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Heat conduction in a weakly anharmonic chain: an analytical approach

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Abstract

The analytical study of heat conduction in an anharmonic chain is considered here. We investigate an one-dimensional system (directly related to the Frenkel–Kontorova model) with anharmonic cosine on-site potential and harmonic interparticle interaction. We start with a stochastic thermal reservoir connected to each site of the system, and analyse the behaviour of the conductivity in the steady state with all the heat baths as we turn off the interior reservoirs, i.e., as we keep the heat baths at the boundaries only. For a weak interparticle potential and small anharmonicity, in a perturbative computation, we derive an analytic expression for the heat conductivity which indicates that the Fourier's law holds only when each site is connected to a heat bath. To show the trustworthiness of our perturbative computation, we also derive an expression for the conductivity by starting from the exact solution of the linear part of the dynamics and compare with the result which comes from the previous perturbative analysis.

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1. Introduction

The analytical derivation of macroscopic phenomenological laws of thermodynamics from microscopic models of interacting particles is a challenging problem of nonequilibrium statistical physics. In particular, the rigorous derivation of Fourier's law of heat conduction is still unknown, even in the 1D context [1, 2]. A pioneering work on this subject is the study of a chain of interacting harmonic oscillators coupled to thermal reservoirs at the boundaries [3]. There, the authors calculate the covariance of the steady Gaussian distribution and show that the heat current is independent of the length of the chain, i.e., the heat conductivity diverges in the thermodynamic limit, and so, the Fourier's law does not hold. Since then, many works have been devoted to the problem of heat conduction and Fourier's law, but almost all of them by means of computer simulations [1]. Besides the difficulty to arrive at correct conclusions from numerical studies, the existence of contradicting results makes clear the necessity of the development of analytical methods of modelling the heat conduction problem.

In this scenario of more accurate studies, the harmonic chain of oscillators has been recently revisited for the case of each site connected to a stochastic Langevin heat bath [4]. Considering the 'self-consistent' condition, which means that there is no heat flow between an inner site and its reservoir, the stationary nonequilibrium state is analysed, and it is shown that Fourier's law holds in such case. Of course, as the coupling between each inner site and its thermal reservoir is turned off, the heat conductivity diverges for the harmonic chain, and Fourier's law is lost, as previously calculated in [3]. Concerning the central problem of heat conduction, i.e., the rigorous treatment of a nonlinear (anharmonic) system, the results are quite few: e.g., it is proved the existence of steady states in [5], and the positivity of entropy production in [6].

In the direction of the development of analytical techniques to treat nonlinear systems, some problems involving small anharmonic interactions have been considered quite recently in [7, 8] (by one of the authors and collaborators). In a perturbative approach, the harmonic chain with thermal bath at each site and a small anharmonic ϕ^4 on-site potential is investigated in [7], and a chain with harmonic on-site potential and cosine-type coupling interaction (a la rotor model) is considered in [8], where a phase transition (Fourier–non-Fourier behaviour) is claimed to appear.

In the present paper, we consider a system related to a commonly used model of physical interest, namely, the Frenkel–Kontorova model, which involves a cosine on-site potential and a harmonic interparticle interaction (the opposite of [8]). We start with a version where each site of the chain is connected to a thermal reservoir (as in [6–8]), and we study the case of small couplings for the interior sites and baths in order to infer the behaviour of the system with heat baths at the boundaries only. We show that, if the coefficient of the on-site cosine potential is small and the interaction between sites is weak, up to first order in a perturbative computation, the anharmonicity does not introduce any change in the thermal conductivity derived from the harmonic chain. It indicates that Fourier's law holds for the system with thermal reservoirs at each site, but not when we turn off the interior heat baths. Our results agree with numerical simulations presented in the literature [9] (recall that we are in the region of small anharmonicity—we give more comments in the section of concluding remarks). Note that the anharmonic cosine potential is bounded, and so, a perturbative analysis of the anharmonicity (taking small the coefficient of the anharmonic potential) might be correct (we turn to this question and recall some related problems involving similar dynamical systems which have been treated perturbatively and also rigorously by one of the authors and collaborators in the concluding remarks). However, as we also treat perturbatively the harmonic interparticle interaction, to show the trustworthiness of our results, we still compute the thermal conductivity by using (for the harmonic part of the interaction) the rigorous result presented in [4] and compare with our previous perturbative analysis.

The rest of the paper is organized as follows. In section 2, we present the model in detail. In section 3, we introduce our formalism, study the heat flow and obtain an expression for the conductivity. This expression is derived again by starting from the exact solution of the linear part of the dynamics [4] in section 4. Section 5 is devoted to the concluding remarks. Some mathematical manipulations related to expressions of sections 3 and 4 are presented in the appendix.

