Absence of thermal rectification in asymmetric harmonic chains with self-consistent reservoirs

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An exact analysis using the Langevin equation approach proves that an asymmetric-inhomogeneous harmonic chain with self-consistent inner reservoirs does not rectify heat, while it may show diffusive heat transport properties. Thus, we argue that the onset of a formal Fourier's law in an asymmetric system does not guarantee an asymmetric heat flow.

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Thermal rectification, namely, an asymmetry of the heat current with respect to the temperature bias has recently attracted considerable theoretical [1–10] and experimental [11,12] interest, demonstrating the effect at the nanoscale. The basic theoretical challenge here is to identify the necessary and sufficient conditions for manifesting this effect in classical [9] and quantum [13] systems. Generally, it was argued that in order to rectify heat the system should include anharmonic interactions, combined with some built in asymmetry [14].

More basically, a long standing challenge in statistical mechanics is a first-principle derivation of the Fourier's law of heat conduction $J \propto -\nabla T$ [15]. While most studies are restricted to classical models, using classical molecular dynamics simulations [16], recent works targeted this problem quantum mechanically [17,18]. Furthermore, analytical methods were recently developed for approaching this challenge rigorously [19–21].

It is obvious that a fully harmonic Hamiltonian system does not follow this diffusional law, as it is lacking a mechanism for local thermalization. A two-terminal harmonic junction rather obeys an elastic Landauer-type expression [22], $J=\int d\omega \omega \mathcal{T}(\omega)[n_B^L(\omega)-n_B^R(\omega)]$. Here $\mathcal{T}$ is a frequency-dependent transmission coefficient and $n_B^{\nu}=[e^{\omega/T_\nu}-1]^{-1}$ is the Bose-Einstein distribution evaluated at T_ν; $\hbar=1$, $k_B=1$. The index $\nu=L,R$ denotes the terminals. This expression does not bring in thermal rectification, irrespective of the existence of impurities or disorder. It is thus natural to ask whether in general there is any connection between the applicability of the Fourier's law of heat conduction and the onset of thermal rectification, and vice versa, given that some spatial asymmetry is presented in the system.

We may pose this question as follows. (i) Suppose a system manifests thermal rectification, does it necessarily obey the Fourier's law $J \propto N^{-1}$, N is the system size? (ii) From the other direction, if an asymmetric system obeys the Fourier's law, does it necessarily rectify heat? The answer to the first question is negative. Extensive numerical simulations of heat transfer in nonlinear-asymmetric systems manifest rectification, while the heat current follows $J \propto N^{\alpha-1}$, with $\alpha > 0$ in general [15]. In particular, the Fermi-Pasta-Ulam model was proved to have anomalous conductivity [23], while its mass-graded version gives rise to rectification [8]. The answer to the second question is not as obvious. Most models attained the Fourier's dynamics based on the existence of explicit nonlinear interactions, leading to the thermal rectification phenomenon when asymmetry is introduced. However, the $J \propto N^{-1}$ dependence can emerge in other cases, e.g., in a disordered harmonic chain with frequency-dependent friction coefficients [24]. Here we present a case study where diffusional dynamics might be reached, yet thermal rectification is absent.

The self-consistent (SC) harmonic chain is a simple model that can be analytically studied. It includes N harmonic oscillators with each inner site $(n=2,3,\ldots,N-1)$ coupled to a SC stochastic reservoir. The temperatures of these interior baths are determined by demanding that in steady state, on average, there is a no net heat flow between the chain and the reservoirs. In contrast, the first and the last particles are coupled to "real" reservoirs with fixed temperatures. This model was established a while ago [25] as an effective mean for incorporating on-site anharmonic potentials: The SC inner reservoirs do not exchange energy with the system in steady state, but they do present a mechanism for phonon scattering. In what follows we also refer to "isolated chains," where in this case the SC reservoirs are turned off. Interestingly, it was recently shown [26] that the heat current of a SC harmonic system follows the Fourier's law for long enough chains. This is, in contrast, to the isolated case, where J is independent of size assuming Markovian baths [15]. The quantum version of the SC harmonic model was investigated using the quantum Langevin equation approach [27–29], manifesting a crossover from ballistic to diffusional thermal transport with increasing size.

