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A stochastic model of anomalous heat transport: analytical solution of the steady state

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Abstract

We consider a one-dimensional harmonic crystal with conservative noise, in contact with two stochastic Langevin heat baths at different temperatures. The noise term consists of collisions between neighbouring oscillators that exchange their momenta, with a rate γ. The stationary equations for the covariance matrix are exactly solved in the thermodynamic limit ($N \to \infty$). In particular, we derive an analytical expression for the temperature profile, which turns out to be independent of γ. Moreover, we obtain an exact expression for the leading term of the energy current, which scales as $1/\sqrt{\gamma N}$. Our theoretical results are finally found to be consistent with the numerical solutions of the covariance matrix for finite N.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Understanding the statistical properties of open, many-particles systems is one of the challenges of nonequilibrium statistical mechanics. From a fundamental point of view, a successful approach would require finding, and possibly computing explicitly, a statistical measure for (at least) systems steadily kept out of equilibrium. Some insight has been gained over the years mostly thanks to the analysis of specific models (for a recent account, see e.g. [1] and references therein). A related open problem is the derivation of phenomenological transport laws from the microscopic dynamics, without any *ad hoc* statistical assumption. An example is the famous law, postulated by Joseph Fourier almost 200 years ago, relating the heat flux J flowing within a solid material to the local temperature gradient,

$$J = -\kappa \nabla T, \tag{1}$$

where the constant of proportionality, κ, is the thermal conductivity.

In the lack of a general framework, simple models are precious to attack such difficult problems [2, 3]. An instance, dating back to 1967, was provided by Rieder, Lebowitz and Lieb who considered heat conduction in a chain of harmonic oscillators connected at its boundaries to two stochastic heat baths [4]. They showed that the invariant measure in phase space (i.e. the stationary solution of the associated Fokker–Planck equation) is a multivariate Gaussian. Furthermore, they proved that, due to the integrability of the underlying dynamics, such a model is not able to support a temperature gradient. However, this is one of the very few systems that have been rigorously solved. Extensions of this model, where anharmonicities are introduced by means of self-consistent local thermostats, were extensively studied [5–7]. In recent years, further attempts to derive Fourier's law in deterministic systems have been reported [8–11].

As a complementary approach, stochastic models have played an important role in understanding how energy is microscopically transported. This is mainly due to the fact that the stochastic approach seems to easily yield results that would require much more efforts by adopting the dynamical approach. In fact, while stochastic models are assumed to be a reduced (mesoscopic) representation of the 'chaotic' microscopic dynamics, they are free from the intricacies of the fractal structures arising in deterministic dynamics. Actually, the leap from such a class of models to even the simplest deterministic, nonlinear ones is still a challenge for the theory [3]. At the simplest level of modeling, energy is assumed to be randomly exchanged between neighbouring sites of a lattice [12–15]. This class of systems has the invaluable advantage of allowing for a mathematically rigorous treatment, which is usually unfeasible in the deterministic case. Recently, systems of harmonic oscillators exchanging energy with 'conservative' noise have been proven to admit a unique stationary state consistent with (1) [16]. However, if the additional constraint that the random process conserves also the linear momentum is imposed, the equilibrium energy–current correlation function decays as $t^{-d/2}$ (d being the lattice dimension) and transport becomes anomalous in $d \leqslant 2$ [17]. This means that (1) breaks down as κ diverges with the system size. The results of [17] thus provide a rigorous basis to the numerical evidence of anomalous transport and diffusion in deterministic nonlinear models with momentum conservation [2], with the only exception of the coupled rotor chain [18, 19].

In this paper, we consider the problem of heat conduction in a chain of harmonic oscillators, coupled at its boundaries with two stochastic heat baths. In addition to the deterministic bulk dynamics, we consider a noise dynamical term, consisting of collisions occurring at a given rate γ, which exchange the momenta of a randomly chosen pair of neighbour oscillators. The stochastic contribution to the dynamics maintains the linearity of the associated Fokker–Planck equation.

Recently, following a principal component analysis, we have numerically found that, in the basis identified by the eigenvectors of the covariance matrix, the nonequilibrium invariant measure of this model can effectively be expressed as the product of independent distributions aligned along collective modes that are spatially localized with power-law tails [20]. Moreover, several variables, such as the amplitudes of these modes, turn out to be Gaussian distributed. Accordingly, it appears that the unavoidable deviations from Gaussian behaviour are confined to not-so-relevant observables, so that the nonequilibrium invariant measure can effectively be considered to be a multivariate Gaussian. Within this approximation, the covariance matrix provides a complete description of the corresponding invariant measure. Here, with the help of a suitable continuum limit, we derive leading order expressions for the covariance matrix in the steady nonequilibrium state, from which explicit formulae for the temperature profile and the energy current are obtained. It should be noted that this is the first example of an analytic

expression for the temperature profile in a system characterized by anomalous heat transport (i.e. diverging conductivity).

This paper is organized as follows. In section 2, we introduce the stochastic model. In section 3, we define the covariance matrix **C** and write the coupled equations governing the evolution of **C** towards its stationary value. The key results of the paper are also summarized there. Section 4 contains the details of the analytical calculation of the stationary covariance matrix in the thermodynamic limit $N \to \infty$. Our approach is based on a suitable continuum approximation, in which the finite-difference equations for the entries of **C** are replaced by partial differential equations for the corresponding field-like variables. We obtain the covariance matrix to leading order in the smallness parameter $\varepsilon = 1/\sqrt{N}$. In section 5, we discuss the physical meaning of the analytic expressions, compare them with the numerical solution for finite size chains and briefly comment on the open problems.

