Changing the heat conductivity: An analytical study

Fernando Barros,* Humberto C. F. Lemos,† and Emmanuel Pereira‡
Departamento de Física-ICEx, UFMG, CP 702, 30.161-970 Belo Horizonte MG, Brazil
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We address the problem of controlling the energy flow in lattice systems: we investigate, in an analytical approach, the properties of the heat conductivity of the harmonic crystal with self-consistent stochastic reservoirs, a single model with normal conductivity. For the case of weak interparticle interaction, in a perturbative analysis, we obtain an expression for the thermal conductivity and show how to decrease and/or increase the heat current inside the system by changing the masses of the particles and/or the on-site potentials. These results may be useful in the construction of devices controlling the heat conduction.

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It is still a challenging problem of nonequilibrium statistical mechanics to derive the dynamical laws of macroscopic phenomena in terms of simple microscopic models. In particular, the precise conditions in microscopic systems of interacting particles that lead to the (macroscopic phenomenological) Fourier's law of heat conduction are still unknown [1]. Many works have been devoted to this problem: there is plenty of numerical simulations (contradictions exist, see e.g., Refs. [2–5]) and some few analytical results (see, e.g., Refs. [6–9] and references there in). We still ignore the precise mechanism behind the Fourier's law, but, after years of intensive research, our understanding of heat conduction is good enough to permit us to investigate, for example, the possibility to control the heat flow inside a one-dimensional (1D) chain, a very interesting problem that opens the possibility to propose new devices such as a thermal rectifier. There are some recent results on such a subject (again) by means of computer simulations [10,11].

In this work, our aim is to present an attempt of an analytical treatment of the problem of controlling the heat conductivity properties of a model that mimics a real system, i.e., a system with normal heat conductivity. Here we consider the model of the harmonic crystal with self-consistent stochastic reservoirs, and show how to increase and/or decrease its heat conductivity. This model consists of a chain of oscillators with harmonic nearest-neighbor interparticle interactions, harmonic on-site potential and a stochastic heat bath coupled to each site. The interior heat reservoirs are interpreted, from a physical point of view, as a schematical representation of the degrees of freedom not included in the harmonic Hamiltonian (i.e., the inner reservoirs represent the anharmonic part of the interaction). This model has been introduced a long time ago [12], and has been recently revisited in Ref. [13], where the authors rigorously show that it obeys the Fourier's law. As well known, for the harmonic version with reservoirs at the boundaries only, i.e., if we turn off the inner heat baths, the Fourier law does not hold [14].

Here, using an analytical approach, for the case of weak interparticle interaction, in a perturbative analysis we obtain an expression for the thermal conductivity which allows us to propose mechanisms to decrease or increase the heat flow in the system. Namely, we show that the conductivity becomes smaller as we take different masses for the interacting oscillators, and also as we take different coefficients for the harmonic on-site potentials.

Let us introduce the model. We take N oscillators with Hamiltonian

$$H(q,p) = \sum_{j=1}^{N} \frac{1}{2}\left(\frac{p_j^2}{m_j} + M_j q_j^2 + \sum_{l\neq j} q_l J_{lj} q_j\right), \tag{1}$$

where J is Hermitian, $J^T=J$; $M_j, m_j > 0$; with the time evolution

$$dq_j = \frac{\partial H}{\partial p_j}dt = \frac{p_j}{m_j}dt,$$
$$dp_j = -\frac{\partial H}{\partial q_j}dt - \zeta_j p_j dt + \gamma_j^{1/2} dB_j, \tag{2}$$

where B_j are independent Wiener processes; ζ_j is the heat bath coupling for the jth site; $\gamma_j = 2m_j\zeta_j T_j$, where T_j is the temperature of the jth thermal reservoir.

The model in the specific case of identical particle masses $m_j=1$ and uniform on-site potential $M_j=M$ has been already studied in Ref. [15]. Now, we turn to this more general version and investigate the effects in the heat conductivity due to changes in m_j and M_j for different sites j, an interesting result not discovered before. Some expressions with similar ones already described in this previous work [15] are presented ahead again in order to make clear the changes due to the different masses and on-site potentials.