Can this model bring in thermal rectification? In a recent paper Pereira *et al.* [30] returned to the classical SC model, and analytically studied the heat conduction properties of its inhomogeneous (mass graded) version. Using a perturbative treatment the authors proved that this system obeys Fourier's law, yet it does not rectify heat. Based on their results they posed the question whether an (effective) anharmonicity combined with an asymmetric inhomogeneity are sufficient to ensure thermal rectification.

In this paper we include a short proof of the absence of thermal rectification in the classical asymmetric SC harmonic system. In our model the particles' masses are distinct, and we also adopt asymmetric couplings (friction) to the L and R solids. Using the Langevin equation formalism we prove that (i) the temperature profiles for forward and reversed bias are symmetric with respect to the average temperature, (ii) the asymmetric SC harmonic chain does not rectify heat. We argue that this is because there is no energy exchange between modes.

The paper is organized as follows. First we present the SC harmonic model and discuss its temperature profile, unique for harmonic systems. Based on this result we proceed and prove that thermal rectification is absent in this model.

Model and dynamics. We study classical heat transfer in a mass-disordered harmonic-chain model, attaching a SC reservoir to each site. The Hamiltonian of the system is given by the sum of quadratic terms

$$H = \sum_{n=1}^{N} \frac{m_n \dot{x}_n^2}{2} + \sum_{n=0}^{N} \frac{(x_{n+1} - x_n)^2}{2}, \tag{1}$$

where m_n is the nth particle mass, x_n is the particle displacement around equilibrium, and we use fixed boundaries $x_0 = x_{N+1} = 0$. The force constants are all set to 1. The atoms are put in contact with independent Ohmic heat reservoirs with coupling strengths expressed in terms of friction coefficients γ_n. We set $\gamma_n = \gamma_c$ for the central particles $n=2,\ldots,N-1$ and $\gamma_1 = \gamma_L$, $\gamma_N = \gamma_R$ for the end atoms. In order to induce spatial asymmetry, we also enforce $\gamma_L \neq \gamma_R$. We define the average temperature $T_a = \frac{T_L + T_R}{2}$ and the difference $\Delta T = T_L - T_R$. The dynamics of this system follows the Langevin equation [27]

$$m_n \ddot{x}_n = -2x_n + x_{n+1} + x_{n-1} - \gamma_n \dot{x}_n + \eta_n, \tag{2}$$

where the thermal-white noise obeys the fluctuation-dissipation relation $\langle \eta_n(t)\eta_{n'}(t')\rangle = 2T_n\gamma_n\delta(t-t')\delta_{nn'}$. The transport properties of the homogeneous model, in the quantum limit, were analyzed in Ref. [27] manifesting a crossover from a ballistic to diffusional dynamics with increasing internal friction γ_c and size. In the linear response regime, $\Delta T \ll T_a$, and for $\gamma_c \ll 1$ it was shown that

$$J \propto \Delta T/(N+l), \tag{3}$$

where $l = 3/\gamma_c$ [28]. We prove next that in the classical limit the system does not rectify heat, i.e., $J(\Delta T) = -J(-\Delta T)$, for arbitrary size N, coupling strengths γ_n, mass distribution, and boundary temperatures $T_{L/R}$.

Thermal baths' temperature profile. The temperatures of the first and last reservoirs are fixed at $T_1 = T_L$ and $T_N = T_R$, respectively, while the temperatures of the interior reservoirs are determined self-consistently by the condition of net zero current from the chain to each side reservoir. In steady state, recognizing that the random forces can be represented as harmonic driving terms [31], we obtain $(N-2)$ linear equations for $n=2,3,\ldots,N-1$ [27],

$$\sum_{p=1}^{N} \gamma_p \gamma_n M_{n,p}(T_n - T_p) = 0, \tag{4}$$

where

$$M_{n,p} = \int_{-\infty}^{\infty} d\omega \frac{\omega^2}{\pi} |G_{n,p}(\omega)|^2. \tag{5}$$

The matrix $G(\omega)$ is the inverse of a tridiagonal matrix with off-diagonal elements equal to -1 and diagonal elements $2 - m_n\omega^2 - i\gamma_c\omega$, except the end points where $2 - m_{1,N}\omega^2 - i\gamma_{L,R}\omega$. A key element in our derivation is the fact that the matrix M does not depend on the temperature difference ΔT. We rearrange Eq. (4) and rewrite the temperature profile as