2. Stochastic model

We consider a homogeneous harmonic chain of N oscillators of unit mass and frequency ω, in contact with two different stochastic Langevin heat baths under its extrema and fixed boundary conditions. The dynamics in the bulk of the chain is governed by the Hamiltonian

$$H(\vec{q}, \vec{p}, t) = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + \frac{\omega^2}{2} (q_{i+1} - q_i)^2 \right]. \tag{2}$$

Furthermore, the 1st and Nth oscillators are coupled to Langevin heat baths at temperatures $T_\pm = T \pm \Delta T/2$ respectively (T is the average temperature $(T_+ + T_-)/2$). Then the equations of motion become

$$\begin{aligned} \dot{q}_n &= p_n \\ \dot{p}_n &= \omega^2(q_{n+1} - 2q_n + q_{n-1}) + \delta_{n,1}(\xi_+ - \lambda \dot{q}_1) + \delta_{n,N}(\xi_- - \lambda \dot{q}_N), \end{aligned} \tag{3}$$

where ξ_- and ξ_+ are independent Wiener processes with zero mean and variance $2\lambda k_B T_-$ and $2\lambda k_B T_+$ respectively. The fixed boundary conditions are enforced by setting $q_0 = q_{N+1} = 0$. In addition, the chain undergoes random binary collisions, at a rate γ, in which the momenta of a couple of neighbouring oscillators are exchanged. Thus, the resulting dynamics conserves both total momentum and energy.

The phase-space probability density $P(\vec{q}, \vec{p}, t)$ of this model is a solution of the Fokker–Planck equation

$$\frac{\partial P}{\partial t} = (\mathcal{L}_0 + \mathcal{L}_{\text{coll}}) P. \tag{4}$$

The first term describing the evolution of the system, as defined by (3), can be written as

$$\mathcal{L}_0 P = \sum_{i,j} \left(\mathbf{A}_{ij} \frac{\partial x_j P}{\partial x_i} + \frac{\mathbf{D}_{ij}}{2} \frac{\partial^2 P}{\partial x_i \partial x_j} \right), \tag{5}$$

where the $2N$ vector $\mathbf{x} = (q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N)$, and the $2N \times 2N$ matrices **A** and **D** are

$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & -\mathbf{1} \\ \omega^2 \mathbf{G} & \lambda \mathbf{R} \end{pmatrix}, \qquad \mathbf{D} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 2\lambda k_B T (\mathbf{R} + \eta \mathbf{S}) \end{pmatrix} \tag{6}$$

with **0** and **1** the null and unit $N \times N$ matrices respectively,

$$\mathbf{R}_{ij} = \delta_{i,j}(\delta_{i,1} + \delta_{i,N}), \qquad \mathbf{S}_{ij} = \delta_{i,j}(\delta_{i,1} - \delta_{i,N}), \tag{7}$$

and $\mathbf{G}$ is the negative of the Laplacian,

$$\mathbf{G}_{ij} = 2\delta_{i,j} - \delta_{i+1,j} - \delta_{i,j+1}. \tag{8}$$

Moreover, we introduce the normalized bath temperatures difference $\eta = \Delta T/T = (T_+ - T_-)/T$. Finally, the second term in (4) associated with stochastic collisions reads

$$\mathcal{L}_{\rm coll} P = \gamma \sum_{j=1}^{N-1} [P(\ldots, p_{j+1}, p_j, \ldots) - P(\ldots, p_j, p_{j+1}, \ldots)]. \tag{9}$$

Each term in the sum expresses the probability balance for each elementary process in which momenta of the pair j, $j+1$ are exchanged.

As we mentioned above, this type of dynamics with conservative noise was originally introduced in [17] where, however, only the equilibrium case was studied. Here we consider the nonequilibrium situation. Moreover, the collision term (9) we consider here has two main differences: first, in the present case, only collisions of pairs (instead of triplets) are necessary. Second, in [16], each evolution step is an infinitesimal variation of the momenta onto the constant-energy hypersurface. This allows us to define a generator of the process as a differential operator acting on the $\vec{p}$-space. In contrast, in the present case the process remains intrinsically discontinuous.

3. Covariance matrix

Consider the covariance matrix $\mathbf{C}$ for the dynamics (3), which we write as

$$\mathbf{C} = \begin{pmatrix} \mathbf{U} & \mathbf{Z} \\ \mathbf{Z}^\dagger & \mathbf{V} \end{pmatrix}, \tag{10}$$

where

$$\mathbf{U}_{i,j} = \langle q_i q_j \rangle, \qquad \mathbf{V}_{i,j} = \langle p_i p_j \rangle, \qquad \mathbf{Z}_{i,j} = \langle q_i p_j \rangle \tag{11}$$

are three $N \times N$ matrices, $\langle . \rangle$ denote an average over $P(\vec{q}, \vec{p}, t)$, and $\dagger$ denotes the transpose operation. There is no need to include mean values, since $\langle p_i \rangle = \langle q_i \rangle = 0$. Note that the matrices $\mathbf{U}$ and $\mathbf{V}$ are symmetric by definition. The evolution equation for $\mathbf{C}$ can be written as

$$\dot{\mathbf{C}} = \dot{\mathbf{C}}_0 + \dot{\mathbf{C}}_{\rm coll} \tag{12}$$

where (see, e.g. equation (63) in [2]),

$$\dot{\mathbf{C}}_0 = \mathbf{D} - \mathbf{A}\mathbf{C} - \mathbf{C}\mathbf{A}^\dagger. \tag{13}$$