2. The model

We consider a crystal chain with harmonic coupling interactions between two different sites and a cosine on-site potential: in the case of nearest-neighbour harmonic interparticle potential (and thermal baths at the boundaries only, details below), we have the Frenkel–Kontorova model, which is commonly used in nonlinear physics [10]. Precisely, we take a scalar field lattice model with N unbounded spin variables and with stochastic Langevin dynamics given by the differential equations

$$\begin{aligned} \mathrm{d}q_j &= p_j\,\mathrm{d}t, && j = 1, 2, \ldots, N, \\ \mathrm{d}p_j &= -\frac{\partial H}{\partial q_j}\,\mathrm{d}t - \zeta_j p_j\,\mathrm{d}t + \gamma_j^{1/2}\,\mathrm{d}B_j, && j = 1, 2, \ldots, N, \end{aligned} \tag{1}$$

where B_j are independent Wiener processes (i.e., $\mathrm{d}B_j/\mathrm{d}t$ are independent white noises); ζ_j is the coupling between the site j and its heat bath; and $\gamma_j = 2\zeta_j T_j$ where T_j is the temperature of the jth thermal reservoir. For the Hamiltonian H we take

$$\begin{aligned} H(q, p) &= \sum_{j=1}^{N}\left[\frac{1}{2}p_j^2 + U^{(1)}(q_j) + \lambda U^{(2)}(q_j) + \frac{1}{2}\sum_{l\neq j} q_j J_{jl} q_l\right], \\ U^{(1)}(q_j) &= Mq_j^2\big/2, \qquad M > 0, \\ \lambda U^{(2)}(q_j) &= \lambda(1 - \cos q_j), \end{aligned} \tag{2}$$

and $J_{jl} = J_{lj}$. Later, we will consider nearest-neighbour interactions, which means a coupling interaction such as (after small adjustments in the $U^{(1)}$ potential)

$$\sum_{j=1}^{N} V(q_j - q_{j-1}), \qquad V(q) = \frac{\omega^2}{2}q^2, \tag{3}$$

and we assume Dirichlet boundary conditions: $q_0 = 0 = q_{N+1}$.

To get the expression for the heat flow, i.e., the energy current in the system, we write the energy of a single spin (oscillator) j as

$$H_j(q, p) = \frac{1}{2}p_j^2 + U(q_j) + \frac{1}{2}\sum_{l\neq j} V(q_j - q_l), \tag{4}$$

where $U(q_j) = U^{(1)}(q_j) + \lambda U^{(2)}(q_j)$ and V follow from (1) above and from $\sum_{j=1}^{N} H_j = H$. We have

$$\left\langle\frac{\mathrm{d}H_j(t)}{\mathrm{d}t}\right\rangle = \langle R_j(t)\rangle - \langle \mathcal{F}_{j\to} - \mathcal{F}_{j\leftarrow}\rangle, \tag{5}$$

where $\langle\cdot\rangle$ means the expectation with respect to the noise distribution. The energy flux between the jth reservoir and the jth site is given by the expression

$$\langle R_j(t)\rangle = \zeta_j\left(T_j - \langle p_j^2\rangle\right), \tag{6}$$

and the heat current inside the chain is given by

$$\mathcal{F}_{j\to} = \sum_{l>j} \nabla V(q_j - q_l)\frac{p_j + p_l}{2}, \qquad \mathcal{F}_{j\leftarrow} = \sum_{l<j} \nabla V(q_l - q_j)\frac{p_j + p_l}{2}. \tag{7}$$

The stationary state, as well known, is characterized by $\langle \mathrm{d}H_j(t)/\mathrm{d}t\rangle = 0$.

To simplify the notation, it is useful to introduce the phase-space vector $\phi = (q, p)$, with $2N$ coordinates. Hence, the equation for the dynamics (1) becomes

$$\begin{aligned} \mathrm{d}\phi_j &= \phi_{j+N}\,\mathrm{d}t, \\ \mathrm{d}\phi_i &= -\mathcal{M}_{i-N,j'}\phi_{j'}\,\mathrm{d}t - \lambda\sin(\phi_{i-N})\,\mathrm{d}t - \zeta_i\phi_i\,\mathrm{d}t + \gamma_i^{1/2}\,\mathrm{d}B_i, \end{aligned} \tag{8}$$

where $\mathcal{M}_{i-N,j} = M\delta_{i-N,j} + J_{i-N,j}$. Above and in what follows, we use the index notation: j for index values in the set $\{1, 2, \ldots, N\}$, i for values in $\{N+1, N+2, \ldots, 2N\}$, and k in $\{1, 2, \ldots, 2N\}$. We also take $\zeta_i = \zeta_{i-N}$, $\gamma_i = \gamma_{i-N}$, and obvious sums over repeated indices will be omitted in future expressions.

In the following section, we will study the dynamics and the heat flow in the steady state (reached as $t \to \infty$) following the approach proposed in previous works [7, 8].

3. The integral formalism and the heat flow

To obtain the integral representation for the correlations (and so, for the heat flow in the steady state), we start with a system without the coupling J among the sites and also without the anharmonic potential. Then, we solve the simple related dynamical problem and, in the following, we introduce the coupling J and the anharmonicity using a well-known tool of theory of stochastic differential equations: the Girsanov theorem [11]. Finally, we investigate the consequences of turning off the interior heat baths.

For clearness, we describe some expressions and procedures already presented in previous papers [7, 8].

