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Symmetry of heat conductivity in inhomogeneous quantum chains

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Abstract
We address the problem of the existence of thermal rectification in inhomogeneous (in particular, graded) chains. Searching for analytical results, we investigate the symmetry properties of the thermal conductivity of the quantum inhomogeneous harmonic chain of oscillators with self-consistent reservoirs, an analytically treatable effective anharmonic model (the inner reservoirs mimic the anharmonic on-site potentials). Considering the linear response regime, i.e., for the system submitted to a small gradient of temperature, we show that, even with quantum effects in the conductivity, there is no thermal rectification. Moreover, as a secondary result, we analyze an old expression derived for the thermal conductivity of pure harmonic chains (i.e., a chain with baths at the boundaries only), and prove that there is no thermal rectification in such inhomogeneous systems, as suggested by numerical simulations in previous works.

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1. Introduction

One of the demands of theoretical non-equilibrium statistical physics is the derivation of macroscopic phenomenological laws of thermodynamic transport from simple microscopic Hamiltonian models. After decades of intensive investigations [1, 2], the understanding of heat conduction from first principles is still quite incomplete. In particular, the precise conditions that a dynamical system of interacting particles must satisfy in order to obey Fourier's law are still unknown: Fourier's law of heat conduction, $\mathcal{F} = -\nabla T$, relates the heat flow $\mathcal{F}$ to the temperature gradient ∇T. One of the main obstacles in the area is that central questions involve nonlinear dynamical systems, and so, with most works limited to numerical simulations, it has been difficult to arrive at conclusive results. Contradictions exist: e.g., in [3] the authors claim that the anharmonicity (soft or hard) of the on-site potential is enough to guarantee

Fourier's law, but in [4] a counterexample is given. To quote some well-known mathematical physicists working on the subject [5], a complete and decisive mathematical study 'is not even on the horizon'. Thus, to carry out the necessary analytical investigations, approximative schemes and/or effective models have been proposed and details studied [5–9]. An example of an effective model proposed a while ago [10, 11], but recently revisited [7, 8, 12–14], is the harmonic chain of oscillators with self-consistent stochastic reservoirs. This model is given by a chain of N harmonic oscillators, where the first and last sites are coupled to 'real' thermal baths with fixed temperatures, and the inner sites are linked to reservoirs with temperatures determined such that, in the steady state, on average, there is no heat flow between them and the chain (the inner baths do not inject heat into the system, and they represent a mechanism for phonon scattering only, mimicking the absent anharmonic interactions).

In this scenario of intensive study of the microscopic physical mechanism of energy transport, and with the advent of nanotechnology, the idea of possible applications emerged: e.g., the possibility to control the heat flow by constructing thermal (nano)instruments such as diodes or rectifiers [15]. A thermal diode is a device in which the heat flow changes if the device is inverted between two heat baths. The theoretical construction of rectifiers involves difficulties similar to those present in the study of the microscopic origin of the heat flow: namely, many works are carried out by means of numerical computations, with few conclusive results. Of course, there are also analytical investigations in simple models (such as the two-level spin-boson model [16]) or in effective systems (such as the billiard systems [17, 18]). In particular, most of the proposed diodes are constructed (via computer simulations) by coupling two or three chains with different nonlinear on-site potentials, a criticized procedure: in [19], the authors claim that it will be difficult to construct such a diode (segmented chain) in practice. However, in a recent experimental work, Chang *et al* [20] build a nanoscale thermal rectifier using a different procedure: namely, they use a graded mass material (nanotubes externally and inhomogeneously mass loaded with heavy molecules). The system is claimed to present asymmetric axial thermal conductance, with greater heat flow in the direction of decreasing mass density. Following this approach, some other authors [21] performed numerical simulations to obtain a theoretical description of diodes (and even thermal transistors [22]) with graded materials. Their results and claims suggest us that a precise mechanism to build thermal rectifiers is given by taking any anharmonic system with its structure gradually changed in space, e.g. an asymmetrically mass-loaded system.