The energy of the oscillator j is

$$H_j = \frac{p_j^2}{2m_j} + \frac{1}{2}M_j q_j^2 + \frac{1}{2}\sum_{l\neq j} q_l J_{lj} q_j = \frac{p_j^2}{2m_j} + U_1(q_j) + \frac{1}{2}\sum_{l\neq j} U_2(q_j - q_l), \tag{3}$$

where U_1 and U_2 comes from (1) and $\Sigma_j H_j = H$. Hence, it follows that

*Electronic address: fbarros@fisica.ufmg.br
†Electronic address: hcfl@fisica.ufmg.br
‡Electronic address: emmanuel@fisica.ufmg.br

$$\left\langle \frac{dH_j}{dt} \right\rangle = \langle R_j(t) \rangle - \langle \mathcal{F}_{j\rightarrow} - \mathcal{F}_{\rightarrow j} \rangle, \tag{4}$$

where $\langle \cdot \rangle$ means the expectation with respect to the noise distribution, and

$$\langle R_j(t) \rangle = \zeta_j(T_j - \langle p_j^2 \rangle / m_j) \tag{5}$$

is the energy flux from the jth bath to the jth site; the energy current inside the system is given by

$$\mathcal{F}_{j\rightarrow} = \sum_{l>j} \nabla U_2(q_j - q_l) \frac{1}{2}\left(\frac{p_j}{m_j} + \frac{p_l}{m_l} \right). \tag{6}$$

Precisely, $\mathcal{F}_{j\rightarrow}$ describes the heat flow from the jth site to the lth sites, and $\mathcal{F}_{\rightarrow j}$ is given by the expression for $\mathcal{F}_{j\rightarrow}$ by changing l with j.

To study the heat flow in the steady state, we follow the approach described in previous works [6,15]. Namely, we start from a system with isolated states, i.e., without interparticle interactions, solve this simple problem and obtain the expression of the heat flow for the complete model (with the interparticle potential) using the Girsanov theorem, a tool of stochastic differential equations [16]. In the sequel, we carry out a perturbative analysis, which is not naive as we comment on later.

We introduce, for convenience, the phase-space vector $\phi=(q,p)$, with $2N$ coordinates, and write the time evolution equations (2) as

$$\dot{\phi} = -A\phi - U_2' - \sigma\eta, \tag{7}$$

where the $2N \times 2N$ matrices A and σ are given by

$$A = \begin{pmatrix} 0 & -\mathfrak{M}^{-1} \\ \mathcal{M} & \Lambda \end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \Gamma^{1/2} \end{pmatrix}, \tag{8}$$

where $\mathcal{M}$, $\mathfrak{M}$, Λ, and Γ are the $N \times N$ diagonal matrices, $\mathcal{M}_{jl}=\delta_{jl}M_l$, $\mathfrak{M}_{jl}=\delta_{jl}m_l$, $\Lambda_{jl}=\delta_{jl}\zeta_l$, and $\Gamma_{jl}=\delta_{jl}\gamma_l$; η are independent white noises; U_2' is the derivative of U_2 in relation to q (note that its contribution to ϕ_k is nonvanishing only for $k>N$). Discarding the interparticle U_2 term, the solution of (7) above is the well-known Ornstein-Uhlenbeck (Gaussian) process

$$\phi(t) = e^{-tA}\phi(0) + \int_0^t ds e^{-(t-s)A}\sigma\eta(s). \tag{9}$$

We take $\phi(0)=0$ for simplicity, and so, the covariance becomes

$$\langle \phi(t)\phi(s) \rangle \equiv \mathcal{C}(t,s) = \begin{cases} e^{-(t-s)A}\mathcal{C}(s,s), & t \geqslant s, \\ \mathcal{C}(t,t)e^{-(s-t)A^T}, & t \leqslant s, \end{cases}$$

$$\mathcal{C}(t,t) = \int_0^t ds e^{-sA}\sigma^2 e^{-sA^T}. \tag{10}$$

It follows, by, e.g., diagonalizing A, that [for a single site $\phi_j=(q_j,p_j)$]

$$\exp(-tA) = e^{-t\zeta_j/2}\left[\cosh(t\rho_j)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{\sinh(t\rho_j)}{\rho_j}\begin{pmatrix} \zeta_j/2 & m_j^{-1} \\ -M_j & -\zeta_j/2 \end{pmatrix} \right],$$

$$\rho_j = \left[\left(\frac{\zeta_j}{2} \right)^2 - \frac{M_j}{m_j} \right]^{1/2}. \tag{11}$$

The complete expression for e^{-tA} involving $2N \times 2N$ matrices easily follows. For the case of isolated states, i.e., $U_2 \equiv 0$, as $t \rightarrow \infty$ we have the convergence to the equilibrium (each isolated site is linked to a unique thermal reservoir) and the Boltzmann-Gibbs stationary state is Gaussian, with mean zero and covariance

$$C = \int_0^\infty ds e^{-sA}\sigma^2 e^{-sA^T} = \begin{pmatrix} \mathcal{T}\mathcal{M}^{-1} & 0 \\ 0 & \mathcal{T}\mathfrak{M} \end{pmatrix}, \tag{12}$$

where $\mathcal{T}$ is a diagonal $N \times N$ matrix with $\mathcal{T}_{jl}=\delta_{jl}T_l$.