The equation of dynamics, for J and $\lambda = 0$, becomes

$$\dot{\phi} = -A^0\phi + \sigma\eta, \tag{9}$$

where A^0 and σ are $2N \times 2N$ matrices given by

$$A^0 = \begin{pmatrix} 0 & -I \\ MI & \Gamma \end{pmatrix}, \qquad \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2\Gamma\mathcal{T}} \end{pmatrix}, \tag{10}$$

I, Γ and $\mathcal{T}$ are diagonal $N \times N$ matrices: $I_{jl} = \delta_{jl}$, $\Gamma_{jl} = \zeta_j\delta_{jl}$, $\mathcal{T}_{jl} = T_j\delta_{jl}$; η are independent white noises. The solution of the linear equation (9) above is the Ornstein–Uhlenbeck process given by

$$\phi(t) = \mathrm{e}^{-tA^0}\phi(0) + \int_0^t \mathrm{d}s\,\mathrm{e}^{-(t-s)A^0}\sigma\eta(s). \tag{11}$$

For simplicity we will take $\phi(0) = 0$. This Gaussian process has the covariance

$$\begin{aligned} \mathcal{C}(t,s) &\equiv \langle\phi(t)\phi(s)\rangle = \begin{cases} \mathrm{e}^{-(t-s)A^0}\,\mathcal{C}(s,s) & \text{if } t \geqslant s, \\ \mathcal{C}(t,t)\,\mathrm{e}^{-(s-t)A^{0T}} & \text{if } t \leqslant s, \end{cases} \\ \mathcal{C}(t,t) &= \int_0^t \mathrm{d}s\,\mathrm{e}^{-sA^0}\sigma^2\,\mathrm{e}^{-sA^{0T}}. \end{aligned} \tag{12}$$

We still have the following useful expression (obtained by, e.g., diagonalizing A^0) for a single site $\phi_j = (q_j, p_j)$

$$\exp(-tA^0) = \mathrm{e}^{(-t\zeta_j/2)}\cosh(t\rho_j)\left\{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{\tanh(t\rho_j)}{\rho_j}\begin{pmatrix} \zeta_j/2 & 1 \\ -M & -\zeta_j/2 \end{pmatrix}\right\}, \tag{13}$$

the expressions for ϕ involving $2N \times 2N$ matrices follow immediately. Above, we have $\rho_j \equiv [(\zeta_j/2)^2 - M]^{1/2}$, with ζ_j, $M > 0$ and ρ_j is real or pure imaginary, depending on ζ_j and

M. Anyway, there is no problem with the time evolution: as $t \to \infty$ there is a convergence to the equilibrium steady distribution that is Gaussian, with mean zero and covariance

$$C = \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-sA^0}\, \sigma^2\, \mathrm{e}^{-s(A^0)^T} = \begin{pmatrix} \frac{\mathcal{T}}{M} & 0 \\ 0 & \mathcal{T} \end{pmatrix}. \tag{14}$$

As each isolated site is connected to a unique thermal reservoir, in the limit of $t \to \infty$, it is governed by a Boltzmann distribution at temperature T_j.

Now we introduce the interparticle interaction and the anharmonic potential by using the Girsanov theorem. This theorem gives a measure ρ for the complete process (8) in terms of the measure μ_C obtained for the process with J and $\lambda = 0$. For example, the two-point correlation function for the complete process can be written as

$$\langle \varphi_u(t_1)\varphi_v(t_2)\rangle = \int \phi_u(t_1)\phi_v(t_2)Z(t)\,\mathrm{d}\mu_C, \qquad t_1, t_2 < t, \tag{15}$$

where φ is the solution for the complete process and ϕ is the solution (11) for the related harmonic and decoupled process (9). And the 'corrective' factor is

$$\begin{aligned} Z(t) &= \exp\left(\int_0^t u\cdot \mathrm{d}B - \frac{1}{2}\int_0^t u^2\,\mathrm{d}s\right), \\ \gamma_i^{1/2}u_i &= -J_{i-N,j}\phi_j - \lambda V'(\phi)_i, \end{aligned} \tag{16}$$

with $\lambda V'(\phi)_i \equiv \lambda \sin(\phi_{i-N})$; the inner products above are in $\mathbb{R}^{2N}$. Mathematical manipulations and details are given in appendix A.

For the particular case of J involving only nearest-neighbour interactions, we have

$$\mathcal{F}_{j\to j+1} = \frac{(J_{j,j+1})^2}{M}\frac{T_{j+1}-T_j}{\zeta_{j+1}+\zeta_j}. \tag{17}$$

And so, as in the steady state we have $\langle \mathrm{d}H_j/\mathrm{d}t\rangle = 0$ (together with $\langle R_j\rangle = 0$ for the inner sites), it follows that

$$\mathcal{F}_\to \equiv \mathcal{F}_{1\to 2} = \mathcal{F}_{2\to 3} = \cdots = \mathcal{F}_{N-1\to N}. \tag{18}$$

With the notation $J_j \equiv J_{j,j+1}$, from (18) above we have

$$\begin{aligned} \mathcal{F}_\to = \frac{J_1^2(T_2-T_1)}{M(\zeta_1+\zeta_2)} &= \frac{J_2^2(T_3-T_2)}{M(\zeta_2+\zeta_3)} \\ &= \frac{J_3^2(T_4-T_3)}{M(\zeta_3+\zeta_4)} \\ &= \cdots \\ &= \frac{J_{N-1}^2(T_N-T_{N-1})}{M(\zeta_{N-1}+\zeta_N)}. \end{aligned} \tag{19}$$