The collision term $\dot{\mathbf{C}}_{\rm coll}$ is evaluated upon multiplying (9) by $x_i x_j$ and thereby integrating over phase space. We obtain

$$\dot{\mathbf{C}}_{\rm coll} = -\gamma \begin{pmatrix} \mathbf{0} & \mathbf{Z}\mathbf{G} \\ \mathbf{G}\mathbf{Z}^\dagger & \mathbf{W}, \end{pmatrix}, \tag{14}$$

where the auxiliary $N \times N$ matrix $\mathbf{W}$ is defined by

$$\mathbf{W}_{ij} \equiv \begin{cases} \mathbf{V}_{i-1,j-1} + \mathbf{V}_{i+1,j+1} - 2\mathbf{V}_{i,j} & i = j \\ \mathbf{V}_{i-1,j} + \mathbf{V}_{i,j+1} - 2\mathbf{V}_{i,j} & i - j = -1 \\ \mathbf{V}_{i+1,j} + \mathbf{V}_{i,j-1} - 2\mathbf{V}_{i,j} & i - j = 1 \\ \mathbf{V}_{i+1,j} + \mathbf{V}_{i-1,j} + \mathbf{V}_{i,j-1} + \mathbf{V}_{i,j+1} - 4\mathbf{V}_{i,j} & |i - j| > 1. \end{cases} \tag{15}$$

Equation (12) is thus exact and closed and describes the approach to the nonequilibrium steady state. In the present work we aim at finding its stationary solution, which amounts to solving the set of linear equations

$$\mathbf{Z}^{\dagger} = -\mathbf{Z}, \tag{16a}$$

$$\mathbf{V} = \omega^2 \mathbf{U}\mathbf{G} + \lambda \mathbf{Z}\mathbf{R} + \gamma \mathbf{Z}\mathbf{G}, \tag{16b}$$

$$\omega^2(\mathbf{G}\mathbf{Z} + \mathbf{Z}^{\dagger}\mathbf{G}) + \lambda(\mathbf{R}\mathbf{V} + \mathbf{V}\mathbf{R}) + \gamma \mathbf{W} = 2\lambda k_{\mathrm{B}} T(\mathbf{R} + \eta \mathbf{S}). \tag{16c}$$

Note that for $T^{+} = T^{-} = T$, namely $\eta = 0$, these equations admit the equilibrium solution

$$\mathbf{U}_{\mathrm{eq}} = \frac{k_{\mathrm{B}} T}{\omega^2} \mathbf{G}^{-1}, \qquad \mathbf{V}_{\mathrm{eq}} = k_{\mathrm{B}} T \mathbf{1}, \qquad \mathbf{Z}_{\mathrm{eq}} = \mathbf{0}. \tag{17}$$

For $\eta \neq 0$, analogously to what found in purely stochastic models [15, 21], we expect the onset of a nonzero heat flux to be accompanied by the appearance of nondiagonal terms.

In the following section we solve analytically the problem (16*a*)–(16*c*) by means of a suitable continuum approximation. The idea is to replace the finite-difference equations (16*a*)–(16*c*) with a set of partial differential equations. Before entering the technical details, it is useful to briefly anticipate the main outcomes of our calculation. The temperature field $T_i = \langle p_i^2 \rangle$ along the chain, as a function of the scaled variable $y \equiv 2i/N - 1$ can be expressed as

$$T(y) = T + \Delta T \Theta(y), \tag{18}$$

where $\Theta(y)$ is defined through the following series,

$$\Theta(y) = \frac{\sqrt{2}}{(\sqrt{8} - 1)\zeta(3/2)} \sum_{\mathrm{odd}\, n} n^{-3/2} \cos\left(\frac{n\pi}{2}(y+1)\right), \tag{19}$$

where $\zeta(3/2) = 2.612\,375\,348\ldots$ is the Riemann ζ-function. It can be seen that $\Theta(y)$ is an odd function of y such that $\Theta(\pm 1) = \mp 1/2$. The leading term of the stationary energy current (see below for the exact definition) is

$$J = \frac{\mathcal{J}}{\sqrt{N}} = \frac{\Delta T}{8(\sqrt{8} - 1)\zeta(3/2)} \sqrt{\frac{\pi^3 \omega^3}{\gamma N}}. \tag{20}$$

As a consequence, the effective conductivity is

$$\kappa \equiv \frac{J}{\Delta T/N} = \frac{1}{8(\sqrt{8} - 1)\zeta(3/2)} \sqrt{\frac{\pi^3 \omega^3 N}{\gamma}}. \tag{21}$$

Comments on the physical meaning of these formulae will be given in the last section.

4. Analytical solution

The solution of (16*a*)–(16*c*) can be efficiently determined numerically by exploiting the sparsity of the corresponding linear problem, as well as the symmetries of the unknowns **U**, **V** and **Z**. This approach has been followed in [20]. Here, we solve the problem analytically treating the 'lattice' equations in the continuum approximation. It must be first recognized that the correct scaling is not known *a priori*, but rather inferred from the numerical solution. Therefore, the correctness of the results has to be checked *a posteriori* by consistency.

