

Thermal conductivity of anharmonic crystals with self-consistent baths: Analytical computation with discrete time

Emmanuel Pereira,^{1,*} Ricardo Falcao,^{2,†} and Humberto C. F. Lemos^{2,‡}¹*Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, CP 702, 30.161-970 Belo Horizonte, Minas Gerais, Brazil*²*Departamento de Física e Matemática, Universidade Federal de São João del-Rei, 36420-000 Ouro Branco, Minas Gerais, Brazil*

(Received 18 January 2013; published 25 March 2013)

We analytically compute the thermal conductivity of anharmonic crystals with self-consistent stochastic reservoirs. We develop an integral representation for the heat current, assume the approximation of discrete times, and in a perturbative analysis that is rigorously supported by a convergent cluster expansion compute the thermal conductivity for a chain with quartic anharmonic on-site potential. In the high anharmonicity regime, the result for the dependence of the conductivity on temperature is the same as for the system without inner reservoirs. The presented formalism is quite general and is also valid for inhomogeneous systems in any space dimension.

DOI: [10.1103/PhysRevE.87.032158](https://doi.org/10.1103/PhysRevE.87.032158)

PACS number(s): 05.70.Ln, 05.40.-a, 44.10.+i

The study of the microscopic mechanism of heat conduction [1] is an old problem, but it is still a challenge in nonequilibrium statistical physics. For a long time, fundamental questions have been investigated, such as the conditions for Fourier's law to hold true [2]; recently, more and more attention has been devoted to problems regarding the control of the heat current, for example, the construction of devices such as thermal diodes [3], transistors [4], and memories [5].

Since the pioneering work of Debye, the usual models for the description of heat conduction in solids are given by systems of anharmonic oscillators, which involve extremely difficult mathematical problems. Consequently, most of the works are carried out with the aid of numerical techniques or computer simulations. In the few analytical studies, to bypass the excessive difficulty some authors make use of toy models and simplified systems [6], or approximate schemes [7,8]. However, more accurate analytical investigations are still highly desirable for both a clear understanding (to resolve conflicting numerical results and open questions) and hints for the building of thermal devices with useful properties.

Hybrid models, that is, systems in which the interaction is a combination of mechanic (determinist) and stochastic potentials, appear as a candidate for a more amenable analytical problem, still related to realistic models, with a precise solution. An important example is the harmonic and the anharmonic lattice of oscillators with self-consistent stochastic reservoirs linked to each site. The self-consistent condition means that, in the steady state, there is no mean heat flow between each inner reservoir and its linked site. In other words, the inner reservoirs do not describe real thermal baths as those given by the baths at the boundaries: They represent only some residual mechanism of phonon scattering not present in the deterministic potential. The simpler case, that is, the harmonic self-consistent chain of oscillators, is an old problem [9] recently revisited [10]. In such a model, it has been proved that

the Fourier law holds, the thermal conductivity is a constant (it does not change with temperature), and the temperature profile is linear. In Ref. [11] the anharmonic version was investigated: The existence of a nonequilibrium stationary state with the self-consistent condition and the boundedness of a thermal conductivity $\mathcal{K}(T)$ as the size of the system goes to infinity were proved. There $\mathcal{K}(T)$ was given by a Green-Kubo formula, but it was not explicitly computed. Again, the immense difficulty of computations in the nonlinear problem was stressed in Ref. [11].

In this context, the present work addresses the presentation of an analytical approach that allows us to compute in detail the heat flow and the thermal conductivity in lattice systems of anharmonic oscillators that may describe realistic features of the heat conduction in solids. We consider these anharmonic crystals with self-consistent reservoirs, develop an integral representation for the correlation functions that give the heat current, and compute the thermal conductivity of the system. The unique approximation used in the analysis is the replacement of continuous time by discrete time. We perform a perturbative computation that is supported by a convergent cluster expansion; the approach is quite general: It works also for inhomogeneous systems and the integral formalism follows for the space dimension (probably requiring, however, a different perturbative analysis). Moreover, our results indicate that at least in the regime of high anharmonicity, anharmonic chains with and without inner reservoirs present similar heat conduction.