Now we turn to the complete process (with interparticle interaction) by using, as said, the Girsanov theorem, which gives us a measure for the complete process in terms of the measure $\mu_{\mathcal{C}}$ obtained for the decoupled process (with $J=0$, i.e., $U_2 \equiv 0$). For example, for the two-point correlation function, the theorem establishes that

$$\langle \varphi_u(t_1)\varphi_v(t_2) \rangle = \int \phi_u(t_1)\phi_v(t_2)Z(t)d\mu_{\mathcal{C}}/\text{norm}, \tag{13}$$

where $t_1, t_2 < t$; φ and ϕ are the solutions for the complete and decoupled processes, respectively. The factor $Z(t)$ is

$$Z(t) = \exp\left(\int_0^t u dB - \frac{1}{2}\int_0^t u^2 ds \right), \quad \gamma_i^{1/2}u_i = -J_{ik}\phi_k,$$

the inner products above are in $\mathbb{R}^{2N}$. In what follows, we will use the index notation: i for index values in the set $\{N+1, N+2, \ldots, 2N\}$, j for values in the set $\{1,2,\ldots,N\}$, and k in $\{1,2,\ldots,2N\}$. For the first term above we have

$$u_i dB_i = \gamma_i^{-1/2}u_i\gamma_i^{1/2}dB_i = -\gamma_i^{-1}J_{ij}\phi_j(d\phi_i + A_{ik}\phi_k dt), \tag{14}$$

and using the Itô formula [16], we get

$$-\gamma_i^{-1}J_{ij}\phi_j d\phi_i = -dF - \gamma_i^{-1}\phi_k A_{ki}^T J_{ij}\phi_j dt,$$

$$F(\phi) = \gamma_i^{-1}\phi_i J_{ij}\phi_j.$$

Hence, it follows that

$$Z(t) = \exp\left(-F(\phi(t)) + F(\phi(0)) - \int_0^t ds W_J(\phi(s)) \right),$$

with

$$W_J(\phi(s)) = -\gamma_i^{-1}m_j^{-1}\phi_i(s)J_{ij}\phi_{j+N}(s) + \gamma_i^{-1}\phi_k(s)A_{ki}^T J_{ij}\phi_j(s) + O(J^2).$$

As previously described in (6), to study the heat current in the steady state we need to investigate $\lim_{t\rightarrow\infty}\mathcal{F}_{j\rightarrow}(t)$, which is given in terms of the correlation functions

$$\lim_{t\to\infty}\langle\varphi_u(t)\varphi_v(t)\rangle=\lim_{t\to\infty}\int \phi_u(t)\phi_v(t)Z(t)d\mu_{\mathcal{C}}/\mathrm{norm}(\phi),$$

for $u\in\{N+1,N+2,\ldots,2N\}$ and $v\in\{1,2,\ldots,N\}$. Before carrying out the computation which involves only Gaussian integrations, we note that the covariance is given by

$$\mathcal{C}(t,s)=\exp[-(t-s)A]C+O\{\exp[-(t+s)\zeta/2]\},$$

for $t>s$, and the effects of the second term on the right-hand side of the equation above vanish in the correlation formula in the steady state, i.e., in the limit of $t\to\infty$. We will consider the case of a small interparticle potential in order to perform a perturbative analysis. Hence, up to first order in J we have (the computation is straightforward and we do not give details here)

$$\lim_{t\to\infty}\langle\varphi_u(t)\varphi_v(t)\rangle=\frac{(J_{v+N,u-N}T_{u-N}-J_{u,v}T_v)(\zeta_{u-N}+\zeta_v)m_v^{-1}}{(m_{u-N}^{-1}M_{u-N}-m_v^{-1}M_v)^2+(\zeta_{u-N}+\zeta_v)(\zeta_v m_{u-N}^{-1}M_{u-N}+\zeta_{u-N}m_v^{-1}M_v)}. \quad (15)$$

For simplicity, in what follows we will restrict the analysis to the case of one-dimensional systems with nearest-neighbor interactions (and still with $J_{1+N,2}=\cdots=J_{j+N,j+1}=\cdots=J$) and we will take uniform coupling to the thermal reservoirs $\zeta_j=\zeta$. Then, the expansion above becomes

$$\lim_{t\to\infty}\langle\varphi_u(t)\varphi_v(t)\rangle=\frac{2J\zeta m_v^{-1}}{(m_{u-N}^{-1}M_{u-N}-m_v^{-1}M_v)^2+2\zeta^2(m_{u-N}^{-1}M_{u-N}+m_v^{-1}M_v)}(T_{u-N}-T_v). \quad (16)$$