Hence we get, for simplicity assuming that $J_1^2 = J_2^2 = \cdots = J_{N-1}^2 \equiv J^2$, summing up $\mathcal{F}_{1\to 2} + \mathcal{F}_{2\to 3} + \cdots + \mathcal{F}_{N-1\to N}$,

$$\mathcal{F}_\to = \frac{J^2}{M(\zeta_1 + 2\zeta_2 + 2\zeta_3 + \cdots + 2\zeta_{N-1} + \zeta_N)}(T_N - T_1). \tag{20}$$

That is, for the particular case of uniform coupling with the heat bath $\zeta_j = \zeta$, Fourier's law holds

$$\mathcal{F}_\to = \chi\frac{T_N - T_1}{N-1}, \qquad \chi = \frac{J^2}{2\zeta M}. \tag{21}$$

But if we make smaller and smaller the coupling with the inner baths, the flux $\mathcal{F}_{\rightarrow}$ goes to

$$\mathcal{F}_{\rightarrow} \rightarrow \frac{J^2}{(\zeta_1 + \zeta_N)M}(T_N - T_1), \tag{22}$$

i.e., the heat flow becomes proportional to the temperature difference instead of to the temperature gradient, and so, Fourier's law no longer holds. Precisely, up to first order in λ, our result indicates a ballistic behaviour for the system, as it happens in the harmonic chain.

4. Using the exact solution of the harmonic part

Our approach allows us, in a perturbative analysis, to obtain analytical expressions for the thermal conductivity, heat flow, etc, and it is valid for quite general interactions. However, one may pose the question of the reliability of the perturbative computations for the interparticle interaction. There is no rigorous results about the conductivity coefficient, etc, on anharmonic systems to compare with our expressions. However, there is a recent rigorous work on harmonic chains with thermal reservoirs at each site [4]. Thus, for a comparison, in this section we derive the expression for the heat conductivity by starting from the exact solution [4] for the linear system and introducing, in the following, the nonlinear terms via Girsanov theorem.

The results of [4] follow for the specific nearest-neighbour interaction

$$J_{lj} = -\omega^2 \Delta_{lj}, \qquad l, j \in \{1, 2, \ldots, N\}, \tag{23}$$

where Δ is the lattice Laplacian (with Dirichlet boundary condition)

$$\Delta_{lj} = -2\delta_{lj} + \delta_{l-1,j} + \delta_{l+1,j}. \tag{24}$$

Now we consider such restriction and also that $\zeta_1 = \cdots = \zeta_j = \cdots \equiv \zeta$. We also take $\omega^2 = \mathcal{O}(\lambda)$.

The equation for the linear dynamics becomes now

$$\dot{\phi} = -A\phi + \sigma\eta, \qquad A = \begin{pmatrix} 0 & -I \\ MI + J & \Gamma \end{pmatrix}, \tag{25}$$

where σ, η and Γ are as previously defined (9) and (10). Then, the solution is given by the Ornstein–Uhlenbeck process, as in the previous section, with the replacement of A^0 by A, i.e., of MI by $MI - \omega^2\Delta$. As computed in section 2 and appendix B of [4], the covariance of the steady distribution is

$$\lim_{t\to\infty} C(t,t) = \int_0^\infty \mathrm{d}s\, \mathrm{e}^{-sA}\, \sigma^2\, \mathrm{e}^{-sA^T} = \begin{pmatrix} U & Z \\ Z^T & V \end{pmatrix}, \tag{26}$$

where any $N \times N$ block of the covariance matrix above (U, V and Z) can be obtained by a linear transformation of the form

$$B_{jj'} = \sum_{r=1}^{N} B_{jj'}^{(r)} T_r, \tag{27}$$

T_r is the temperature of the rth bath, and

$$
\begin{aligned}
B^{(r)}_{jj'} &= \sum_{j_1,j_2=1}^{N} F_{j,j_1} F_{j',j_2} f^{(B)}(c_{j_1}, c_{j_2}) F_{r,j_1} F_{r,j_2},\\
F_{j,j'} &= \sqrt{\frac{2}{N+1}} \sin\left(\frac{\pi j j'}{N+1}\right),\\
c_j &= \cos\left(\frac{\pi j}{N+1}\right),\\
f^{(U)}(x,y) &= \frac{\zeta^2}{\omega^4}\frac{1}{G(x,y)},\\
f^{(V)}(x,y) &= 1 - \frac{(x-y)^2}{G(x,y)},\\
f^{(Z)}(x,y) &= \frac{\zeta}{\omega^2}\frac{y-x}{G(x,y)},\\
G(x,y) &= (x-y)^2 + \frac{\zeta^2}{\omega^2}\left(\frac{M}{\omega^2} + 2 - x - y\right),
\end{aligned}
\tag{28}
$$

where F is the matrix which diagonalizes the lattice Laplacian Δ, and F has the properties: $F = F^T = F^{-1}$.