Let us introduce the model. For simplicity, we consider a one-dimensional space. Precisely, we take N oscillators with the Hamiltonian

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

where $M_j > 0$, $J_{jl} = J_{lj}$, and \mathcal{P} is the anharmonic on-site potential, with the dynamics given by

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

*emmanuel@fisica.ufmg.br

†rfalcao@ufsj.edu.br

‡humbertolemos@ufsj.edu.br

where B_j are independent Wiener processes, ζ_j is the coupling between site j and its reservoir, and $\gamma_j = 2\zeta_j m_j T_j$, where T_j is the temperature of the j th bath. We will restrict the analysis to nearest-neighbor interactions only.

The energy current, i.e., heat flow, inside the system is given by $\langle F_{j,j+1} \rangle \equiv \mathcal{F}_{j,j+1}$, where $\langle \cdot \rangle$ means the expectation with respect to the noise distribution and

$$F_{j,j+1} = J_{j,j+1}(q_j - q_{j+1}) \left(\frac{p_j}{2m_j} + \frac{p_{j+1}}{2m_{j+1}} \right). \quad (2)$$

Precisely, $\mathcal{F}_{j,j+1}$ describes the mean heat flow from the j th to the $(j+1)$ th site. Given the temperatures T_1 and T_N at the boundaries, the self-consistent condition (no mean heat flow between an inner reservoir and its site in the steady state) is reached with the choice of T_2, T_3, \dots, T_{N-1} such that

$$\mathcal{F}_{1,2} = \mathcal{F}_{2,3} = \dots = \mathcal{F}_{N-1,N}. \quad (3)$$

In order to make clear the usefulness of the approach to be presented here, we recall some previous results and show the difficulty of the investigation in the specific case of crystals of anharmonic oscillators with self-consistent reservoirs. In our initial works [12], inspired by the Feynman-Kac formula, we develop an integral formalism with a Gaussian measure related to the harmonic potential part. The formalism works well for the simpler harmonic models and allows us to describe the nontrivial behavior of systems with alternating masses [13] and the absence of rectification in general graded harmonic chains [14]. However, the derivation of the anharmonic model features by starting from this Gaussian measure (i.e., from the harmonic interaction) seems to be impracticable. Hence, to make profitable the integral formalism, in Ref. [15] we proposed some modifications involving uncontrolled approximations, e.g., the replacement of instantaneous value of $q(t)$ and $p(t)$ by their mean values $\langle q(t) \rangle$ and $\langle p(t) \rangle$ (a kind of mean field approximation) and the replacement of the measure evolving in time by the stationary measure. It is interesting to note that such approximations work very well for the simpler case of harmonic models (where the existence of rigorous results allow a comparison; see Ref. [15]). Moreover, for the anharmonic systems, such an approximate scheme was useful enough to give us some qualitative understanding of the onset of thermal rectification in graded models (with the result extended and confirmed for different models in other works [16,17]) and the occurrence of negative differential thermal resistance. However, given the uncontrolled changes introduced in the formalism, it is clear that a more precise approach is still necessary. Thus, in the present work, we assume one approximation (discrete time) and by performing rigorous procedures develop an alternative approach as described in detail.

For simplicity, we restrict the analysis to one-dimensional homogeneous systems ($\lambda_j = \lambda$, $M_j = M$, etc.) with particle mass $m = 1$. We stress, however, that similar procedures follow the investigation of inhomogeneous models.

For clarity and to give an essentially self-contained description of our method, the expressions (4) and (10), already derived in previous works, are repeated below. We introduce the notation of the phase-space vector $\varphi = (q, p)$, with $2N$

coordinates. The dynamics becomes

$$\dot{\varphi} = -A\varphi - \lambda\mathcal{P}'(\varphi) + \sigma\eta, \quad (4)$$

where $A = A^0 + \mathcal{J}$ and σ are $2N \times 2N$ matrices

$$A^0 = \begin{pmatrix} 0 & -I \\ \tilde{\mathcal{M}} & \Gamma \end{pmatrix}, \quad \mathcal{J} = \begin{pmatrix} 0 & 0 \\ J & 0 \end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2\Gamma\mathcal{T}} \end{pmatrix},$$

