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Thermal rectification in quantum graded mass systems

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ABSTRACT

We show the existence of thermal rectification in the graded mass quantum chain of harmonic oscillators with self-consistent reservoirs. Our analytical study allows us to identify the ingredients leading to the effect. The presence of rectification in this effective, simple model (representing graded mass materials, systems that may be constructed in practice) indicates that rectification in graded mass quantum systems may be an ubiquitous phenomenon. Moreover, as the classical version of this model does not present rectification, our results show that, here, rectification is a direct result of the quantum statistics.

A fundamental challenge in statistical physics is the derivation of macroscopic phenomenological laws of thermodynamic transport from the underlying microscopic Hamiltonian systems. However, after decades, a first-principle derivation of the Fourier's law of heat conduction, for instance, is still a puzzle [1]. Many works have been devoted to the theme [2], most of them by means of computer simulations. But, in these problems where the central question involves the convergence or divergence of thermal conductivity, sometimes there is a significant difficulty to arrive at precise conclusions from numerical results [3]. Thus, the necessity of analytical studies together with the huge complexity of the associated nonlinear dynamical systems led to several works considering approximative schemes or simplified models [4] – since the pioneering work of Debye, the microscopic models to describe heat conduction are mainly given by systems of anharmonic oscillators, leading to problems without analytical solutions. Many works involve, e.g., the use of approximations such as Boltzmann equations, master equations for effective models, the analysis of Green–Kubo formula, etc. An example of simple (effective) model that can be analytically studied is the classical or quantum harmonic chain of oscillators with self-consistent reservoirs. It has been proposed a while ago [5,6], but it is always revisited [7,8]. In such model, each site of the chain is coupled to a reservoir; the first and last sites are coupled to "real" thermal baths, while the inner reservoirs only mimic the absent anharmonic interactions. The self-consistent condition means that there is no heat flow between an inner reservoir and its site in the steady state: the inner baths act only as a phonon scattering mechanism, such as the on-site anharmonic potential in more elaborated systems. This model, the classical and also the quantum version, in opposition to a standard harmonic system, obeys the Fourier's law [7].

In this scenario of intensive study of the heat mechanism, problems involving the possibility to control the heat flow by constructing thermal nano-instruments such as thermal diodes, and even transistors, thermal gates and memories, have recently attracted considerable theoretical [9–11] and experimental [12] interest. A thermal diode, or rectifier, is a device in which the magnitude of the heat current changes as we invert the device between two thermal baths. That is, in a thermal diode, heat flows preferably in one direction. There are some analytical attempts to explain the phenomenon of thermal rectification and/or design a diode by using simple models (see e.g. the spin-boson nanojunction [13,14], and the billiard system [15]) but, again, most of the works consider numerical computations [9–11]. It is worth to recall the extensive work of B. Li and collaborators: e.g. thermal rectification in asymmetric graphene ribbons is studied by using molecular dynamics simulations in Ref. [16]; also in carbon nanocone structures [17]; at silicon–amorphous polyethylene interfaces [18]; in carbon nanotube intramolecular junctions [19], etc. A commonly used design of diodes is given by the sequential coupling of two or three chains with different anharmonic potentials [9–11]. It is frequently studied, but it is also criticized due to the difficulty to be constructed in practice [10]. Recently, Chang et al. [12], considering a different procedure, built a nanoscale thermal rectifier in an experimental work: they use a graded material, namely, nanotubes externally and inhomogeneously mass-loaded with heavy molecules, a system with asymmetric-axial thermal conductance. Graded materials are also considered in other numerical studies of diodes [20,21], and the interesting results made some authors suggest that thermal rectification is guaranteed by the use of graded materials with anharmonic interactions.

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Having in mind the investigation of this suggested relation between graded (anharmonic) materials and rectification, in a recent paper [22] we study the classic harmonic chain of oscillators with self-consistent reservoirs (CSC). We show the absence of thermal rectification for the CSC model with graded masses or graded interparticle interactions by using the method developed in Refs. [23,24]. In [25], Segal obtains similar results by using the approach of [8]. We, and other authors [5,7], understand the SC models as effective anharmonic models (the inner reservoirs mimic the absent anharmonic potentials), but it is not a consensus. Anyway, even if we discard any relation with anharmonicity, these results show, at least, that the onset of Fourier's law does not guarantee thermal rectification in asymmetric classic models – we recall that the Fourier's law does not hold in standard harmonic systems (i.e., harmonic models with reservoirs at the boundaries only), but it holds in the SC models.

