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Approximative analytical method for some Langevin dynamical systems

Emmanuel Pereira *

Departamento de Física-ICEx, UFMG, CP 702, 30.161-970 Belo Horizonte MG, Brazil

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ABSTRACT

We develop an approach which leads to an analytically treatable integral representation for the steady state correlation functions of some Langevin dynamical systems, which are related to the microscopic Hamiltonian description of the heat mechanism. For the simpler case of harmonic interactions (where rigorous results exist and a comparison with our method is possible), we perform the computations for the thermal conductivity (given by two-point functions) and show that our approximative scheme works perfectly well.

1. Introduction

We address here the investigation of some stochastic Langevin systems used to describe the mechanism of heat conduction. The dynamical equations and our procedures are quite general, but we are specifically interested in the study of the microscopic description of the heat flow.

The problem of understanding the properties of heat conduction in solids, starting from microscopic models of matter, is one of the most fundamental, and it is still a challenge in non-equilibrium physics. In particular, the phenomenological Fourier's law, proposed in 1822 and present in basic textbooks, states that, when a gradient of temperature ∇T is applied to a material, the local heat current is given by

$$\mathcal{F}(x) = -\kappa(x)\nabla T(x),$$

where the heat conductivity κ is a function of the local temperature $T(x)$. This law is experimentally observed in many materials, from gases to solids, and in a considerable range of temperatures, but its derivation from first principles is still unknown.

Since the pioneering work of Debye, the microscopic models to describe heat conduction are mainly given by systems of anharmonic oscillators. Many works have been devoted to this problem (a review is presented in Ref. [1]), almost all by means of computer simulations—recall, e.g., the seminal work of Fermi, Pasta and Ulam [2]. However, there are several conflicting results, and the precise conditions in interacting models of particles which lead to the Fourier's law are still ignored. We recall some conflicting works. In Ref. [3], the authors claim that one-dimensional translational invariant systems (i.e., systems with momentum conservation) have anomalous conductivity (Fourier's law does not hold), but in [4], the authors obtain finite conductivity for an one-dimensional momentum conserving system. See Refs. [5,6] for comments on the physical reason of such finite conductivity. In Ref. [7], it is claimed that any amount of anharmonicity in the on-site potential of the particle model is enough to guarantee the Fourier's law (in a recent work [8], the authors argue in

* Corresponding author. Tel.: +55 31 3499 6617; fax: +55 31 3499 5600.
E-mail address: emmanuel@fisica.ufmg.br.

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the same direction, but for the specific case of disordered systems); however, in Ref. [9], counterexamples are given. It is worth recalling that the role of on-site potentials has been discussed first in Ref. [10]. In specific, two pioneering papers related to the study of quartic on-site potentials are given by Refs. [11,12]. As emphasized in Ref. [13], the computational difficulties of investigation of the heat conductivity, in many of these problems, are not a result of ineffective procedures or weak computers: unavoidable technical problems (correlation time and length very large) indicate that the study of the convergence of the thermal conductivity requires some analytical treatment.

Concerning the analytical investigation of the problem, one of the first works on this subject was the rigorous study of the harmonic chain of oscillators with thermal baths at the boundaries [14]. In this work, it is proved that, for such systems, the Fourier's law does not hold: the heat current does not depend on the length of the chain. In Ref. [15], periodic harmonic chains are analyzed, and, again, the thermal conductivity is shown to be anomalous. Harmonic systems are related to linear dynamical problems, and so, they are obviously much simpler than the nonlinear systems related to the anharmonic potentials. For this reason, several analytical works have been devoted to their analysis. We give a few other examples. Disordered harmonic chains were investigated a long time ago, in Ref. [16], and rigorously studied in Ref. [17]: they also do not obey the Fourier's law. Harmonic systems with thermal baths at each site (introduced to simulate the absent anharmonic on-site potentials) are proposed as effective anharmonic models in Ref. [18], and are recently revised and rigorously studied in Refs. [19,20]. In such a model, the Fourier's law holds and the temperature profile is linear. Of course, the limit of the coupling between the inner site and its bath is going to be zero (i.e., if we turn off the inner reservoirs), the thermal conductivity diverges and Fourier's law does not hold anymore. The quantum version of the harmonic chain with reservoirs at each site is presented in Ref. [21], and it is recently revisited in Refs. [22,23] (which considers the case of alternate masses in the chain). A system of harmonic oscillators perturbed by nonlinear stochastic dynamics conserving momentum and energy is proposed in Refs. [24,25]. It is shown that the thermal conductivity diverges in space dimensions $d = 1$ and 2, but it is finite if $d \geq 3$.