where I is the unit $N \times N$ matrix; J is the $N \times N$ matrix for the interparticle interaction J_{jl} ; and $\tilde{\mathcal{M}}$, Γ , and \mathcal{T} are diagonal $N \times N$ matrices $\tilde{\mathcal{M}}_{jl} = M_j \delta_{jl}$, $\Gamma_{jl} = \zeta_j \delta_{jl}$, and $\mathcal{T}_{jl} = T_j \delta_{jl}$. Here η are independent white noises; $\mathcal{P}'(\varphi)$ is a $2N \times 1$ matrix with $\mathcal{P}'(\varphi)_j = 0$ for $j = 1, \dots, N$ and $\mathcal{P}'(\varphi)_i = d\mathcal{P}(\varphi_{i-N})/d\varphi_{i-N}$ for $i = N+1, \dots, 2N$. In what follows we use the following index notation: i for index values in the set $[N+1, N+2, \dots, 2N]$, j for values in the set $[1, 2, \dots, N]$, and k for values in $[1, 2, \dots, 2N]$. We omit the sum over repeated indices.

To derive the integral representation for the heat current (given by two-point correlation functions) we start from the decoupled harmonic system, i.e., with $\mathcal{J} = 0$ and $\lambda = 0$, as in our previous works. The solution of the dynamical equation with $\mathcal{J} = 0$ and $\lambda = 0$ is the Ornstein-Uhlenbeck Gaussian process

$$\phi(t) = e^{-tA^0} \phi(0) + \int_0^t ds e^{-(t-s)A^0} \sigma \eta(s), \quad (5)$$

where, for the simple case of $\phi(0) = 0$, the covariance of the process is given by

$$\langle \phi(t)\phi(s) \rangle_0 \equiv \mathcal{C}(t,s) = \begin{cases} e^{-(t-s)A^0} \mathcal{C}(s,s), & t \geq s \\ \mathcal{C}(t,t) e^{-(s-t)A^{0\dagger}}, & t \leq s, \end{cases} \quad (6)$$

$$\mathcal{C}(t,t) = \int_0^t ds e^{-sA^0} \sigma^2 e^{-sA^{0\dagger}}. \quad (7)$$

As $t \rightarrow \infty$ we have a convergence to the Gaussian distribution with covariance

$$C = \int_0^\infty ds e^{-sA^0} \sigma^2 e^{-sA^{0\dagger}} = \begin{pmatrix} \mathcal{T}\mathcal{M}^{-1} & 0 \\ 0 & \mathcal{T} \end{pmatrix}, \quad (8)$$

where \mathcal{T} is a diagonal $N \times N$ matrix with $\mathcal{T}_{j,j'} = T_j \delta_{j,j'}$.

Now we obtain a preliminary integral representation for the correlation functions of the complete process with the interparticle interaction \mathcal{J} and the anharmonic potential by using the Cameron-Martin-Girsanov theorem, which describes a relation between the correlations for the complete and the decoupled harmonic processes. Precisely, for the two-point function we have

$$\langle \varphi_{u_1}(t)\varphi_{u_2}(t) \rangle = \int \varphi_{u_1}(t)\varphi_{u_2}(t) Z(t) d\mu_C, \quad (9)$$

where

$$Z(t) = \exp \left(\int_0^t u dB - \frac{1}{2} \int_0^t u^2 ds \right),$$

$$\gamma_i^{1/2} u_i(s) = -\mathcal{J}_{i,j} \phi_j(s) - \lambda \mathcal{P}'(\phi_{i-N})(s).$$

For the parameters γ_i , T_i , etc., we have $\gamma_i \equiv \gamma_{i-N}, \dots$. After simple manipulations (using the dynamical equation for ϕ to

replace dB), we get

$$Z(t) = \exp \left(- \int_0^t [\phi_j(s) \mathcal{J}_{ji}^\dagger \gamma_i^{-1} d\phi_i(s) + \gamma_i^{-1} \lambda \mathcal{P}'(\phi_{i-N}(s)) d\phi_i(s)] - \int_0^t ds \left[\phi_j(s) \mathcal{J}_{ji}^\dagger \gamma_i^{-1} A_{ik}^0 \phi_k(s) \right. \right. \\ \left. \left. + \gamma_i^{-1} \lambda \mathcal{P}'(\phi_{i-N}(s)) A_{ik}^0 \phi_k(s) + \frac{1}{2} \phi_{j'}(s) \mathcal{J}_{j'i}^\dagger \gamma_i^{-1} \mathcal{J}_{ij} \phi_j(s) + \frac{1}{2} \gamma_i^{-1} \lambda^2 [\mathcal{P}'(\phi_{i-N}(s))]^2 + \gamma_i^{-1} \lambda \mathcal{P}'(\phi_{i-N}(s)) \mathcal{J}_{ij} \phi_j(s) \right] \right). \quad (10)$$