4.1. The continuum limit

The first step consists of mapping the discrete variables i and j into two suitable continuous variables x and y, so that an $N \times N$ matrix $\mathbf{M}_{ij}$ can be transformed into a 'field variable' $\mathbf{M}(x, y)$ and the associated discrete equation turned into a partial differential equation. In

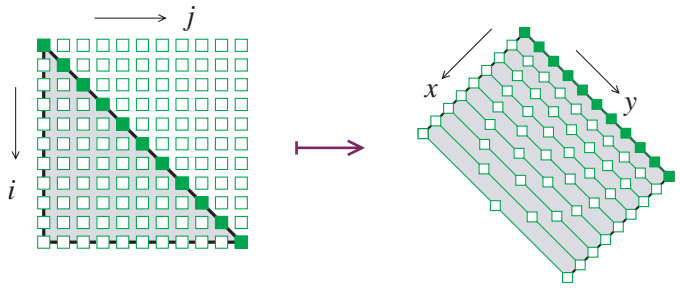

Figure 1. Schematic representation of the mapping from the matrix indices i, j (left) to the continuous variables (x, y) (right). The latter vary in the domain $\mathcal{D}$, definition (23) (shaded region). The square symbols represent matrix elements (bolded along the diagonal, $i = j$). Diagonals are parametrically obtained as $x =$ constant, and antidiagonals as $y =$ constant. The denominator in the definition of y (22) takes into account that the length of the diagonals depends on their value of x so that the domain of y is independent of x.

order to do so, it is first necessary to introduce a smallness parameter that vanishes as $N \to \infty$. In [20], it was found that while neighbouring elements along the diagonal differ by $O(1/N)$, across the diagonal the difference is $O(1/\sqrt{N})$. This suggests defining the smallness parameter as $\varepsilon = 1/\sqrt{N}$. In addition, it is convenient to introduce a further stretching of the longitudinal variable y so as to ensure a constant elongation in the (x, y) representation. This is achieved through the following transformation:

$$x \equiv (i - j)\varepsilon \qquad y \equiv \frac{(i + j)\varepsilon^2 - 1}{1 - |i - j|\varepsilon^2}. \tag{22}$$

that is schematically represented also in figure 1. The nonlinear transformation complicates the expansions along y, but is essential to set the boundary conditions correctly. Although (22) is singular for $|i - j| = N$, this is harmless, since its location diverges to infinity and is thus located outside the region of interest. In the infinite volume limit, the variables (x, y) belong to the domain

$$\mathcal{D} \equiv \{(x, y) | x \in [0, \infty);\ y \in [-1, 1]\}. \tag{23}$$

Note that $x =$ const corresponds to moving along a diagonal direction, $x = 0$ corresponding to the main diagonal.

In order to determine the continuum limit of equations (16*a*)–(16*c*), it is necessary to deal with the infinitesimal changes of x and y that arise from Δi and Δj shifts of i and j. It is convenient to introduce the integer functions $f, s : \mathbb{Z}^2 \mapsto \mathbb{Z}$

$$f(\Delta i, \Delta j) \equiv \Delta i - \Delta j, \qquad s(\Delta i, \Delta j) \equiv \Delta i + \Delta j. \tag{24}$$

With the help of these shift functions, the coordinates of a point shifted by $(\Delta i, \Delta j)$ read

$$x' = x + f\varepsilon; \qquad y' = \frac{(i + j)\varepsilon^2 - 1 + s\varepsilon^2}{1 - (i - j)\varepsilon^2 - f\varepsilon^2} \tag{25}$$

where we assume that $i \geqslant j$ to get rid of the absolute value. Accordingly,

$$y' = \left(y + \frac{\varepsilon^2 s}{1 - \varepsilon x}\right) \frac{1}{1 - \varepsilon^2 f/(1 - \varepsilon x)}, \tag{26}$$

and, up to fourth order in ε,

$$y' = (y + \varepsilon^2 s(1 + \varepsilon x + \varepsilon^2 x^2))(1 + \varepsilon^2 f(1 + \varepsilon x + \varepsilon^2 x^2) + \varepsilon^4 f^2), \tag{27}$$

which is conveniently written as

$$y' = y + \varepsilon^2(1 + \varepsilon x + \varepsilon^2(x^2 + f))(s + fy) \equiv y + \varepsilon^2 R_{f,s}, \tag{28}$$

where

$$R_{f,s} = [1 + \varepsilon x + \varepsilon^2(x^2 + f)](fy + s). \tag{29}$$

With these definitions, an infinitesimal change in x involves terms of $\mathrm{O}(\varepsilon)$ and an infinitesimal change in y generates terms of $\mathrm{O}(\varepsilon^2)$, $\mathrm{O}(\varepsilon^3)$ and $\mathrm{O}(\varepsilon^4)$. However, for the estimate of the leading contributions, it is sufficient to consider $R_{f,s} = (1 + \varepsilon x)\,(fy + s)$.

Altogether, the above relations provide a useful tool for investigating the continuum limit. For later applications, the above results are summarized in the rule

$$\mathbf{M}_{i+\Delta i, j+\Delta j} = \mathbf{M}(x + f\varepsilon,\, y + \varepsilon^2 R_{f,s}) \tag{30}$$

that is written in a convenient form for an expansion in powers of ε. Here and in what follows, we keep the bold-face notation for the continuous functions derived from the matrix variables.