In relation to the main problem, namely, the analytical study of the (genuine) anharmonic system, some mathematical–physicists have recently turned to the question, with several, say, partial results, but a complete solution is still unknown. The existence of a stationary nonequilibrium state for a quite general anharmonic potential is proved in Ref. [26]. Using a Boltzmann type equation, for a small anharmonic quartic potential and in the limit of the temperature going to zero, the thermal conductivity for a one-dimensional system with quartic anharmonic potential is (approximately) computed in Ref. [27], and it is normal. Using a truncation (approximation) of the formula for the two-point function in the steady state, and still considering the small anharmonicity, the temperature gradient and the coupling with the thermal reservoirs, in Refs. [28,29], it is shown that the Fourier's law holds for a system with a small quartic on-site potential and large pinning (quadratic on-site potential). See also Ref. [30] for similar results.

To emphasize one more time the difficulty of the analytical study of the thermal conductivity for anharmonic systems, we quote the (mathematical–physicists) authors of some previous references: "despite its fundamental nature, a derivation of Fourier's law from first principles lies well beyond what can be mathematically proven" [28]; "a first principle derivation of the law is missing and, many would say, is not even on the horizon" [29]; "a rigorous treatment of a non-linear system, even the proof of the conductivity coefficient, is out of the reach of current mathematical techniques" [24].

To overcome these difficulties, besides the approximative schemes, many times simplified or effective models have been investigated: a review of recent results on theoretical studies of heat conduction in simple, yet nontrivial, models is presented e.g. in Ref. [31].

As repeatedly said, our ignorance on the precise mechanism behind the Fourier's law and the thermal conductivity still prevails, but after years of intensive studies, we know enough to start the investigation on the possibility to control the heat flow (e.g., to increase or decrease the current inside a one-dimensional system), and even to propose new technical devices such as thermal rectifiers [32,33] (we remark that, up to now, the theoretical study on such subject is mainly carried out by means of computer simulations; there are some analytical investigations on simple or effective models such as the spin–boson system [34], chaotic billiard [35], etc). A thermal diode, or rectifier, is a device in which the magnitude of the heat current changes as we invert the system between two thermal baths. There are still other important works related to the control of heat flow, such as the study of thermal transistor [36], thermal logic gate [37], and thermal memory [38]. Moreover, detailed experimental measurements, even of one-dimensional systems, is now becoming possible [39].

This scenario makes clear the importance of new analytical approaches to the investigation of heat conduction from first principles: even tentative schemes such as effective models and approximative studies are welcome in order to shed some light into the problem.

In the present paper, we develop an approximative method which leads to an analytically treatable integral representation for the correlation functions in the steady state (i.e., in the limit $t \to \infty$) of some systems with Langevin dynamics, models related to the microscopic Hamiltonian description of the heat mechanism. Now we obtain an integral formalism, e.g., for the heat flow in the steady state, where the intricate time dependence of our previous methods (used in some papers) is essentially "washed out", which will allow us to analyze systems with more complicated (and realistic) interactions. We show that our approximative scheme works perfectly well for the simpler case of harmonic interactions (where a comparison is possible due to the existence of exact results).

The rest of the paper is organized as follows. In Section 2 we present the model and some expressions for the energy current. The integral formalism and the approximative scheme for the correlation functions in the steady state is developed in Section 3. In Section 4, we use our scheme to analyze the energy current in the steady state for the simpler case of a