Before carrying out an analysis that differs from that in our previous works, let us first note that it is possible to rewrite the integrals with $d\phi$ above as integrals in ds with functions of ϕ (by turning to the equations of dynamics and using Itô's calculus [12]), but we would still stay with a formalism involving a Gaussian measure coming from the harmonic interaction. Hence, recalling hints from field theory, to proceed we introduce an ultraviolet cutoff, precisely, we take discrete times $t = 0, 1, \dots, \tau - 1, \tau$. As our interest is related to properties of the steady state reached as $\tau \rightarrow \infty$, we believe that the absence of short times will not introduce considerable changes. Functionally, it is similar to averaging over the dynamical variables over only short times instead of using the average over the whole process (which is the approximation assumed in a previous work [15]). We believe that this ultraviolet cutoff is appropriate since, by considering the power spectra of hydrodynamic currents in the model, it is found that the lower frequencies dominate the transport on a large scale (the scale of the whole chain). An interesting related discussion is presented in Ref. [18]. Moreover, now in a space-time lattice, it is possible to join anharmonic terms to the Gaussian measure in order to get a different measure (an anharmonic single spin distribution) suitable for the problem. The important physical consequence of the replacement of the initial Gaussian measure by an anharmonic one in the integral formalism must be recalled: It means that, in the following perturbative analysis, we will start from the correct point, namely, from the core of the anharmonic interaction, not from the harmonic potential (related to the Gaussian measure) whose properties are completely different from those associated with the complete system. Thus, in what follows,

$$t \in \{0, 1, \dots, \tau - 1, \tau\}, \quad d\phi(t) = \phi(t+1) - \phi(t).$$

We recall that, for these chains of oscillators with anharmonic on-site potential, one expects that the thermal conductivity remains finite as the inner reservoirs are turned

off, in opposition to the harmonic chain where Fourier's law does not hold in the absence of the inner reservoirs. The behavior of the system as we make smaller and smaller the inner reservoirs is a difficult problem (although very interesting) and it will not be considered in the present work. Thus, in what follows, for simplicity we take the coupling constant between the site and reservoir as $\zeta_j = 1$.

From the expressions (6)–(8) for the covariance \mathcal{C} of the quadratic measure above, it follows that

$$\exp(-tA^0) = e^{-t(\zeta/2)} \cosh(t\rho) \\ \times \left\{ \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} + \frac{\tanh(t\rho)}{\rho} \begin{pmatrix} \frac{\zeta}{2} & I \\ -\mathcal{M} & -\frac{\zeta}{2} \end{pmatrix} \right\}, \quad (11)$$

where $\rho = [(\zeta/2)^2 - M]^{1/2}$. We also note that

$$\mathcal{C}(t, s) = \exp[-(t-s)A^0] \mathcal{C} + O\{\exp[-(t+s)\zeta/2]\}, \quad (12)$$

where the effects on the correlation function formula of the second term on the right-hand side vanish in the limit $t \rightarrow \infty$; \mathcal{C} is the covariance as $t \rightarrow \infty$ (8). As we take $\zeta = 1$, for ease of computation we also take M slightly larger than 2. Hence, considering discrete times, from the expressions above, proper bounds follow for $\mathcal{C}_{k,k'}^{-1}(s, s')$, i.e., for the contribution of the Gaussian measure

$$d\mu_{\mathcal{C}} = \exp \left(- \frac{1}{2} \sum_{s,s'} \sum_{k,k'} \phi_k(s) \mathcal{C}_{k,k'}^{-1}(s, s') \phi_{k'}(s') \right) \\ \times \prod_{k,s} d\phi_k(s) / \mathcal{N},$$

where \mathcal{N} denotes normalization. In particular, the contribution for $\mathcal{C}_{k,k'}^{-1}(s, s')$ coming from terms beyond the next-nearest-neighbor time interaction is very small and may be discarded.