4.2. Field variables

The disadvantage of representation (11) is that $\mathbf{U}_{\mathrm{eq}}$ is a full matrix whose diagonal elements are $\mathrm{O}(N)$. This hinders the formulation of a proper perturbation scheme to compute the nonequilibrium corrections. For the sake of the numerical solution carried out in [20], this difficulty has been overcome by looking at correlators involving relative rather than absolute displacements, i.e., $\mathbf{Z}'_{i,j} = \langle (q_i - q_{i+1}) p_j \rangle$ and $\mathbf{U}'_{i,j} = \langle (q_{i+1} - q_i)(q_{j+1} - q_j) \rangle$. In fact, in this representation, $\mathbf{U}'$ turns out to be diagonal at equilibrium with diagonal elements of $\mathrm{O}(1)$. On the other hand, $\mathbf{Z}'_{i,j}$ loses the antisymmetry of $\mathbf{Z}_{i,j}$, a very useful property for our analytical treatment. Therefore, we have decided to keep the definition of $\mathbf{Z}$ as in (11) while introducing a new matrix $\mathbf{Y}_{i,j} \equiv \omega^2 \langle (q_{i+1} - q_i)(q_{j+1} - q_j) \rangle$, which is conveniently expressed in terms of $\mathbf{U}$ as,

$$\mathbf{Y}_{i,j} \equiv \omega^2 [\mathbf{U}_{i,j} - \mathbf{U}_{i,j+1} - \mathbf{U}_{i+1,j} + \mathbf{U}_{i+1,j+1}]. \tag{31}$$

Note that the diagonal elements are proportional to the average bond potential energy Φ_i,

$$\mathbf{Y}_{i,i} \equiv \omega^2 \langle (q_{i+1} - q_i)^2 \rangle \equiv 2\Phi_i. \tag{32}$$

The next step consists of choosing the proper order of magnitude of the three fields $\mathbf{V}$, $\mathbf{Y}$ and $\mathbf{Z}$. This will be done by exploiting the knowledge of the equilibrium case and the information arising from the previous numerical solution [20]. First, since $\mathbf{Y}_{i,i}$ and $\mathbf{V}_{i,i}$ are proportional to the mean potential and kinetic energy, respectively, they are both of $\mathrm{O}(1)$ as in equilibrium. On the other hand, the off-diagonal elements turn out to be of $\mathrm{O}(\varepsilon)$. Hence, for the consistency of the continuum approximation, we must consider independently diagonal and off-diagonal (bulk) entries of $\mathbf{V}$ and $\mathbf{Y}$. The matrix $\mathbf{Z}$ exhibits somehow complementary behaviour. Since it is antisymmetric in x, there are no diagonal terms,

$$\mathbf{Z}(0, y) = 0, \tag{33}$$

while the numerics suggests that in the bulk it is $\mathrm{O}(1)$. We thus define the following field variables: in the bulk ($i \neq j, x > 0$)

$$\mathbf{Y}_{i,j} = \varepsilon \mathbf{Y}(x, y) + \text{h.o.t.}, \qquad \mathbf{V}_{i,j} = \varepsilon \mathbf{V}(x, y) + \text{h.o.t.}, \qquad \mathbf{Z}_{i,j} = \mathbf{Z}(x, y) + \text{h.o.t.} \tag{34}$$

and for the diagonal ($i = j, x = 0$) terms

$$\mathbf{V}_{i,i} = T(y) + \text{h.o.t.}, \qquad \mathbf{Y}_{i,i} = 2\Phi(y) + \text{h.o.t.}. \tag{35}$$

The scaling properties of the first corrections to the leading order are not known and the comparison with the numerical results discussed in the final section shows the existence of a singular dependence on ε. As a consequence, it is not possible to set up a standard perturbation expansion scheme and it is therefore necessary to rely on expressions dominated by the leading contributions. In the following section we demonstrate that by manipulating equations (16*a*)–(16*c*) and suitable combinations of them, it is possible to obtain a set of partial differential equations whose solution gives the covariance matrices at leading order.

4.3. Stationary equation in the bulk

Using definitions (6), (7) and (8), the equation (16*b*) is written as

$$\omega^2(2\mathbf{U}_{i,j} - \mathbf{U}_{i,j+1} - \mathbf{U}_{i,j-1}) - \mathbf{V}_{i,j} + \gamma(2\mathbf{Z}_{i,j} - \mathbf{Z}_{i,j-1} - \mathbf{Z}_{i,j+1}) = 0. \tag{36}$$

The reader should note that the term $\mathbf{ZR}$ appearing in (16*b*), can be written as

$$\lambda\mathbf{ZR} = \lambda(\mathbf{Z}(-x,-1) + \mathbf{Z}(x,1)). \tag{37}$$

This term only contributes at the boundaries and consequently, we have omitted it in (36). In the subsequent treatment, this omission will be justified later when we fix the boundary conditions of $\mathbf{Z}$.

In order to write the equations in terms of the new variable $\mathbf{Y}$ let us first rewrite (16*b*) with i replaced by $i+1$:

$$\omega^2(2\mathbf{U}_{i+1,j} - \mathbf{U}_{i+1,j+1} - \mathbf{U}_{i+1,j-1}) - \mathbf{V}_{i+1,j} + \gamma(2\mathbf{Z}_{i+1,j} - \mathbf{Z}_{i+1,j-1} - \mathbf{Z}_{i+1,j+1}) = 0. \tag{38}$$

Subtracting (38) from (36), and using the definition of the matrix $\mathbf{Y}$ we obtain

$$\begin{aligned}\mathbf{Y}_{i,j} - \mathbf{Y}_{i,j-1} + \mathbf{V}_{i+1,j} - \mathbf{V}_{i,j} + \gamma[&-2\mathbf{Z}_{i+1,j} + 2\mathbf{Z}_{i,j} \\ &+ \mathbf{Z}_{i+1,j-1} - \mathbf{Z}_{i,j-1} + \mathbf{Z}_{i+1,j+1} - \mathbf{Z}_{i,j+1}] = 0.\end{aligned} \tag{39}$$