Then, as previously planned out, we introduce the nonlinear terms in the dynamics via the Girsanov theorem. We obtain (following the steps of section 3)

$$
\begin{aligned}
\langle \varphi_u(t_1)\varphi_v(t_2)\rangle &= \int \phi_u(t_1)\phi_v(t_2) Z(t)\, \mathrm{d}\mu_C(\phi), \qquad t_1, t_2 < t,\\
Z(t) &= \exp\left[-F_\lambda(\phi(t)) + F_\lambda(\phi(0)) - \int_0^t W_\lambda(\phi(s))\,\mathrm{d}s\right],
\end{aligned}
\tag{29}
$$

with F_λ given by (A.2) and W_λ by (A.4) after the replacement $A^0 \leftrightarrow A$. In order to compare the results coming from the expression above with those described in the previous section, we carry out the computation of the Gaussian integrals up to first order in λ and ω^2 (which means first order in J). Note that $Z(t)$ is the exponential of a term of order λ, and so, in the computation of the parts involving such $Z(t)$ terms, the measure covariance shall contribute only with its part involving A^0 (recall that $A = A^0 - \omega^2\Delta$), otherwise we get terms of order $\lambda\omega^2$. Hence, we have

$$
\lim_{t\to\infty} \langle \varphi_u(t)\varphi_v(t)\rangle = Z_{u-N,v} + T^{(1)}_\lambda + T^{(2)}_\lambda + T^{(3)}_\lambda, \tag{30}
$$

where $Z_{u-N,v}$ comes from the Z block of covariance C (26)–(28), and $T^{(n)}_\lambda$ (with $n = 1, 2, 3$) are given by (A.7). The computation of the covariance term above is presented in appendix B.

For the heat flow we obtain (see appendix B)

$$
\mathcal{F}_{v\to v+1} = \frac{\omega^4}{2\zeta M'}(T_{v+1} - T_v), \tag{31}
$$

that is, exactly the same result of section 3 (see expression (17)), with $\zeta_{j+1} = \zeta_j = \zeta$, M replaced by M' and J by ω^2.

5. Concluding remarks

The understanding of heat conduction (in particular, the validity of Fourier's Law) in one-dimensional lattices is, say, a classical problem of nonequilibrium statistical physics. Many works (computer simulations in the great majority) are dedicated to this problem, with several conflicting results. We recall one of these disagreements: in [12] the authors claim that any one-dimensional momentum conserving system has anomalous conductivity, but in [13, 14] a momentum conserving model with normal conductivity is described. As pointed out in [15], in many cases the computational difficulties are not just a result of weak computer or ineffective procedures: it has become clear that the complete solution of the heat conduction problem requires the development of new analytical methods of modelling.

The present paper considers the development of an approach which leads to an analytic expression for the heat conductivity. We study a system related to a particular model of physical interest (namely, the Frenkel–Kontorova model). We show that, for a weak anharmonicity, if we keep the thermal reservoir at the boundaries only, Fourier's law does not hold at any temperature. For a comparison between the effects of the on-site and the coupling potentials, we recall that our model has a harmonic coupling and a cosine on-site potential, and that in the opposite case, i.e., cosine coupling and harmonic on-site potential, there is a phase transition (Fourier–non-Fourier at high–low temperatures, respectively) as described in [8]. It is worth recalling that our result is in agreement with computer simulations: in [9]—see figure 7 and note that $g \approx 1/\lambda$—for small λ (large g), the numerical simulations indicate a divergent conductivity for all temperatures, i.e. Fourier's law does not hold in this case.

In relation to this contrast between, say, Fourier behaviour for the chain with harmonic on-site potential and cosine interparticle interaction (as claimed in [8] for high temperature) and non-Fourier behaviour for the system with harmonic coupling and cosine on-site potential, we recall that such a contrast appears also in the comparison between the rotor model, with cosine coupling (without the on-site potential), and the Frenkel–Kontorova model with small anharmonicity. A definite interpretation of such a phenomenon is still unknown. In fact, some authors [16] claim that it is still necessary to understand even the Fourier behaviour for the rotor model (a chain with a translational invariant interaction). It shows how intricate are the microscopic mechanisms behind Fourier's law.

To show the reliability of our treatment involving a perturbative expansion in the coupling J, we study the heat flow by starting also from the exact solution of the linear part of the dynamics, and we obtain the same result as our previous treatment. And in favour of the perturbative computation in λ (i.e., in the anharmonicity), we recall some previous works on nonconservative stochastic Langevin systems with heat baths at the same temperature: a problem involving related dynamical stochastic equations and with similar integral representations for the correlations functions . The four-point function is rigorously studied in [17], and there we show that the complete treatment adds only small corrections to the first-order perturbative analysis [18], in the case of low temperatures and weak coupling interactions. Moreover, there the perturbative potential involves, say, a 'hard' anharmonicity, i.e., the potential is a polynomial (unbounded) expression; here, in the present paper we have a 'soft' (bounded) anharmonic perturbation. For high temperatures, a cluster expansion developed in [19] supports the perturbative treatment described in [20].

Finally, we emphasize that our analytical approach is quite general and that we expect to use it in the study of more intrincate problems, e.g., a system with strong anharmonicity.

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Appendix A

We describe here some mathematical manipulations related to the two-point correlation function of section 3.