Finally, with discrete times, the integral representation for the two-point function (heat current) in a space-time lattice becomes

$$\langle \varphi_{u_1}(t) \varphi_{u_2}(t) \rangle = \int \phi_{u_1}(t) \phi_{u_2}(t) \exp \left(- \sum_{s,i,j,\dots} \left\{ \phi_j(s) \mathcal{J}_{ji}^\dagger \gamma_i^{-1} \phi_i(s+1) + \gamma_i^{-1} \lambda \mathcal{P}'(\phi_{i-N}(s)) \phi_i(s+1) \right. \right. \\ \left. \left. + \phi_j(s) \mathcal{J}_{ji}^\dagger \gamma_i^{-1} M_{i-N} \phi_{i-N}(s) + \gamma_i^{-1} \lambda \mathcal{P}'(\phi_{i-N}(s)) M_{i-N} \phi_{i-N}(s) + \frac{1}{2} \phi_{j'}(s) \mathcal{J}_{j'i}^\dagger \gamma_i^{-1} \mathcal{J}_{ij} \phi_j(s) \right. \right. \\ \left. \left. + \frac{1}{2} \gamma_i^{-1} \lambda^2 [\mathcal{P}'(\phi_{i-N}(s))]^2 + \gamma_i^{-1} \lambda \mathcal{P}'(\phi_{i-N}(s)) \mathcal{J}_{ij} \phi_j(s) + \frac{1}{2} \phi_k(s) \mathcal{C}_{k,k'}^{-1}(s, s') \phi_{k'}(s') \right\} \right) \prod_{s,k} d\phi_k(s) / \mathcal{N}. \quad (13)$$

The integral representation above for the correlation functions (and thus for the heat current) is the main technical achievement of the present paper. Now, to carry out the computation, we take as a measure a properly chosen single spin distribution (SSD) involving the higher powers of ϕ_j and ϕ_i ; a perturbative analysis may be rigorously implemented, supported by a convergent polymer expansion as described in Ref. [19]. We stress that the unique approximation used is the assumption of discrete times. We turn to a concrete example to make clear the usefulness of our approach.

We consider now, as an example, the investigation of the chain of oscillators with a weak next-nearest-neighbor interaction, i.e., $\mathcal{J}_{ij} \neq 0 \iff i = (j + N) \pm 1$, $|\mathcal{J}_{ij}| \ll 1$, and quartic anharmonic on-site potential $\mathcal{P}(\phi_j) = \phi_j^4/4$. For simplicity, besides the regimes already considered ($\zeta = 1$, $m = 1$, and $M = 2 + \varepsilon$), we still take high anharmonicity and temperature.

The integral formalism involves sites $j \in \{1, 2, \dots, N\}$ and $i \in \{N + 1, \dots, 2N\}$ (the index k , as previously stated, runs over $\{1, \dots, 2N\}$). In the SSD, instead of fields in sites j and i always in separate cells, we join in the same cell the pairs $\phi_j(s)$ and $\phi_i(s + 1)$ with $i = j + N$ [of course, $\phi_j(\tau)$ and $\phi_i(0)$ do not have pairs]. Thus our SSD is given by

$$\begin{aligned} & dv[\phi_j(s), \phi_{i=j+N}(s + 1)] \\ &= \exp \left\{ -\frac{1}{2} \lambda^2 \gamma_j^{-1} \phi_j^6(s) - \frac{1}{2T_i} \phi_i^2(s + 1) \right. \\ &\quad \left. - \gamma_j^{-1} \lambda \phi_j^3(s) \phi_i(s + 1) + \dots \right\} d\phi_j(s) d\phi_i(s + 1) / N, \end{aligned} \quad (14)$$

where the ellipsis denotes subdominant terms, N is the normalization, and $\phi_i^2(s + 1)$ was extracted from $(\phi, \mathcal{C}^{-1}\phi)$. Essentially, ϕ_i^2 and ϕ_j^6 rule the computations, i.e., the behavior of the SSD above. Hence the integral representation for the two-point function is given as a product of these SSDs (with cells of sites $[j, s]$ and $[i = j + N, s + 1]$) and the exponential of terms involving the weak interaction J , which couples different cells, and the remaining terms from $(\phi, \mathcal{C}^{-1}\phi)$, which are also small: For example, for the part involving ϕ_j , in the regime of large anharmonicity, by rescaling the dominant term $\lambda^2 \phi_j^6$ as $\tilde{\phi}_j^6$ in the SSD, this part will involve $\tilde{\phi}_j$ and powers of $1/\lambda$.