With the help of rule (30), the continuous version of (39) in the bulk is readily written as

$$\begin{aligned}\mathbf{Y}(x,y) - \mathbf{Y}(x+\varepsilon, y+\varepsilon^2 R_{1,-1}) + \mathbf{V}(x+\varepsilon, y+\varepsilon^2 R_{1,1}) - \mathbf{V}(x,y) \\ + \gamma[-2\mathbf{Z}(x+\varepsilon, y+\varepsilon^2 R_{1,1}) + 2\mathbf{Z}(x,y) + \mathbf{Z}(x+2\varepsilon, y+\varepsilon^2 R_{2,0}) \\ - \mathbf{Z}(x+\varepsilon, y+\varepsilon^2 R_{1,-1}) + \mathbf{Z}(x, y+\varepsilon^2 R_{0,2}) - \mathbf{Z}(x-\varepsilon, y+\varepsilon^2 R_{-1,1})] = 0.\end{aligned} \tag{40}$$

The leading order of (40) is of $\mathrm{O}(\varepsilon^2)$ and can be written as

$$\mathbf{\Omega}_x(x,y) = 0, \tag{41}$$

where the subscripts denote the partial derivative with respect to the corresponding variable and for reasons that will be clear below, we have introduced the function

$$\mathbf{\Omega}(x,y) \equiv \mathbf{Y}(x,y) - \mathbf{V}(x,y). \tag{42}$$

Furthermore, by exchanging i with j in equation (39) and adding the result to (39), we find a symmetrized equation in the bulk, given by

$$\begin{aligned}2\mathbf{Y}_{i,j} - \mathbf{Y}_{i,j-1} - \mathbf{Y}_{i-1,j} + \mathbf{V}_{i+1,j} + \mathbf{V}_{i,j+1} - 2\mathbf{V}_{i,j} + \gamma[&\mathbf{Z}_{i,j+1} - \mathbf{Z}_{i+1,j} \\ &+ \mathbf{Z}_{i+1,j-1} - \mathbf{Z}_{i-1,j+1} + \mathbf{Z}_{i-1,j} - \mathbf{Z}_{i,j-1}] = 0.\end{aligned} \tag{43}$$

The continuous version of (43) is

$$\begin{aligned}2\mathbf{Y}(x,y) - \mathbf{Y}(x+\varepsilon, y+\varepsilon^2 R_{1,-1}) - \mathbf{Y}(x-\varepsilon, y+\varepsilon^2 R_{-1,-1}) - 2\mathbf{V}(x,y) \\ + \mathbf{V}(x+\varepsilon, y+\varepsilon^2 R_{1,1}) + \mathbf{V}(x-\varepsilon, y+\varepsilon^2 R_{-1,1}) + \gamma[\mathbf{Z}(x-\varepsilon, y+\varepsilon^2 R_{-1,1}) \\ - \mathbf{Z}(x+\varepsilon, y+\varepsilon^2 R_{1,1}) + \mathbf{Z}(x+2\varepsilon, y+\varepsilon^2 R_{2,0}) - \mathbf{Z}(x-2\varepsilon, y+\varepsilon^2 R_{-2,0}) \\ + \mathbf{Z}(x-\varepsilon, y+\varepsilon^2 R_{-1,-1}) - \mathbf{Z}(x+\varepsilon, y+\varepsilon^2 R_{1,-1})] = 0,\end{aligned} \tag{44}$$

whose leading contribution yields

$$-\mathbf{\Omega}_{xx}(x, y) + 2[\mathbf{Y}_y(x, y) + \mathbf{V}_y(x, y)] + 2\gamma \mathbf{Z}_{xxx}(x, y) = 0. \tag{45}$$

By using (41), the above equation becomes

$$\mathbf{Y}_y(x, y) + \mathbf{V}_y(x, y) + \gamma \mathbf{Z}_{xxx}(x, y) = 0. \tag{46}$$

Furthermore, integrating (41) on x we obtain that $\mathbf{\Omega}(x, y)$ does not depend on the transversal coordinate x, namely

$$\mathbf{\Omega}(x, y) \equiv \mathcal{F}(y). \tag{47}$$

By using this in (46) to replace $\mathbf{Y}$ with $\mathbf{V}$, we obtain

$$\mathbf{V}_y(x, y) = -\frac{\gamma}{2}\mathbf{Z}_{xxx}(x, y) - \frac{1}{2}\mathcal{F}(y). \tag{48}$$

Proceeding as before, with the help of (15), the stationary equation (16*c*) in the continuum is

$$\begin{aligned}\omega^2[&\mathbf{Z}(x+\varepsilon, y+\varepsilon^2 R_{1,-1}) + \mathbf{Z}(x-\varepsilon, y+\varepsilon^2 R_{-1,1}) - \mathbf{Z}(x-\varepsilon, y+\varepsilon^2 R_{-1,-1}) \\ &- \mathbf{Z}(x+\varepsilon, y+\varepsilon^2 R_{1,1})] + \gamma[\mathbf{V}(x+\varepsilon, y+\varepsilon^2 R_{1,1}) + \mathbf{V}(x-\varepsilon, y+\varepsilon^2 R_{-1,-1}) \\ &+ \mathbf{V}(x+\varepsilon, y+\varepsilon^2 R_{1,-1}) + \mathbf{V}(x-\varepsilon, y+\varepsilon^2 R_{-1,1}) - 4\mathbf{V}(x, y)] = 0.\end{aligned} \tag{49}$$