In a previous paper [14], having in mind the accurate investigation of the conditions which are sufficient to obtain an asymmetric heat conductivity, we analytically study the heat flow in the harmonic crystal with self-consistent stochastic reservoirs and arbitrary structures (including the graded one), an effective and analytically treatable anharmonic model: in opposition to the pure harmonic models, it obeys Fourier's law [7]. We perform a perturbative and rigorous [23] computation of the thermal conductivity, and show that it is symmetric (i.e., there is no thermal rectification) even for the graded system.

Now, in the present work, we consider the quantum version of this harmonic chain with self-consistent reservoirs and inhomogeneous structure in order to investigate if quantum effects may induce the asymmetric behavior: again, we recall that Fourier's law also holds in such quantum model [8]. As well known [8, 13], quantum effects cannot be neglected in the study of heat conduction in low temperatures: for example, in homogeneous self-consistent chains [8], the thermal conductivity becomes an explicit function of the temperature in the quantum case and low temperature regime, but it does not change in the classical one (or in the high temperature regime). Here, considering a small temperature gradient, i.e., in the linear response regime, we show that the thermal conductivity, although presenting a more intricate structure, is still symmetric, even for the graded system.

The rest of the paper is organized as follows. For a more complete description of the problem involving inhomogeneity and asymmetry in the heat flow, in section 2 we first analyze pure harmonic inhomogeneous chains with baths at the boundaries only, and we also review the classical harmonic chain with self-consistent reservoirs. In section 3, we investigate the thermal conductivity of the quantum inhomogeneous chain with self-consistent reservoirs. Section 4 is devoted for concluding remarks.

2. Symmetry of thermal conductivity in some classical inhomogeneous models

Graded materials, i.e. inhomogeneous systems whose composition and/or structure change gradually in space, have recently attracted great attention [24]. Their physical properties are of interest to many areas: material sciences, engineering, optics, etc. Their thermal characteristics, however, are not well known. In a recent paper [21], the heat flow is investigated, by means of computer simulations, in a harmonic graded mass model and also in a specific anharmonic graded mass chain, with a Fermi–Pasta–Ulam β potential. The authors find a symmetric flow for the harmonic case, and a thermal rectification for the anharmonic chain with fixed boundary conditions.

In this section, for a more general understanding of the relation between inhomogeneity and symmetry in thermal conductivity, we briefly describe some results in classical graded systems. First, by using a rigorous expression derived by Casher and Lebowitz a while ago [25], we show that, as indicated by the simulations in the recent paper mentioned above [21], the heat flow is symmetric in any inhomogeneous pure harmonic chains (i.e., harmonic chains with reservoirs at the boundaries only). In what follows, we review our results [14] obtained for the heat conductivity in the inhomogeneous classical harmonic chain with self-consistent stochastic reservoirs.

Let us show the symmetry in the heat flow for an arbitrary pure harmonic chain. Consider an one-dimensional lattice with N particles (sites), with arbitrary masses (which may be graded: $m_1 < m_2 < \cdots < m_N$, or not), and the Hamiltonian

$$H = \sum_{j=1}^{N} \left[\frac{p_j^2}{2m_j} + \frac{1}{2} \sum_{k=1}^{N} q_j \Phi_{jk} q_k \right] = \sum_{j=1}^{N} H_j, \tag{1}$$

where Φ is a positive matrix. As usual, the time evolution is given by the stochastic differential equations

$$\begin{aligned} \frac{\mathrm{d}q_j}{\mathrm{d}t} &= \frac{\partial H}{\partial p_j} = \frac{p_j}{m_j}, \\ \frac{\mathrm{d}p_j}{\mathrm{d}t} &= -\frac{\partial H}{\partial q_j} - \zeta_j p_j + \gamma_j^{1/2} \eta_j = -(\Phi q)_j - \zeta_j p_j + \gamma_j^{1/2} \eta_j, \end{aligned} \tag{2}$$

where $\zeta_j = (\delta_{j,1} + \delta_{j,N})\zeta$ is the dissipative constant; $\gamma_j = 2m_j \zeta_j T_j (\delta_{j,1} + \delta_{j,N})$ and η_j are white noises describing the thermal reservoirs at the boundaries ($j = 1$ and $j = N$), with the expectations

$$\langle \eta_j(t) \rangle = 0; \qquad \langle \eta_j(t) \eta_{j'}(t') \rangle = \delta_{j,j'} \delta(t - t'). \tag{3}$$