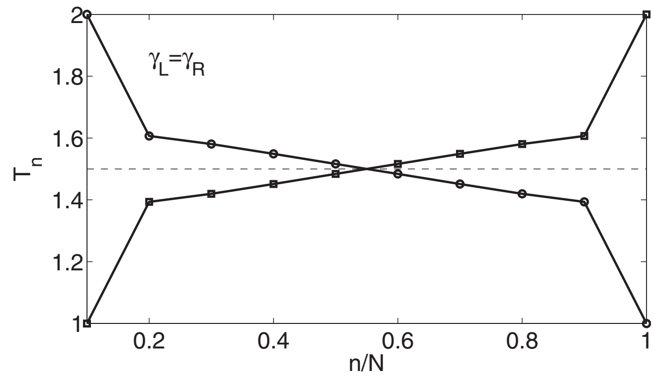

FIG. 1. Temperature profile in a symmetric-homogeneous SC harmonic chain $\gamma_L = \gamma_R = 1$, $\gamma_c = 0.1$, $N=10$, $m=1$. $\beta_L = 0.5$, $\beta_R = 1$ (circle); $\beta_L = 1$, $\beta_R = 0.5$ (square). The dashed line marks the average temperature $T_a = 1.5$.

$$\mathbf{T} = T_a A^{-1} v^+ + \frac{\Delta T}{2} A^{-1} v^-, \tag{6}$$

where A is an $(N-2)\times(N-2)$ matrix with diagonal elements $A_{n,n} = \sum_{p\neq n} \gamma_{n+1}\gamma_p M_{n+1,p}$ $(p=1\cdots N)$ and nondiagonal elements $A_{n,n'} = -\gamma_{n+1}\gamma_{n'} M_{n+1,n'}$. The vectors $v^{\pm}$ are defined as $v_n^{\pm} = \gamma_{n+1}\gamma_1 M_{n+1,1} \pm \gamma_{n+1}\gamma_N M_{n+1,N}$ and $\mathbf{T}$ is the vector of the steady-state temperature at the $2,3,\ldots,N-1$ inner sites. Next we interchange the temperatures T_L and T_R and attain a new profile $\tilde{\mathbf{T}}$

$$\tilde{\mathbf{T}} = T_a A^{-1} v^+ - \frac{\Delta T}{2} A^{-1} v^-. \tag{7}$$

The sum of the last two equations is a constant $\tilde{\mathbf{T}} + \mathbf{T} = 2T_a A^{-1} v^+$. Moreover, evaluating Eq. (6) with $\Delta T = 0$ reveals that $A^{-1}v^+ = I$, a vector of $N-2$ ones, concluding that

$$\tilde{T}_n + T_n = T_L + T_R. \tag{8}$$

We can also rewrite the last relation as

$$T_n = T_L + \frac{\Delta T}{2}(\alpha_n - 1), \quad \tilde{T}_n = T_R - \frac{\Delta T}{2}(\alpha_n - 1), \tag{9}$$

with $\alpha_n \equiv (A^{-1}v^-)_n$. This is a unique property of our system: The temperature profiles for forward and reversed bias are symmetric, with the mirror line at T_a. Note that Eq. (9) does not necessarily imply a linear $T_n \propto n$, profile. It also holds for arbitrary sizes, not only in the asymptotic $N \to \infty$ limit, as in Refs. [26–28].

Simulating Eq. (9), Fig. 1 shows that for a fully symmetric system the temperature profile has two reflection symmetries, with respect to both the coordinate and the temperature. When we break the spatial symmetry by taking $\gamma_L \neq \gamma_R$, the symmetry with respect to T_a still holds, see Fig. 2.