The leading order contribution is of $\mathrm{O}(\varepsilon^3)$,

$$\mathbf{V}_{xx}(x, y) = \frac{2\omega^2}{\gamma}\mathbf{Z}_{xy}(x, y). \tag{50}$$

By integrating in x, we obtain

$$\mathbf{V}_x(x, y) = \frac{2\omega^2}{\gamma}\mathbf{Z}_y(x, y) + \mathcal{G}(y), \tag{51}$$

where $\mathcal{G}(y)$ is a suitable integration constant that will be determined by imposing the boundary conditions. Now, taking the derivative of (48) w.r.t. x, and the derivative of (51) w.r.t. y, and summing the results, we obtain a differential equation for the behaviour of $\mathbf{Z}$ in the bulk,

$$\mathbf{Z}_{xxxx}(x, y) - \frac{4\omega^2}{\gamma^2}\mathbf{Z}_{yy}(x, y) = \frac{2}{\gamma}\mathcal{G}_y(y). \tag{52}$$

This is the general equation, whose solution yields the behavior of the various fields in the bulk.

4.4. Boundary conditions

In this section, we impose all boundary conditions. The various constraints allow us not only to uniquely determine the behaviour in the bulk, but also to establish a link with the physically relevant observables, such as the temperature profile. Analogously to the previous section, we proceed into two steps by separately analysing the implications of (16*b*) and of (16*c*).

By setting $i = j$ in (39), we obtain

$$\mathbf{Y}_{i,i} - \mathbf{Y}_{i,i-1} + \mathbf{V}_{i+1,i} - \mathbf{V}_{i,i} + \gamma[-2\mathbf{Z}_{i+1,i} + 2\mathbf{Z}_{i,i} + \mathbf{Z}_{i+1,i-1} - \mathbf{Z}_{i,i-1} + \mathbf{Z}_{i+1,i+1} - \mathbf{Z}_{i,i+1}] = 0. \tag{53}$$

We recall that in order to avoid the complication of the absolute value in the denominator of (28), we have assumed that $i \geqslant j$. Accordingly, the use of (28) requires considering always

the lower (by convention) triangle of all the matrices. In order to satisfy this condition, we exploit the antisymmetry of $\mathbf{Z}$ to obtain

$$\mathbf{Y}_{i,i} - \mathbf{Y}_{i,i-1} + \mathbf{V}_{i+1,i} - \mathbf{V}_{i,i} + \gamma(-\mathbf{Z}_{i+1,i} + \mathbf{Z}_{i+1,i-1} - \mathbf{Z}_{i,i-1}) = 0,$$

and, in field variables,

$$\begin{aligned} 2\Phi(y) - \mathbf{Y}(\varepsilon, y + \varepsilon^2 R_{1,-1}) + \mathbf{V}(\varepsilon, y + \varepsilon^2 R_{1,1}) - T(y) + \gamma(-\mathbf{Z}(\varepsilon, y + \varepsilon^2 R_{1,1}) \\ + \mathbf{Z}(2\varepsilon, y + \varepsilon^2 R_{2,0}) - \mathbf{Z}(\varepsilon, y + \varepsilon^2 R_{1,-1})) = 0. \end{aligned} \tag{54}$$

The leading contribution of (54) is O(1), as expected for the diagonal terms, yielding a boundary condition for $\mathbf{\Omega}$:

$$\Omega(y) = 2\Phi(y) - T(y) = 0. \tag{55}$$

This last expression is just a local version of the virial theorem for the harmonic oscillators.

The reader can verify that the leading term of (40) in the upper diagonal ($i = j - 1$) does not give further information. However, adding the equation for the upper diagonal to (53), we obtain, in field variables,

$$\begin{aligned} \mathbf{Y}(x + \varepsilon, y + \varepsilon^2 R_{1,1}) - \mathbf{Y}(x + \varepsilon, y + \varepsilon^2 R_{1,-1}) + T(y + \varepsilon^2 R_{0,2}) - T(y) \\ + \gamma[-2\mathbf{Z}(x + \varepsilon, y + \varepsilon^2 R_{1,1}) - \mathbf{Z}(x + \varepsilon, y + \varepsilon^2 R_{1,3}) + \mathbf{Z}(x + 2\varepsilon, y + \varepsilon^2 R_{2,2}) \\ + \mathbf{Z}(x + 2\varepsilon, y + \varepsilon^2 R_{2,0}) - \mathbf{Z}(x + \varepsilon, y + \varepsilon^2 R_{1,-1})] = 0. \end{aligned} \tag{56}$$

This equation gives rise to two relations of leading order. The first is redundant as it confirms that $\mathbf{Z}$ is zero along the diagonal. The second relation is, instead, a differential equation for $T(y)$,

$$T_y(y) + \gamma \mathbf{Z}_{xx}(0, y) = 0. \tag{57}$$

It allows determining the temperature profile, once $\mathbf{Z}(x, y)$ has been determined.