The first term in $Z(t)$ (A.3) may be rewritten as

$$\begin{aligned} u_i\,\mathrm{d}B_i &= \gamma_i^{-1/2} u_i \gamma_i^{1/2}\,\mathrm{d}B_i \\ &= \gamma_i^{-1/2} u_i \left(\mathrm{d}\phi_i + A^0_{i,k}\phi_k\,\mathrm{d}t\right) \\ &= -\gamma_i^{-1}[J_{i-N,j}\phi_j + \lambda\sin(\phi_{i-N})]\left(\mathrm{d}\phi_i + A^0_{i,k}\phi_k\,\mathrm{d}t\right). \end{aligned} \tag{A.1}$$

For the terms with $\mathrm{d}\phi_i$, the Itô formula gives

$$\begin{aligned} &-\gamma_i^{-1} J_{i-N,j}\phi_j\,\mathrm{d}\phi_i = -\mathrm{d}F_J - \gamma_i^{-1}\phi_i J_{i-N,j} A^0_{jk}\phi_k\,\mathrm{d}t, \\ &F_J(\phi) = \gamma_i^{-1}\phi_i J_{i-N,j}\phi_j, \\ &-\gamma_i^{-1}\lambda\sin(\phi_{i-N})\,\mathrm{d}\phi_i = -\mathrm{d}F_\lambda + \gamma_i^{-1}\phi_i\lambda\cos(\phi_{i-N})\,\mathrm{d}\phi_{i-N}, \\ &F_\lambda(\phi) = \gamma_i^{-1}\lambda\sin(\phi_{i-N})\phi_i. \end{aligned} \tag{A.2}$$

Hence, we have

$$\begin{aligned} Z(t) &= \exp\{-F_\lambda(\phi(t)) - F_J(\phi(t)) + F_\lambda(\phi(0)) + F_J(\phi(0))\} \\ &\quad\times\exp\left\{-\int_0^t W_J(\phi(s))\,\mathrm{d}s - \int_0^t W_\lambda(\phi(s))\,\mathrm{d}s - \int_0^t W_{\lambda J}(\phi(s))\,\mathrm{d}s\right\}, \end{aligned} \tag{A.3}$$

where F_J and F_λ are as previously defined in (A.2), and

$$\begin{aligned} W_J(\phi(s)) &= \gamma_i^{-1}\phi_i(s)J_{i-N,j}A^0_{jk}\phi_k(s) + \phi_k(s)A^{0^T}_{ki}\gamma_i^{-1}J_{i-N,j}\phi_j(s) \\ &\quad + \tfrac{1}{2}\phi_{j'}(s)J^T_{j',i-N}\gamma_i^{-1}J_{i-N,j}\phi_j(s), \\ W_\lambda(\phi(s)) &= \gamma_i^{-1}\phi_i(s)\lambda\cos(\phi_{i-N}(s))A^0_{i-N,k}\phi_k(s) + \gamma_i^{-1}\lambda\sin(\phi_{i-N}(s))A^0_{ik}\phi_k(s) \\ &\quad + \tfrac{1}{2}\gamma_i^{-1}\lambda^2\sin^2(\phi_{i-N}(s)), \\ W_{\lambda J}(\phi(s)) &= \gamma_i^{-1}\lambda\sin(\phi_{i-N}(s))J_{i-N,j}\phi_j(s). \end{aligned} \tag{A.4}$$

In short, we have an integral representation a la Feynman–Kac formula for the correlations.

Turning to the energy flux, from (7) we have

$$\mathcal{F}_{j\to} = \sum_{r>j} J_{j,r}(\varphi_j - \varphi_r)(t)\frac{\varphi_{j+N} + \varphi_{r+N}}{2}, \qquad r\in\{1,2,\ldots,N\}. \tag{A.5}$$

To carry out the computation of $\lim_{t\to\infty}\langle\mathcal{F}_{j\to}\rangle$, we first note that

$$\mathcal{C}(t,s) = \exp(-(t-s)A^0)C + \mathcal{O}(\exp[-(t+s)\zeta/2]), \qquad \text{for}\quad t>s, \tag{A.6}$$

and the effects of the second term on the right-hand side of the equation above vanish as $t\to\infty$. Hence, from (15)–(A.4), for $\langle\varphi_u\varphi_v\rangle \equiv \lim_{t\to\infty}\langle\varphi_u(t)\varphi_v(t)\rangle$, with $u>N, v\leqslant N$, we have, up to first order in λ and J,

$$\langle\varphi_u\varphi_v\rangle = T^{(1)}_\lambda + T^{(2)}_\lambda + T^{(3)}_\lambda + T^{(1)}_J + T^{(2)}_J + T^{(3)}_J, \tag{A.7}$$