The heat flow at site j, in the steady state, is given by

$$\mathcal{F}_j - \mathcal{F}_{j-1} = -\lim_{t \to \infty} \left\langle \frac{\mathrm{d}H_j}{\mathrm{d}t} \right\rangle. \tag{4}$$

As $\mathcal{F}_{j-1} = \mathcal{F}_j = \mathcal{F}_{j+1} = \cdots$, in the steady state, we use the notation $\mathcal{F}$ for the heat flow, i.e. we drop the index j. Following Casher and Lebowitz [25], we have

$$\mathcal{F} = (T_1 - T_N)\frac{\zeta^2 m_1 m_N}{\pi} \times \int_{-\infty}^{+\infty} \mathrm{d}\omega \frac{\omega^2 |C_{1,N}(\omega)|^2}{(K_{1,N} - \zeta^2\omega^2 m_1 m_N K_{2,N-1})^2 + \zeta^2\omega^2(m_1 K_{2,N} + m_N K_{1,N-1})^2}, \tag{5}$$

where $K_{l,m}(\omega)$ is the determinant of $(\Phi - \omega^2 M)$ for a chain which starts from the lth particle and ends with the mth one; M is the diagonal matrix for the particle masses; $C_{1,N}$ is the cofactor of $Z_{1,N}$, where $Z = \Phi - \mathrm{i}\omega M L - \omega^2 M$, L is a diagonal matrix with $L_{j,j} = \zeta$ if $j = 1$ or N, otherwise $L_{j,j} = 0$. Note that, as well known, Fourier's law does not hold for the harmonic chain: the heat flow is proportional to the temperature difference $(T_1 - T_N)$ instead of to the temperature gradient $(T_1 - T_N)/(N-1)$. The solution of the integral above may be very complicate: an explicit formula for the thermal conductivity is known only for some specific values of the mass, e.g. for $m_1 = m_2 = \cdots = m_N$. Anyway, for formula (5) above, it is clear that when we invert the system between the thermal reservoirs, i.e., if we keep T_1 and T_N but replace the particle 1 by N, 2 by $N-1$, etc, the thermal conductivity does not change: in formula (5), after the replacement, $K_{1,N}$ becomes $K_{N,1}$, which has an identical value; the same for $K_{2,N-1}$; m_1 becomes m_N and vice versa. Finally, $m_1 K_{2,N}$ becomes $m_N K_{N-1,1}$ and $m_N K_{1,N-1}$ is replaced by $m_1 K_{N,2}$. In short, for any value of the masses $m_1, \ldots, m_N$, the heat flow is symmetric in the pure harmonic chain (as we invert the system between two heat baths).

Now we turn to the effective anharmonic model, namely, to the harmonic chain with self-consistent reservoirs. It is given by the previous equations (1)–(3), now with $\zeta_j = \zeta$ for $j = 1, 2, \ldots, N$. We recall the results of [14], where we make a perturbative, but rigorous [23], investigation of such model. First, we write the Hamiltonian of the system as

$$H = \sum_{j=1}^{N}\left[\frac{1}{2}\left(\frac{p_j^2}{m_j} + M_j q_j^2\right) + \frac{1}{2}\sum_{l=1}^{N} q_j J_{j,l} q_l\right] = \sum_{j=1}^{N} H_j, \tag{6}$$

with J being Hermitian, $J_{j,l} = J_{l,j}$. We define $Q_j \equiv q_j\sqrt{m_j}$ and $P_j \equiv p_j/\sqrt{m_j}$, to get

$$H_j = \frac{P_j^2}{2} + \frac{M}{2}Q_j^2 + \frac{1}{2}\sum_{l=1}^{N} Q_l D_{l,j} Q_j, \tag{7}$$