Now, from (6), for the heat current we have

$$\mathcal{F}_{j\to j+1}\equiv\langle\mathcal{F}_{j\to}\rangle=\frac{J}{2}\left\langle(\varphi_j-\varphi_{j+1})\left(\frac{\varphi_{j+N}}{m_j}+\frac{\varphi_{j+1+N}}{m_{j+1}}\right)\right\rangle.$$

Thus, in the steady state where $\langle dH_i/dt\rangle=0$, using that

$$\lim_{t\to\infty}\langle\varphi_u(t)\varphi_u(t)\rangle=m_{u-N}T_{u-N},\quad u\in\{N+1,\ldots,2N\},$$

which gives us $\lim_{t\to\infty}\langle R_j(t)\rangle=0$, we have

$$\mathcal{F}_{1\to 2}=\mathcal{F}_{2\to 3}=\cdots=\mathcal{F}_{N-1\to N}\equiv\mathcal{F}. \quad (17)$$

Using the notation

$$J_j\equiv\frac{2J^2\zeta m_j^{-1}m_{j+1}^{-1}}{\left(\frac{M_j}{m_j}-\frac{M_{j+1}}{m_{j+1}}\right)^2+2\zeta^2\left(\frac{M_j}{m_j}+\frac{M_{j+1}}{m_{j+1}}\right)}$$

and from (17) we have

$$\mathcal{F}=J_1(T_2-T_1)=\cdots=J_{N-1}(T_N-T_{N-1}).$$

And so, we can write

$$\mathcal{F}=\frac{\chi}{N-1}(T_N-T_1),$$

where we have for the conductivity

$$\frac{\chi}{N-1}=\left(\frac{1}{J_1}+\frac{1}{J_2}+\cdots+\frac{1}{J_{N-1}}\right)^{-1}. \quad (18)$$

Let us consider the case of masses and on-site potentials with values alternating in the sets $\{m_1,m_2\}$ and $\{M_1,M_2\}$, i.e., $m_j=m_1$ for j odd and $m_j=m_2$ for j even, etc. From (18), we have

$$\chi=\frac{2J^2\zeta m_1^{-1}m_2^{-1}}{\left(\frac{M_1}{m_1}-\frac{M_2}{m_2}\right)^2+2\zeta^2\left(\frac{M_1}{m_1}+\frac{M_2}{m_2}\right)}. \quad (19)$$

For $m_1=m_2$ and $M_1=M_2$, the conductivity becomes

$$\chi=\frac{J^2}{2\zeta mM}, \quad (20)$$

i.e., the conductivity is proportional to the inverse of the particle mass and to the inverse of the coefficient of the on-site potential. In short, from the expressions (19) and (20) above we obtain mechanisms to change the heat conductivity. For example, for a system of particles with equal masses but with on-site potentials with alternating values, the conductivity becomes proportional to the inverse of the square of the difference between the on-site potential values (instead of proportional to the inverse of the on-site potential). Similar results follow if we alternate the masses of the particles.

We make some comments now. Concerning the physical interest of the models with unequal masses and/or on-site potentials, we recall that the study of systems with different masses is recurrent [17–19]. For example, for 1D harmonic chain with baths at the boundaries only, the model with equal masses has been rigorously studied a long time ago in Ref. [14], where the authors show that the heat current is independent of the system size (in a system where the Fourier law holds, one has the heat current depending on the system size as $\mathcal{F}\sim 1/N$). In sequel, the case of unequal masses has been studied, e.g., by Lebowitz *et al.* [17]. In particular, for a random mass distribution, it is rigorously shown that $\mathcal{F}\sim N^{-1/2}$ [18]. Unfortunately, these models do not obey the Fourier law. We do not know of any similar study for different on-site potentials which, however, have well-known physical meaning: e.g., low-dimensional lattice structures are usually grown on a substrate which exerts a pinning force on the atoms, and such force is represented by an on-site potential.

To show the trustworthiness of our perturbative computation, we turn to the model with equal masses and on-site potentials, and recall that the expressions for the heat conductivity obtained by our first-order perturbative computation and the exact one described in Ref. [13] are the same one (see Ref. [15] for details). In fact, the perturbative treatment of the harmonic chain with stochastic reservoirs is rigorously correct, i.e., the perturbative series is convergent [20].

As a final comment, we remark that the results presented here may be useful in the (theoretical) construction of devices such as thermal rectifiers, which have been recently proposed as a mix of two systems with different heat conductivity.

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