$$
\begin{aligned}
T_\lambda^{(1)} &= -\lambda \left\langle \phi_u(t)\phi_v(t)\gamma_i^{-1} \frac{\mathrm{e}^{+\mathrm{i}\phi_{i-N}(t)} - \mathrm{e}^{-\mathrm{i}\phi_{i-N}(t)}}{2\mathrm{i}} \phi_i(t) \right\rangle_0 \\
&= -\lambda \frac{T_v}{2M\zeta_v} \exp\left(-\frac{1}{2}\frac{T_v}{M}\right) \delta_{u-N,v}, \\
T_\lambda^{(2)} &= -\lambda \int_0^t \mathrm{d}s \left\langle \phi_u(t)\phi_v(t)\gamma_i^{-1}\phi_i(s) \frac{\mathrm{e}^{+\mathrm{i}\phi_{i-N}(s)} + \mathrm{e}^{-\mathrm{i}\phi_{i-N}(s)}}{2} A^0_{i-N,k}\phi_k(s) \right\rangle_0 \\
&= \lambda \frac{T_v^2}{4M^2\zeta_v} \exp\left(-\frac{1}{2}\frac{T_v}{M}\right) \delta_{u-N,v}, \\
T_\lambda^{(3)} &= -\lambda \int_0^t \mathrm{d}s \left\langle \phi_u(t)\phi_v(t)\gamma_i^{-1} \frac{\mathrm{e}^{+\mathrm{i}\phi_{i-N}(s)} - \mathrm{e}^{-\mathrm{i}\phi_{i-N}(s)}}{2\mathrm{i}} A^0_{i,k}\phi_k(s) \right\rangle_0 \\
&= \lambda \frac{T_v}{2M\zeta_v} \exp\left(-\frac{1}{2}\frac{T_v}{M}\right) \delta_{u-N,v} - \lambda \frac{T_v^2}{4M^2\zeta_v} \exp\left(-\frac{1}{2}\frac{T_v}{M}\right) \delta_{u-N,v}, \\
T_J^{(1)} &= -\left\langle \phi_u(t)\phi_v(t)\gamma_i^{-1}\phi_i(t) J_{i-N,j}\phi_j(t) \right\rangle_0 = -\frac{J_{u-N,v}T_v}{2M\zeta_{u-N}}, \\
T_J^{(2)} &= -\int_0^t \mathrm{d}s \left\langle \phi_u(t)\phi_v(t)\gamma_i^{-1}\phi_i(s) J_{i-N,j} A^0_{jk}\phi_k(s) \right\rangle_0 = 0, \\
T_J^{(3)} &= -\int_0^t \mathrm{d}s \left\langle \phi_u(t)\phi_v(t)\gamma_i^{-1} J_{i-N,j}\phi_j(s) A^0_{ik}\phi_k(s) \right\rangle_0 \\
&= \frac{J_{v,u-N}T_{u-N}}{M(\zeta_{u-N}+\zeta_v)} + \frac{J_{u-N,v}T_v\zeta_v}{2M\zeta_{u-N}(\zeta_{u-N}+\zeta_v)} - \frac{J_{u-N,v}T_v}{2M(\zeta_{u-N}+\zeta_v)}.
\end{aligned}
$$

Note that $T_\lambda^{(1)} + T_\lambda^{(2)} + T_\lambda^{(3)} = 0$, i.e., up to first order in λ, the anharmonic potential does not change the heat flow; the notation $\langle\cdot\rangle_0$ above means the average for the process with J and $\lambda = 0$. The expressions involve several, but straightforward, Gaussian integrations.

Appendix B

Let us analyse the covariance term in (30), section 4.

With the notation $M' \equiv M + 2\omega^2$, where $\omega^2 \ll M$, we have

$$
\begin{aligned}
Z^{(r)}_{jj'} &= \sum_{j_1,j_2=1}^{N} F_{j,j_1}F_{j',j_2} f^{(Z)}(c_{j_1}, c_{j_2}) F_{r,j_1}F_{r,j_2} \\
&\approx \frac{\omega^2}{\zeta M'} \sum_{j_1,j_2=1}^{N} F_{j,j_1}F_{j',j_2}(c_{j_1} - c_{j_2}) F_{r,j_1}F_{r,j_2}.
\end{aligned}
\tag{B.1}
$$

And to analyse each c_j term, we use the notation $\nu \equiv \exp[\mathrm{i}\pi/(N+1)]$. Hence, we can rewrite the matrix F as

$$
F_{j,j'} = \sqrt{\frac{2}{N+1}} \sin\left(\frac{\pi j j'}{N+1}\right) = \sqrt{\frac{2}{N+1}} \frac{\nu^{+jj'} - \nu^{-jj'}}{2\mathrm{i}}.
\tag{B.2}
$$

We have

$$
\begin{aligned}
\sum_{j_1,j_2=1}^{N} F_{j,j_1}F_{j',j_2}c_{j_1}F_{r,j_1}F_{r,j_2} &= \delta_{j',r}\sum_{j_1=1}^{N} F_{j,j_1}c_{j_1}F_{r,j_1} \\
&= \delta_{j',r}\sum_{j_1=1}^{N} \sqrt{\frac{2}{N+1}} \frac{\nu^{+jj_1} - \nu^{-jj_1}}{2\mathrm{i}} \cdot \frac{\nu^{+j_1} + \nu^{-j_1}}{2} \cdot \sqrt{\frac{2}{N+1}} \frac{\nu^{+rj_1} - \nu^{-rj_1}}{2\mathrm{i}}
\end{aligned}
$$

$$= -\delta_{j',r}\frac{1}{8}\frac{2}{N+1}\sum_{j_1=1}^{N}(\nu^{(1+j+j')j_1} + \nu^{(-1+j+j')j_1} - \nu^{(1-j+j')j_1} - \nu^{(-1-j+j')j_1}$$
$$- \nu^{(1+j-j')j_1} - \nu^{(-1+j-j')j_1} + \nu^{(1-j-j')j_1} + \nu^{(-1-j-j')j_1}). \tag{B.3}$$