where for technical reasons, we keep a quadratic term Q_j^2 with constant coefficient $M/2$ (the difference between M and M_j/m_j is included in the diagonal part of D): it is more difficult to treat a system with M_j instead M, i.e., with the coefficient changing at each site. Note that, essentially (discarding the details in the diagonal), we have $D = \mathcal{M}^{-1/2} J \mathcal{M}^{-1/2}$, where $\mathcal{M}$ is the diagonal matrix for the particle masses. Thus, for a weak interparticle interaction D (which may be given, e.g. by any interaction J and heavy particle masses), after analytical computations we obtain, up to $\mathcal{O}(D^3)$,

$$\mathcal{F} = \kappa \frac{T_1 - T_N}{N-1}, \tag{8}$$

i.e. Fourier's law holds with thermal conductivity κ given by

$$\frac{\kappa}{N-1} = \left(\frac{1}{\mathcal{G}_1} + \frac{1}{\mathcal{G}_2} + \cdots + \frac{1}{\mathcal{G}_{N-1}}\right)^{-1}, \tag{9}$$

$$\mathcal{G}_j = \mathcal{D}_{j+N,j+1}\left[\frac{\mathcal{D}_{j+N,j+1}}{2\zeta M} - \frac{\mathcal{D}_{j+N,j+1}}{4\zeta M^2}\frac{\mathcal{D}_{j+N,j} + \mathcal{D}_{j+1+N,j+1}}{2}\right], \tag{10}$$

where $\mathcal{D}$ is the $2N \times 2N$ matrix involving the $N \times N$ matrix D

$$\mathcal{D} = \begin{pmatrix} 0 & 0 \\ D & 0 \end{pmatrix}. \tag{11}$$

The symmetry in the thermal conductivity is transparent: nothing changes when we invert the chain, since $\mathcal{D}_{j+N,j+1} = D_{j,j+1}$ and D is Hermitian. In [14] we still give arguments which indicate that the symmetry follows for the remaining terms of the perturbative series. Anyway, a possible contribution of these terms is insignificant: $\mathcal{O}(D^4)$.

3. Conductivity in quantum inhomogeneous chains

Now we consider the quantum version of the harmonic oscillators chain with self-consistent baths, as said before, an analytically treatable effective anharmonic model.

The investigation of quantum models is a must for the understanding of the thermal conductivity: to describe the heat flow at low temperatures, it is necessary to take into account quantum effects, which may introduce significant changes. For example, as said before, in the classical description of the self-consistent harmonic chain with the same mass for the particles, Fourier's law holds, and the thermal conductivity does not depend on the temperature [7]. But, in the quantum version, the thermal conductivity (which is still normal) changes with temperature [8]: in particular, for the low-temperature regime, the dependence on temperature for thermal conductivity of the system with pinning on-site is quite different from that without such potential. These properties suggest us to investigate if quantum effects may be responsible for the origin of asymmetry in inhomogeneous materials.

Here, to describe the quantum system and its evolution to the steady state, we use a Ford–Kac–Mazur approach [26], as details presented in [8]. Such an approach considers the baths (connected to the chain) modeled also as mechanical harmonic systems, with initial coordinates and momenta determined by some statistical distribution (that is the origin of the stochasticity of the system). The expression for the heat flow in the steady state is obtained by solving the quantum dynamical equations, and by taking the stochastic distribution for the initial coordinates of the baths, as well as the limit $t \to \infty$.

Let us describe the model (for clearness, we keep the notation of [8], where all details are presented). Our system is given by a chain (W) with harmonic interparticle and on-site potentials, with each site connected to a bath (B), also with harmonic interactions. The Hamiltonian of the system (chain and baths) is given by