From Eq. (2), to get the heat current in the steady state, we need to study the averages of $\varphi_{i-N}(\tau)\varphi_{i+1}(\tau)$, $\varphi_{i-N}(\tau)\varphi_i(\tau)$, etc., as $\tau \rightarrow \infty$. Performing a perturbative computation from Eq. (13), for small J , large λ , and T it follows that the main contributions for $\varphi_{i-N}(\tau)\varphi_{i+1}(\tau)$ come from expressions similar to those below. The first one is given by

$$\begin{aligned} & \int [\phi_{i-N}(\tau)\phi_{i+1}(\tau)] [\lambda \gamma_{i+1}^{-1} \phi_{i+1-N}^3(\tau - 1) \phi_{i+1}(\tau)]_* \\ & \times [\lambda \gamma_{i+1}^{-1} \phi_{i+1-N}^3(\tau - 1) \mathcal{J}_{i+1, i-N} \phi_{i-N}(\tau - 1)] \\ & \times [\phi_{i-N}(\tau - 1) \mathcal{C}_{i-N, i-N}^{-1}(\tau - 1, \tau) \phi_{i-N}(\tau)] d\tilde{v}(\phi) \\ & \sim c' J \frac{1}{\lambda^{4/3}} \frac{T_{i+1}^{2/3}}{T_i}, \end{aligned}$$

where $[\cdot]_*$ comes from the cross term in the SSD, $d\tilde{v}$ is the main part of the SSD (involving ϕ_i^2 and ϕ_j^6), and c' is a numerical

factor. A second important contribution comes from terms similar to

$$\begin{aligned} & \int [\phi_{i-N}(\tau)\phi_{i+1}(\tau)] [\phi_{i-N}(\tau - 1) \mathcal{J}_{i-N, i+1}^{\dagger} \gamma_{i+1}^{-1} \phi_{i+1}(\tau)] \\ & \times [\phi_{i-N}(\tau - 1) \mathcal{C}_{i-N, i-N}^{-1}(\tau - 1, \tau) \phi_{i-N}(\tau)] d\tilde{v}(\phi) \\ & \sim c'' J \frac{1}{\lambda^{4/3}} \frac{1}{T_i^{1/3}}. \end{aligned}$$

Hence, summing up all leading terms (with $\tau \rightarrow \infty$) and considering a small difference between T_{i+1} and T_i [such that $T_{i+1}^{\alpha} - T_i^{\alpha} \approx \alpha T_i^{\alpha-1} (T_{i+1} - T_i)$], we get

$$\mathcal{F}_{j, j+1} \approx -c \frac{J^2}{\lambda^{4/3}} \frac{1}{T_j^{4/3}} (T_{j+1} - T_j). \quad (15)$$

Now the computation of the heat current in terms of the temperatures at the boundaries is straightforward. The self-consistent condition in the steady state gives

$$\mathcal{F}_{1,2} = \mathcal{F}_{2,3} = \dots = \mathcal{F}_{N-1,N} \equiv \mathcal{F}. \quad (16)$$

These equations, together with Eq. (15), give us

$$\begin{aligned} \mathcal{F}(\mathcal{C}T_1^{\alpha}) &= T_1 - T_2, \\ \mathcal{F}(\mathcal{C}T_2^{\alpha}) &= T_2 - T_3, \\ &\vdots \\ \mathcal{F}(\mathcal{C}T_{N-1}^{\alpha}) &= T_{N-1} - T_N. \end{aligned}$$

Summing up the expressions above, we find

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

where

$$\mathcal{K} = \{\mathcal{C}T_1^{\alpha} + \mathcal{C}T_2^{\alpha} + \dots + \mathcal{C}T_{N-1}^{\alpha}\}^{-1} (N - 1),$$

with $\mathcal{C}^{-1} = c \frac{J^2}{\lambda^{4/3}}$ and $\alpha = 4/3$. If $T_j \approx T$, we have the Fourier law in the chain with thermal conductivity

$$\mathcal{K} \sim c \frac{J^2}{\lambda^{4/3} T^{4/3}}. \quad (17)$$

We must recall that, as is well known, detailed numerical simulations for a chain of oscillators with quartic anharmonic on-site potential and reservoirs only at the boundaries lead to a thermal conductivity $\mathcal{K} \sim 1/T^{1.35}$ [20], essentially the same result described above. This indicates that, at least in the regime of high anharmonicity, the inner reservoirs do not play an important role. In other words, the models of anharmonic oscillators with self-consistent reservoirs and anharmonic oscillators with reservoirs only at the boundaries have similar heat conduction and thus we may use this hybrid model for further investigations of realistic features of the heat problem.