Denoting by $R_\alpha, \alpha = 1, 2, \ldots, 8$ each term of the sum above, we have (note that $1 + j + j'$, $-1 + j + j', 1 - j - j', -1 - j - j' \neq 0$)

$$R_1 + R_2 + R_7 + R_8 = 2[-1 + (-1)^{j+j'}],$$
$$R_3 + R_4 + R_5 + R_6 = 2N\delta_{j,j'+1} + 2N\delta_{j+1,j'} + [-1 + (-1)^{j+j'}](1 - \delta_{j,j'+1}) + [-1 + (-1)^{j+j'}](1 - \delta_{j+1,j'}), \tag{B.4}$$

where we have used the identity

$$\sum_{j_1=1}^{N} \nu^{lj_1} = \begin{cases} N & \text{for } l = 0, \\ \dfrac{\nu^l - (-1)^l}{1 - \nu^l} & \text{for } l \neq 0. \end{cases} \tag{B.5}$$

Thus, we get

$$\sum_{j_1,j_2=1}^{N} F_{j,j_1}F_{j',j_2}c_{j_1}F_{r,j_1}F_{r,j_2} = \delta_{j',r}\begin{cases} \dfrac{1}{2} & \text{for } j = j'+1 \text{ or } j' = j+1, \\ 0 & \text{otherwise,} \end{cases} \tag{B.6}$$

and an analogous expression for the sum involving c_{j_2}. Finally, we obtain

$$Z_{j,j'} = \sum_{r=1}^{N} Z_{j,j'}^{(r)}T_r$$
$$= \frac{\omega^2}{\zeta M'}\sum_{r=1}^{N}\left[\frac{1}{2}\delta_{j',r}(\delta_{j,j'+1} + \delta_{j+1,j'})T_r - \frac{1}{2}\delta_{j,r}(\delta_{j,j'+1} + \delta_{j+1,j'})T_r\right]. \tag{B.7}$$

Hence, as the $T_\lambda^{(n)}$ sum vanishes, for the heat flow we have

$$\mathcal{F}_{\upsilon\to\upsilon+1} = -\frac{\omega^2}{2}\langle\varphi_\upsilon\varphi_{(\upsilon+1)+N}\rangle + \frac{\omega^2}{2}\langle\varphi_{\upsilon+1}\varphi_{\upsilon+N}\rangle$$
$$= -\frac{\omega^4}{2\zeta M'}\left(\frac{1}{2}T_\upsilon - \frac{1}{2}T_{\upsilon+1}\right) + \frac{\omega^4}{2\zeta M'}\left(\frac{1}{2}T_{\upsilon+1} - \frac{1}{2}T_\upsilon\right), \tag{B.8}$$
$$\mathcal{F}_{\upsilon\to\upsilon+1} = \frac{\omega^4}{2\zeta M'}(T_{\upsilon+1} - T_\upsilon).$$

References

[1] Lepri S, Livi S and Politi A 2003 *Phys. Rep.* **377** 1–80
[2] Bonetto F, Lebowitz J L and Rey-Bellet L 2000 *Fourier's Law: A Challenge to Theorists, Mathematical Physics 2000* (London: Imperial College Press) pp 128–50
[3] Rieder Z, Lebowitz J L and Lieb E 1967 *J. Math. Phys.* **8** 1073–78
[4] Bonetto F, Lebowitz J L and Lukkarinen J 2004 *J. Stat. Phys.* **116** 783–813
[5] Eckmann J P, Pillet C A and Rey-Bellet L 1999 *Commun. Math. Phys.* **201** 657–97
[6] Eckmann J P, Pillet C A and Rey-Bellet L 1999 *J. Stat. Phys.* **95** 305–31
[7] Pereira E and Falcao R 2004 *Phys. Rev.* E **70** 46105
[8] Pereira E and Falcao R 2006 *Phys. Rev. Lett.* **96** 100601
[9] Savin A V and Gendelman O V 2003 *Phys. Rev.* E **67** 041205
[10] Braun O M and Kivshar Y S 1998 *Phys. Rep.* **306** 1–108

[11] Øksendal B 2003 *Stochastic Differential Equations: An Introdution with Applications* 6th edn (Berlin: Springer)
[12] Prosen T and Campbell D K 2000 *Phys. Rev. Lett.* **84** 2857–60
[13] Gendelman O V and Savin A V 2000 *Phys. Rev. Lett.* **84** 2381–84
[14] Giardiná C, Livi R, Politi A and Vassalli M 2000 *Phys. Rev. Lett.* **84** 2144–47
[15] Gendelman O V and Savin A V 2004 *Phys. Rev. Lett.* **92** 074301
[16] Baowen L, Casati G, Wang J and Prosen T 2004 *Phys. Rev. Lett.* **92** 254301
[17] Faria da Veiga P A, O'Carroll M, Schor R and Pereira E 2001 *Commun. Math. Phys.* **220** 377–402
[18] Schor R, Barata J C A, Faria de Veiga P A and Pereira E 1999 *Phys. Rev.* E **59** 2689–94
[19] Thebaldi R S, Pereira E and Procacci A 2005 *J. Math. Phys.* **46** 053302
[20] Pereira E 2002 *Phys. Rev.* E **65** 056605