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_W + \sum_{i=1}^{N}\mathcal{H}_{B_i} + \sum_{i=1}^{N}\mathcal{V}_i, \\
\mathcal{H}_W &= \frac{1}{2}\dot{X}_W^T M_W \dot{X}_W + \frac{1}{2}X_W^T \Phi_W X_W, \\
\mathcal{H}_{B_i} &= \frac{1}{2}\dot{X}_{B_i}^T M_{B_i} \dot{X}_{B_i} + \frac{1}{2}X_{B_i}^T \Phi_{B_i} X_{B_i}, \\
\mathcal{V}_i &= X_W^T V_{B_i} X_{B_i},
\end{aligned} \tag{12}$$

where M_W and M_{B_i} are the particle-mass diagonal matrices for the chain and baths, Φ_W and Φ_{B_i} are symmetric matrices representing the interparticle and on-site harmonic interactions, and V_{B_i} describes the interaction between the i-site and its bath (details ahead). For each part,

$X = [X_1, X_2, \ldots, X_{N_s}]^T$, where X_r is the position operator of the rth particle; $\dot{X} = M^{-1}P$, where P_l is the momentum operator of the lth particle. We have $[X_r, P_l] = \mathrm{i}\hbar\delta_{r,l}$. The dynamics of the system is given by the Heisenberg equations

$$\begin{aligned} M_W \ddot{X}_W &= -\Phi_W X_W - \sum_i V_{B_i} X_{B_i}, \\ M_{B_i} \ddot{X}_{B_i} &= -\Phi_{B_i} X_{B_i} - \sum_i V_{B_i}^T X_W. \end{aligned} \tag{13}$$

The heat currents inside the chain and from the reservoir to the chain are related to $\langle X_W \dot{X}_W^T \rangle$ and $\langle X_B \dot{X}_W^T \rangle$. To find the exact expressions, we turn to the Heisenberg equations above (13), treat the equations of the baths as linear inhomogeneous equations, plug these solutions into the equations for the chain, and then we take the average over the initial conditions of the baths, which we assume to be distributed according to equilibrium phonon distributions with properly chosen temperatures (recall that we want the self-consistent condition, that is, we need to take the temperatures of the inner baths such that there is no heat flow between an inner bath and its site). The steady state is reached by taking the limit $t \to \infty$ (for technical reasons we still take $t_0 \to -\infty$, and consider the Fourier transform of t). We stress that the formalism is detailed in [8], and references there in. The heat flow, thermal conductivity, etc, are analyzed for sites in the bulk of a very large chain, i.e. sites far from the boundaries. The expression for the heat flow from the lth reservoir to the chain is given by

$$\mathcal{F}_l = \sum_{m=1}^{N} \zeta^2 \int_{-\infty}^{+\infty} \mathrm{d}\omega\, \omega^2 \left|\left[G_W^+(\omega)\right]_{l,m}\right|^2 \frac{\hbar\omega}{\pi} [f(\omega, T_l) - f(\omega, T_m)], \tag{14}$$

where ζ is the dissipation constant; it controls the coupling strength to the reservoirs, which are taken to be Ohmic, as usual:

$$G_W^+(\omega) = \left[-\omega^2 M_W + \Phi_W - \sum_l \Sigma_l^+(\omega)\right]^{-1}, \tag{15}$$

with the matrix Σ_l^+ having only one non-vanishing element: $\left(\Sigma_l^+\right)_{l,l} = \mathrm{i}\zeta\omega$; $f(\omega, T_l)$ is the phonon distribution for the lth bath

$$f(\omega, T_l) = \left[\exp\left(\frac{\hbar\omega}{k_B T_l}\right) - 1\right]^{-1}, \tag{16}$$

and the variable ω in the expressions above comes from the Fourier transform

$$\widetilde{X}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}t\, X(t)\, \mathrm{e}^{\mathrm{i}\omega t}. \tag{17}$$

Let us assume the linear response regime, i.e., the difference between the temperatures T_1 and T_N is small, precisely, $\Delta T = |T_1 - T_N| \ll T = (T_1 + T_N)/2$. It leads to simplifications in the expression for the heat flow. In particular, for $\mathcal{F}_l$ above (14), we obtain

$$\mathcal{F}_l = \zeta^2 \int_{-\infty}^{+\infty} \mathrm{d}\omega \frac{\hbar\omega^3}{\pi} \frac{\partial f(\omega, T)}{\partial T} \sum_{m=1}^{N} \left|\left[G_W^+(\omega)\right]_{l,m}\right|^2 (T_l - T_m). \tag{18}$$