The temperature profile along an isolated-chain model ($\gamma_c = 0$) with explicit internal anharmonic interactions, assuming asymmetric couplings at the ends, can be obtained by directly simulating the Langevin equation. In this case we

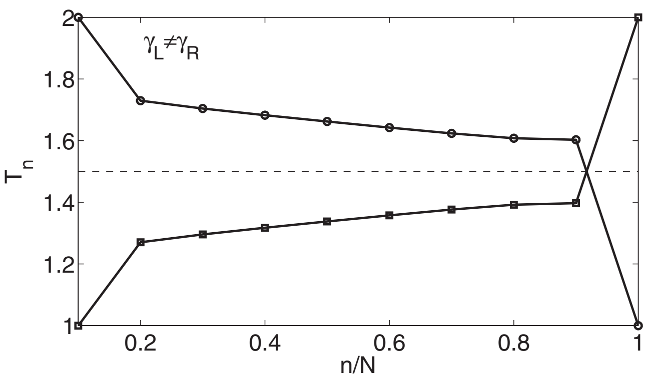

FIG. 2. Temperature profile in an asymmetric-mass homogeneous SC harmonic system $\gamma_L=1$, $\gamma_R=5$, $\gamma_c=0.1$, $m=1$, $N=10$, $\beta_L=0.5$, $\beta_R=1$ (circle); $\beta_L=1$, $\beta_R=0.5$ (square). The dashed line marks $T_a=1.5$.

found that the forward and backward profiles significantly differ [3], revealing that the SC harmonic model is fundamentally different from genuine anharmonic models.

Absence of thermal rectification. We prove next that thermal rectification is absent in the asymmetric SC harmonic model. The steady-state current through the chains' bonds is given by [27,28]

$$J_{n,n+1} = -\sum_{p=1}^{N} \gamma_p T_p S_{n,p}, \tag{10}$$

with the coefficients

$$S_{n,p} = \int_{-\infty}^{\infty} d\omega \frac{\omega}{\pi} \mathrm{Im}[G_{n,p}(\omega)G^*_{n+1,p}(\omega)]. \tag{11}$$

The explicit notation $J=J_{n,n+1}$ marks the position along the chain where the current is calculated. In equilibrium ($\Delta T=0$), $T_a=T_L=T_R$, and we should trivially retrieve a constant temperature profile $T_n=T_a$ with zero interparticle current. Using Eq. (10) we find that the $S_{n,p}$ coefficients must therefore satisfy the relation

$$\sum_{p=1}^{N} \gamma_p S_{n,p} = 0. \tag{12}$$

Next we interchange the L and R temperatures, resulting in the new profile $\tilde{T}_n=T_L+T_R-T_n$, see Eq. (8). The reversed heat current (10) becomes

$$\tilde{J}_{n,n+1} = -\sum_{p=1}^{N} \gamma_p (T_L + T_R - T_p) S_{n,p}$$
$$= \sum_{p=1}^{N} \gamma_p T_p S_{n,p} - (T_L + T_R) \sum_{p=1}^{N} \gamma_p S_{n,p}. \tag{13}$$

Utilizing Eq. (12) we conclude that the second term here vanishes, thus $\tilde{J}_{n,n+1}=-J_{n,n+1}$, i.e., thermal rectification is absent in the system. Note that we derived this result without calculating explicitly neither the internal baths' temperatures, nor the heat current in the system. The SC harmonic model can thus establish a Fourier's type dynamics for long systems [27,28], but it cannot bring in thermal rectification irrespective of system size, mass distribution, and coupling strength. This is the main message of our paper: The onset of a formal Fourier law (in an asymmetric system) does not guarantee thermal rectification. While a $J \propto N^{-1}$ dynamics may result from several effects, e.g., the spectral properties of the reservoirs [24], thermal rectification is a phenomenon originating from nonlinear interactions [13].

To conclude, based on the Langevin equation approach we obtained two interesting characteristics of the asymmetric SC harmonic model. (i) The internal baths' temperature profiles for forward and reversed bias are mirror reflected with respect to the average temperature T_a, irrespective of structural asymmetry and disorder. (ii) Thermal rectification is absent. Our results could be also generalized to the asymmetric force constant case, and it is of interest to extend them to the quantum regime.

Finally, we argue that one should interpret Eqs. (10) and (11) as a multiterminal elastic transport expression, where the heat flux is given by the sum of independent frequency terms. Therefore, though the system develops a local temperature profile, in contrast to the isolated ($\gamma_c=0$) case, this results from the interaction with several thermal reservoirs, and not due to energy exchange processes between phonon modes.

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