpha \neq 0$, i.e., the precise dependence on temperature of the sites in the bulk does not matter.

Similar linear stochastic dynamical systems have already been investigated exhaustively [17,18], and detailed expressions for the heat current, in different situations, have been derived. In the steady state, for the heat flow between sites j and $j+1$, in the case of weak nearest-neighbor interparticle interaction [i.e., small J in $J(\phi_{j+1} - \phi_j)^2$], uniform $\mu_j = \mu$, and $c_\lambda = c$, we have for the leading order in an expansion in powers of J,

$$\mathcal{F}_{j,j+1} = \frac{2J^2\zeta m_j^{-1} m_{j+1}^{-1}}{\left(\frac{\mu + cT_j^\alpha}{m_j} - \frac{\mu + cT_{j+1}^\alpha}{m_{j+1}}\right)^2 + 2\zeta^2\left(\frac{\mu + cT_j^\alpha}{m_j}\right)}(T_j - T_{j+1}). \tag{16}$$

Therefore, taking for example a system with graded mass distribution $m_1 < m_2 < \cdots < m_N$, in the formula $\mathcal{F}_{j,j+1} = \kappa(T_j,T_{j+1},m_j,m_{j+1})(T_j - T_{j+1})$, with κ as given above, we note that we have sufficient ingredients for the occurrence of thermal rectification, as described in detail in Ref. [12]: namely, we have a Fourier-like expression for the local heat flow, local thermal conductivity that is dependent on temperature, and other local parameters with graded distribution, such as the particle masses. Here, for these systems with inner stochastic baths, we have the condition of normal heat transport that was absent in the previous section. That is, after detailed computations, a Fourier-like expression for current appears. Note, however, that we do not take it as part of the starting assumptions. As was mentioned earlier, it emerged after the calculations.

IV. FINAL REMARKS

A central issue in the study of energy transport in nonequilibrium statistical physics is the theoretical understanding of thermal rectification mechanisms. It is a problem with both theoretical and experimental concerns, which are motivated by the need for efficient thermal diodes to be used in the manipulation and control of heat flow.

In this context, in the present paper we propose an analytical investigation of some effective harmonic toy models related to more intricate systems, i.e., those built after a profitable linearization of their stochastic dynamics.

We do not know how different these toy models are from the related anharmonic ones, but it is clear that these minimalistic structures retain some of the features of the more realistic versions. The main message of this paper is the occurrence of thermal rectification even in a poor, quite simplified model. As we already mentioned, when searching for the minimal ingredients needed for a given phenomenon to occur, an analysis of toy models may enable us to discard complicated but unimportant details. In addition, the use of minimalistic models allows us to unveil the basic properties of more intricate systems. For example, in Ref. [8] a simple chain of elastically colliding particles of two different kinds (bars and bullets) is used to show the ubiquitous occurrence of thermal rectification in graded materials. A minimal model of heat and particle transport based on zero-dimensional dynamics is considered in Ref. [31] in order to understand thermoelectric and thermochemical efficiency. Local hierarchical models are built to clarify the intricate properties of renormalization-group flow in quantum field theory [32].

Some improvements to the analysis carried out herein are possible. For example, we can improve the choice of the effective harmonic potential that is dependent on temperature: for the case of original systems with translational invariance, the effective potential could be taken as $c_\lambda(T_j,T_{j+1})(\phi_{j+1} - \phi_j)^2$, as commented on in a previous section. In any case, the results described in the present work are already enough to reveal the ingredients needed for the occurrence of thermal rectification in a chain. Specifically, the phenomenon holds if the system has asymmetric inner parameters that are related to its own structure, e.g., a graded mass distribution, and some other inner parameters or features related to temperature. Our results also show which of those parameters are linked to the baths at the ends. Note that the anharmonic potentials in more realistic versions of oscillator systems do not explicitly depend on temperature, but they indeed bring some temperature dependence to the heat flow problem. For example, in a chain with normal transport, anharmonic potentials lead (due to an intricate nonlinear dynamics) to a local thermal conductivity that depends on temperature.

Once again, our approach is not limited by the validity of Fourier's law, which was assumed in some previous analytical studies of thermal rectification mechanisms. To conclude, it is worthwhile to stress that the description of rectification in a simple model, with minimal ingredients, shows the ubiquity of rectification, and it may serve to guide additional work in the search for effective thermal diodes.

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