And for the heat flow inside the chain (to be specific, we take the flux from the lth to the $(l+1)$ th site)

$$\begin{aligned} \mathcal{F}_{l,l+1} = \Phi_{l,l+1} \langle X_l \dot{X}_{l,l+1} \rangle = -\frac{\Phi_{l,l+1}\zeta}{\pi} \int_{-\infty}^{+\infty} \mathrm{d}\omega\, \omega \left(\frac{\hbar\omega}{2k_B T}\right)^2 \operatorname{cosech}^2\left(\frac{\hbar\omega}{2k_B T}\right) \\ \times \sum_{m=1}^{N} k_B T_m \operatorname{Im}\left\{\left[G_W^+(\omega)\right]_{l,m} \left[G_W^+(\omega)\right]_{l+1,m}^*\right\}, \end{aligned} \tag{19}$$

where $*$ denotes the complex conjugate, and Im the imaginary part. In the formula above for $\mathcal{F}_{l,l+1}$ and in what follows, we restrict the interparticle interaction to nearest neighbors only. Let us say, once more time, that formula (19) above and previous expressions are already described in [8].

To perform the computation (i.e., the sum and the integration in (19)) in order to obtain a precise expression for the heat flow, we need to specify the matrix G_W^+, i.e. the particle masses M_W and the interparticle potential Φ_W, as well as the temperature profile, which is found by assuming that $\mathcal{F}_l = 0$ for any inner site. The determination of $G_W^+(\omega)$, the inverse matrix given by equation (15), may be a very hard task—a precise solution is known only for some specific cases: e.g., for a homogeneous interparticle interaction Φ connecting next-neighbors sites, and for all particles with the same mass $M_W = mI$ [8]; and also for the case of particles with alternate masses, i.e. $m_j = m_1$ for j odd, and $m_j = m_2$ for j even [13]. However, for the question of existence or absence of symmetry in the heat flow inside the chain, a precise answer is still possible even in the case of a generic next-neighbor interparticle interaction and an inhomogeneous matrix for the particle masses (graded or not), as we show below.

Let us analyze the formula for $\mathcal{F}_{l,l+1}$ (19). First, we need to know the temperature profile. Instead of trying to obtain it from equation (18) in the self-consistent condition $\mathcal{F}_l = 0$ for any inner site l, we follow the strategy used in the works on homogeneous and alternate mass chains [8, 13]: we take the profile obtained for the classical model [14]. The trustworthiness of such a procedure comes from the fact that, as $|G_W^+(\omega)|^2$ does not depend on T, the solution of $\mathcal{F}_l = 0$ has a smooth behavior as a function of T, that is, the obtained expression for the temperature profile shall be valid for high and also low T. Moreover, in the high-temperature regime, the quantum and classical behaviors coincide. Thus, we can use here the expression for the temperature profile obtained in the analysis of the classical inhomogeneous chain [14]. We recall first that, in this previous work, we show that a change of variables maps (without loss of generality) a system with inhomogeneous particle masses into another one where the particles have unit mass, but the interparticle interaction changes. Hence, from now on, we treat a system with unit masses and arbitrary interparticle potential. From equation (26) of [14] and previous expressions there in, we obtain

$$T_k = T_1 + \frac{\mathcal{G}_1^{-1} + \cdots + \mathcal{G}_{k-1}^{-1}}{\mathcal{G}_1^{-1} + \cdots + \mathcal{G}_{N-1}^{-1}}(T_N - T_1), \tag{20}$$

where $\mathcal{G}_j$ is given by equation (10) above. We turn to the expression for $\mathcal{F}_{l,l+1}$ (19), to recall that

$$\mathcal{F}_{l,l+1} \propto \sum_{m=1}^{N} T_m \mathrm{Im}\{G_{l,m} G_{l+1,m}^*\},$$

where, for ease of notation, we write $G_W^+(\omega)$ as G. Now, let us keep our chain and invert the thermal reservoirs at the boundaries. If there exists a thermal rectification in the system, then the sum of the previous heat flow and the new one (for the chain with inverted reservoirs) does not vanish: i.e., the absolute value of the heat flow changes as we invert the thermal reservoirs. For the system with inverted reservoirs, the temperature profile becomes

$$T_k' = T_N + \frac{\mathcal{G}_1^{-1} + \cdots + \mathcal{G}_{k-1}^{-1}}{\mathcal{G}_1^{-1} + \cdots + \mathcal{G}_{N-1}^{-1}}(T_1 - T_N).$$