To conclude, we stress that the approach described here is quite general. For example, the integral formalism is valid in any space dimension, although, as is well known from equilibrium statistical physics (where similar integral representations appear in several problems), the polymer expansion in the perturbative analysis will require different arrangements for different dimensions. Moreover, our integral formalism is also

suitable for the investigation of inhomogeneous models, that is, it may be useful in detailed analytical studies of thermal rectification and other properties of the heat current.

The authors thank the referee for several comments that improved the presentation of the paper. This work was partially supported by CNPq (Brazil).

-
- [1] A. Dhar, *Adv. Phys.* **57**, 457 (2008); S. Lepri, R. Livi, and A. Politi, *Phys. Rep.* **377**, 1 (2003).
- [2] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, *Mathematical Physics 2000*, edited by A. Fokas *et al.* (Imperial College Press, London, 2000), pp. 128–150.
- [3] M. Terraneo, M. Peyrard, and G. Casati, *Phys. Rev. Lett.* **88**, 094302 (2002); B. Li, L. Wang, and G. Casati, *ibid.* **93**, 184301 (2004); B. Hu, L. Yang, and Y. Zhang, *ibid.* **97**, 124302 (2006).
- [4] B. Li *et al.*, *Appl. Phys. Lett.* **88**, 143501 (2006).
- [5] L. Wang and B. Li, *Phys. Rev. Lett.* **99**, 177208 (2007).
- [6] C. Bernardin and S. Olla, *J. Stat. Phys.* **121**, 271 (2005); G. Basile, C. Bernardin, and S. Olla, *Phys. Rev. Lett.* **96**, 204303 (2006).
- [7] K. Aoki, J. Lukkarinen, and H. Spohn, *J. Stat. Phys.* **124**, 1105 (2006).
- [8] J. Bricmont and A. Kupiainen, *Phys. Rev. Lett.* **98**, 214301 (2007); *Commun. Math. Phys.* **274**, 555 (2007).
- [9] M. Bosterli, M. Rich, and W. M. Visscher, *Phys. Rev. A* **1**, 1086 (1970).
- [10] F. Bonetto, J. L. Lebowitz, and J. Lukkarinen, *J. Stat. Phys.* **116**, 783 (2004).
- [11] F. Bonetto, J. L. Lebowitz, J. Lukkarinen, and S. Olla, *J. Stat. Phys.* **134**, 1097 (2009).
- [12] E. Pereira and R. Falcao, *Phys. Rev. E* **70**, 046105 (2004); *Phys. Rev. Lett.* **96**, 100601 (2006).
- [13] F. Barros, H. C. F. Lemos, and E. Pereira, *Phys. Rev. E* **74**, 052102 (2006).
- [14] E. Pereira and H. C. F. Lemos, *Phys. Rev. E* **78**, 031108 (2008); E. Pereira, L. M. Santana, and R. Ávila, *ibid.* **84**, 011116 (2011).
- [15] E. Pereira, *Phys. Rev. E* **82**, 040101(R) (2010); *Physica A* **390**, 4131 (2011).
- [16] E. Pereira, *Phys. Rev. E* **83**, 031106 (2011).
- [17] J. Wang, E. Pereira, and G. Casati, *Phys. Rev. E* **86**, 010101(R) (2012).
- [18] L. Delfini, S. Lepri, R. Livi, and A. Politi, *Phys. Rev. E* **73**, 060201(R) (2006).
- [19] R. S. Thebaldi, E. Pereira, and A. Procacci, *J. Math. Phys.* **46**, 053302 (2005).
- [20] K. Aoki and D. Kusnezov, *Phys. Lett. A* **265**, 250 (2000).