Still searching for the mechanism behind the rectification in graded mass systems, we recall that, at low temperatures, quantum effects may introduce significant changes. The thermal conductivity for the quantum self-consistent harmonic chain (QSC), for example, depends on temperature [8,26], in opposition to the CSC thermal conductivity [7]. Thus, searching for possible quantum effects in the mechanism of thermal rectification, in a quite recent work [27], we turn to the inhomogeneous QSC and, in the linear response regime, i.e., for the chain submitted to a very small gradient of temperature and considering only linear corrections in computations with changes in the temperature, we show the absence of thermal rectification despite quantum effects in the conductivity. However, we may still ask about the possibility of a rectification for the quantum system submitted to a large gradient of temperature or, at least, for some effect beyond linear corrections. It is, indeed, a very important question: in Ref. [28], the authors show that there is a significative rectification in some chaotic billiard systems "provided the temperatures (of the two sides of the system) are strongly different ...".

In the present work, with the focus on the onset of rectification in inhomogeneous systems, we revisit the graded mass QSC model, and study it by using an analytical approach valid for any temperature gradient, i.e., beyond the linear response regime. For this quantum model, we show that, in opposition to the behavior of its classical version, there is a thermal rectification. We offer an explanation for this difference: in the quantum version, the expression for the heat flow (3) involves a distribution for the phonon frequencies (the frequencies in the system) that depends on temperature (5), leading to a mix of temperature, frequencies and also particle masses (see Eqs. (3), (4)). It does not happen in the classical system – see the comments for the high temperature limit at the end of this manuscript. This intricate mix of temperature, masses and frequencies makes the heat current change as we invert the graded mass system between two thermal reservoirs. The presence of rectification in this quite simple, say, bare model is of considerable interest: it indicates the generality of such phenomenon in the experimentally realizable class of graded mass systems, i.e., it indicates that rectification is not related to intricate interactions in the microscopic systems. Moreover, as far as we know, this work is the first demonstration of a "purely" quantum thermal rectifier, in the sense that, for such model, the rectification is a direct result of the quantum statistics: i.e., rectification is absent in the classical version of the model.

Let us introduce the QSC model. We use a Ford–Kac–Mazur approach, as detailed presented in Ref. [8], in order to describe the quantum system and its time evolution to the steady state. Here, all the baths connected to the chain are modeled as mechanical harmonic systems, with initial coordinates and momenta determined by some statistical distribution. Then, we solve the quantum dynamics given by Heisenberg equations, take the stochastic distribution for the initial coordinates of the baths, as well as the limit $t \to \infty$, and obtain the expression for the heat flow in the steady state.

The Hamiltonian of our system, a chain (W) with harmonic interparticle and on-site potentials, with each site connected to a bath (B), also with harmonic interactions, is given by

$$\mathcal{H} = \mathcal{H}_W + \sum_{i=1}^{N} \mathcal{H}_{B_i} + \sum_{i=1}^{N} X_W^T V_{B_i} X_{B_i},$$
$$\mathcal{H}_S = \frac{1}{2}\dot{X}_S^T M_S \dot{X}_S + \frac{1}{2} X_S^T \Phi_S X_S, \tag{1}$$

where $S = W$ or B_i; M_W, M_{B_i} are the particle-mass diagonal matrices for the chain and baths; Φ_W and Φ_{B_i} are symmetric matrices describing the interparticle and on-site harmonic interactions; and V_{B_i} gives the interaction between the i-site and its bath (more details below). We have, 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. Of course, it follows that $[X_r, P_l] = i\hbar\delta_{r,l}$. Finally, the dynamics is given by the Heisenberg equations

$$M_W \ddot{X}_W = -\Phi_W X_W - \sum_i V_{B_i}^T X_{B_i},$$
$$M_{B_i} \ddot{X}_{B_i} = -\Phi_{B_i} X_{B_i} - \sum_i V_{B_i}^T X_W. \tag{2}$$

The formulas for the heat currents inside the chain and from each reservoir to the chain are related to $\langle X_W \dot{X}_W^T \rangle$ and $\langle X_B \dot{X}_W^T \rangle$. Before presenting the formulas, let us give a very short resume of their derivation. To find the expressions, we turn to the Heisenberg equations (2), treat the equations of the baths as linear inhomogeneous equations, and plug these solutions into the equations for the chain. Then, we take the average over the initial conditions of the baths, which are assumed to be distributed according to equilibrium phonon distributions with properly chosen temperatures, determined such that the self-consistent condition holds, that is, we must take the temperatures of the inner baths such that there is no heat flow between an inner bath and its site. We reach the steady state 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 note that, by plugging the solutions of the baths back into the equations of motion for the system, we get a quantum Langevin equation. Remember that, for our model, all particles are connected to heat reservoirs that are taken to be Ohmic. The coupling strength to the reservoirs is controlled by the dissipation constant ζ defined by an expression involving the matrix V presented in the Hamiltonian above (see Ref. [8]).

The expression for the heat flow from the lth reservoir to the chain is given by

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

where ζ is the dissipation constant;

$$\left[G_W(\omega) \right]^{-1} = -\omega^2 M_W + \Phi_W - \sum_l \Sigma_l^+(\omega), \tag{4}$$

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

$$f(\omega, T_l) = 1/\left[\exp(\hbar\omega/KT_l) - 1 \right]; \tag{5}$$