Hence, if we sum up the flows, we obtain

$$\begin{aligned}
\mathcal{F}_{l,l+1} + \mathcal{F}'_{l,l+1} &= C \sum_{m=1}^{N} (T_m + T'_m)\, \mathrm{Im}(G_{l,m} G^*_{l+1,m}) \\
&= C \sum_{m=1}^{N} (T_1 + T_N)\, \mathrm{Im}(G_{l,m} G^*_{l+1,m}) \\
&= C(T_1 + T_N) \sum_{m=1}^{N} \mathrm{Im}\big(G_{l,m} G^\dagger_{m,l+1}\big) \\
&= C(T_1 + T_N)\, \mathrm{Im}(GG^\dagger)_{l,l+1}.
\end{aligned}$$

We recall that

$$G = [\Phi - \omega^2 M - \mathrm{i}\zeta\omega I]^{-1},$$

in fact, with the change of variables, we also have $M = I$. Hence,

$$\begin{aligned}
GG^\dagger &= [\Phi - \omega^2 M - \mathrm{i}\zeta\omega I]^{-1}[\Phi - \omega^2 M + \mathrm{i}\zeta\omega I]^{-1} \\
&= \{[\Phi - \omega^2 M + \mathrm{i}\zeta\omega I][\Phi - \omega^2 M - \mathrm{i}\zeta\omega I]\}^{-1} \\
&= \{(\Phi - \omega^2 M)^2 + \zeta^2\omega^2 I\}^{-1},
\end{aligned}$$

and so, all the elements of $GG^\dagger$ are real $\Rightarrow \mathrm{Im}(GG^\dagger)_{l,l+1} = 0$. That is,

$$\mathcal{F}_{l,l+1} + \mathcal{F}'_{l,l+1} = 0 \quad \Rightarrow \quad \mathcal{F}_{l,l+1} = -\mathcal{F}'_{l,l+1}.$$

Precisely, there is no thermal rectification in the quantum chain with self-consistent reservoirs for the system submitted to a small gradient of temperature (i.e., in the linear response regime).

4. Final remarks

In this paper, we address the question of a possible thermal rectification in inhomogeneous (in particular, graded) chains. Searching for analytical results, we consider the pure harmonic chain (a system with harmonic interactions and thermal reservoirs at the boundaries only) and the harmonic chain with self-consistent anharmonic reservoirs, which is an effective anharmonic system where the anharmonic on-site interactions are mimicked by baths connected to each site. Using a well-known result of Casher and Lebowitz, we show the symmetry in the heat flow (absence of thermal rectification) in inhomogeneous pure harmonic chains. And, after revisiting our previous result on classical self-consistent harmonic chains, we analyze the symmetry properties of quantum inhomogeneous self-consistent harmonic chains in the linear response regime, and we show that, even with quantum effects in the conductivity, there is no thermal rectification.

As already recalled, the classical and also the quantum harmonic chain with self-consistent baths obey Fourier's law of heat conduction, a property of some anharmonic Hamiltonian systems. Moreover, such a model is rich enough to present other nontrivial properties, such as the phenomenon of crossover from ballistic to diffusive thermal transport as the system size is increased [27]. If we consider this model as a good representant of the anharmonic systems, then our results reinforce the message that inhomogeneity and anharmonicity in a chain are not sufficient to guarantee asymmetry in the heat flow (in spite of some authors' opinion). They also show that the origin of thermal rectification is more intricate than the origin of normal conductivity: the effective mechanism presented in the self-consistent chain is enough to assure Fourier's law, but the inhomogeneous (classical or quantum) version of such model does not present thermal rectification.

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