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Heat transport and current fluctuations in harmonic crystals

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HIGHLIGHTS

- This article is a pedagogic review on heat transport across a harmonic crystal.
- Heat baths are modeled through generalized quantum Langevin equations.
- The Landauer formula for phonon heat transport is derived.
- Applications of the Landauer formula to ordered and disordered harmonic chains is discussed.
- Current fluctuations are studied, again using the Langevin equations approach, and a formula for the cumulant generating function is derived.

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ABSTRACT

The approach of studying heat conduction in harmonic crystals, using generalized Langevin equations and phonon Green's functions, is explained in this review. We present the detailed derivation of the Landauer formula for phonon heat transfer using this approach. Some applications of the Landauer formula to understanding heat conduction in one-dimensional ordered and mass-disordered harmonic chains are given. It is explained how different boundary conditions lead to completely different system-size dependence of the average current in disordered chains. Finally we discuss the fluctuations in the total heat transferred in a fixed large interval of time and show how the Langevin approach is also useful in computing properties of these fluctuations in a harmonic system. In particular we derive the general formula for the cumulant generating function of these fluctuations.

1. Introduction

Phenomenologically, heat transport in solids has been understood in terms of Fourier's law, which states that the local heat current density J in a solid is proportional to the gradient in the local temperature T, *i.e* $J = -\kappa \nabla T$. The constant of proportionality κ is the thermal conductivity of the material. Linear response theory predicts that this can be related to the temporal decay of the equilibrium heat current auto-correlation function. Proving Fourier's law from first principles has been an outstanding problem in theoretical physics [1] and currently it is believed that this law is not valid in low-dimensional systems [2,3].

For a system such as a purely harmonic crystal we do not expect Fourier's law to be valid. Heat in such a system is carried by phonons and, if there is no scattering mechanism, then clearly we cannot get diffusive heat transfer as is implied by Fourier's law. A simple way to introduce scattering of phonons, *while still retaining the harmonic description*, is to introduce disorder in the system. Disorder can be in the form of random masses, or random force constants, or defects in the system.

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Does one recover Fourier's law in this case? Surprisingly the answer has been proved to be negative for one-dimensional systems [4–8] and there are indications that this may be the case even for higher-dimensional lattices [9,10].

The most direct way of studying heat conduction from a microscopic view-point is to take a system with purely Hamiltonian dynamics and connect its boundary points to heat baths at different temperatures and then measure the heat current in such a system. Harmonic systems provide a class of models for which this direct microscopic calculational approach can be carried through quite rigorously and where some exact results are available. The approach is very similar to the Landauer formalism for electron transport in non-interacting systems and this is what is described in this tutorial. The main result of the formalism is an explicit formula for the heat current in a general harmonic system. One can analyze this formula in specific cases to see if Fourier's law is valid. Secondly we also discuss how the approach can be extended to study current fluctuations in the system. While the formalism is easily extendable to systems in arbitrary dimensions, here for simplicity we consider one-dimensional chains.

There are several ways of dealing with the problem of a system coupled to multiple heat baths, for example the Keldysh nonequilibrium Green's function approach [11,12] is one. Here we use the Langevin equations approach. The final results from different approaches is the same. The main strategy of the Langevin equation approach is as follows. We model the heat baths by writing Langevin equations for the particles of the system that are in contact with the heat baths. The noise in the Langevin equation could be white, but one can also consider correlated noise in which case one has what are called generalized Langevin equations. We point out how these equations arise naturally by modeling the heat baths themselves as infinite collection of oscillators. The generalized Langevin equations are linear equations and can be solved simply by taking Fourier transforms, in time, of the equations of motion. These solutions involve phonon Green's functions and after some manipulations lead to the Landauer formula for the heat current. The current fluctuations are also obtained using a similar approach but here we show that Fourier series solutions are more useful.

In Section 2 we describe the Langevin equation approach of studying heat transport. The solution of the Langevin equations and the derivation of the Landauer formula for the average heat current is given. We then show how the Landauer formula can be used to obtain current properties for ordered and disordered harmonic chains. In Section 3 we study current fluctuations and discuss various notions such as that of the large deviation functions, cumulant generating functions and fluctuation theorems. Finally we conclude with a summary in Section 4.

2. Heat transport across a one-dimensional harmonic chain

One of the simplest ways to model heat baths is to write a Langevin dynamics for a particle, as was first done by Langevin for the description of the motion of a colloidal particle moving inside a fluid. In the Langevin formulation, the effect of the forces from all the fluid molecules is captured through two extra terms in the equation of motion of the colloidal particle, corresponding to dissipation and noise. Thus, for example, the Langevin equation of motion for a single particle inside a fluid and in the presence of an external harmonic trapping potential is given by

$$m\ddot{x} = -kx - \gamma\dot{x} + \eta(t), \tag{1}$$

where x represents a single positional degree of freedom of the particle with mass m, k is the spring constant, γ the dissipation constant and the Gaussian noise η has zero mean and satisfies the fluctuation–dissipation relation

$$\langle \eta(t)\eta(t')\rangle = 2\gamma k_B T\delta(t-t'). \tag{2}$$

A few comments on this dynamics:

1. The above equations are for a classical system. In this case it can be shown that the particle will eventually reach a state of thermal equilibrium. If $v = \dot{x}$ it can be shown that the phase space distribution $P(x, v, t)$ evolves as $t \to \infty$ to the Boltzmann distribution $P_{eq} \propto \exp[-\beta(mv^2/2 + kx^2/2)]$ where $\beta = 1/(k_B T)$.
2. The heat bath forces have two parts, a deterministic dissipative part $-\gamma\dot{x}$ and a stochastic part $\eta(t)$, and they are related through the fluctuation–dissipation relation in Eq. (2).
3. The heat bath force $-\gamma\dot{x}+\eta(t)$ emerges as a result of integrating out the bath degrees of freedom. One of the simplest way to see this is to model the heat baths as a Hamiltonian system described by an infinite collection of harmonic oscillators with a continuous spectrum of frequencies. The bath is initially prepared in thermal equilibrium. Then, after writing the dynamics of the coupled system-plus-bath, one can show exactly that the bath degrees of freedom in the equations of motion of the system can be replaced by Langevin type terms comprising of a deterministic and of a stochastic part [13].
4. In the quantum case, writing a phenomenological equation such as Eq. (1) and proving equilibration is non-trivial [14] and here it is necessary to start with the Hamiltonian heat bath model as described in the previous paragraph [13]. One then finds that the quantum Langevin equation for a single harmonic oscillator is given by

$$m\ddot{x} = -kx + \int_{-\infty}^{t} dt'\,\Sigma^{+}(t-t')x(t') + \eta(t) \tag{3}$$

with

$$\frac{1}{2}\langle \tilde{\eta}(\omega)\tilde{\eta}(\omega') + \tilde{\eta}(\omega')\tilde{\eta}(\omega)\rangle = \frac{\hbar\Gamma(\omega)}{2\pi}\coth\frac{\hbar\omega}{2k_B T}\delta(\omega+\omega'), \tag{4}$$