We now turn our attention to (16*c*). Along the diagonal ($i = j$), it is[1]

$$\gamma(2\mathbf{V}_{i,i} - \mathbf{V}_{i-1,i-1} - \mathbf{V}_{i+1,i+1}) + 2\omega^2(\mathbf{Z}_{i,i-1} - \mathbf{Z}_{i+1,i}) = 0. \tag{58}$$

It is straightforward to show that the above equation is equivalent to

$$\frac{\gamma}{2}(\mathbf{V}_{i,i} - \mathbf{V}_{i-1,i-1}) + \omega^2 \mathbf{Z}_{i,i-1} = -J, \tag{59}$$

where the integration constant J is nothing but the average heat flux. In fact, the energy flux J_i between the particles $i - 1$ and i is the sum of two contributions, a deterministic one $J_i^{(d)}$, due to the interaction with the neighbours, and a stochastic one $J_i^{(s)}$, originating from the collisions,

$$J_i = J_i^{(d)} + J_i^{(s)} \tag{60}$$

with

$$J_i^{(d)} \equiv \omega^2 \langle q_{i-1} p_i \rangle = \omega^2 \mathbf{Z}_{i-1,i}, \tag{61}$$

$$J_i^{(s)} \equiv \frac{\gamma}{2}\left(\langle p_{i-1}^2 \rangle - \langle p_i^2 \rangle\right) = \frac{\gamma}{2}(\mathbf{V}_{i-1,i-1} - \mathbf{V}_{i,i}), \tag{62}$$

where in both definitions we have adopted the convention that a positive flux corresponds to energy travelling from smaller to larger i coordinates. Accordingly, (59) states the physical

[1] The reader can easily check that if one identifies $T(-1)$ with the left temperature T^+ and $T(+1)$ with the right temperature T^-, then the boundary terms in (16*c*) cancel each other, namely $(\mathbf{RV} + \mathbf{VR}) = 2k_B T\,(\mathbf{R} + \eta\mathbf{S})$.

fact that the heat flux is constant along the chain (i.e., independent of i). In the continuum limit, equation (59) is written as

$$\frac{\gamma}{2}[T(y) - T(y + \varepsilon^2 R_{0,-2})] + \omega^2 \mathbf{Z}(\varepsilon, y + \varepsilon^2 R_{1,-1}) = -J. \tag{63}$$

The leading contribution of the lhs is of $O(\varepsilon)$ and so must be J ($J = \mathcal{J}\varepsilon$). As a result, we can write

$$\omega^2 \mathbf{Z}_x(0, y) = -\mathcal{J}. \tag{64}$$

This is a relevant piece of information that will allow us to uniquely determine $\mathbf{Z}(x, y)$ in the bulk.

Finally, for the upper diagonal ($i = j + 1$), (16*c*) becomes

$$\omega^2[\mathbf{Z}(0, y) - \mathbf{Z}(2\varepsilon, y + \varepsilon^2 R_{2,2}) + \mathbf{Z}(2\varepsilon, y + \varepsilon^2 R_{2,0}) - \mathbf{Z}(0, y + \varepsilon^2 R_{0,2})] + \gamma[\mathbf{V}(2\varepsilon, y + \varepsilon^2 R_{2,0}) + \mathbf{V}(2\varepsilon, y + \varepsilon^2 R_{2,2}) - 2\mathbf{V}(\varepsilon, y + \varepsilon^2 R_{1,1})] = 0, \tag{65}$$

from where we obtain to leading order

$$2\omega^2 \mathbf{Z}_y(0, y) + \gamma \mathbf{V}_x(0, y) = 0, \tag{66}$$

that, by virtue of (33), implies

$$\mathbf{V}_x(0, y) = 0. \tag{67}$$

For (16*c*), combinations of the diagonal and upper diagonal relations give no further information.

4.5. Solution of the equations

In this section, we solve the differential equations of covariance matrices to leading order in ε. From this solution we derive analytical expressions for the temperature profile and the energy flux. We start noting that the function $\mathcal{G}(y)$ appearing in (51) is identically equal to zero. This is seen by setting $x = 0$ and using (33) and (67). As a result, (52) simplifies to

$$\mathbf{Z}_{xxxx}(x, y) - \frac{4\omega^2}{\gamma^2} \mathbf{Z}_{yy}(x, y) = 0. \tag{68}$$

The form of the above equation suggests looking for a solution by the method of separation of variables. Furthermore, the numerical solution of the stationary solution (16*a*) suggests that $\mathbf{Z}(x, y) = 0$ at the boundaries of the domain $\mathcal{D}$. Therefore, we assume the following Ansatz:

$$\mathbf{Z}(x, y) = \sum_n B_n(x) \sin[\beta_n(y + 1)], \qquad \beta_n \equiv \frac{n\pi}{2}, \tag{69}$$

which, upon substitution into (68), gives

$$\frac{\mathrm{d}^4 B_n}{\mathrm{d}x^4} = -\left(\frac{n\pi\omega}{\gamma}\right)^2 B_n. \tag{70}$$

This is readily solved by finding the four roots of the associated characteristic polynomial. Two of the four eigenvalues having a positive real part would lead to an unphysical divergence in x and have to be discarded. Another constraint is imposed, by recalling that $\mathbf{Z}(0, y) = 0$. Altogether, the coefficients B_n can be written as

$$B_n(x) = A_n \exp(-\alpha_n x) \sin(\alpha_n x), \qquad \alpha_n \equiv \left(\frac{n\pi\omega}{2\gamma}\right)^{1/2}. \tag{71}$$

Finally, the constants A_n can be determined by imposing (64)

$$\mathbf{Z}(x, y) = -\frac{2\mathcal{J}}{\omega^2} \sum_{\text{odd}\, n} \frac{1}{\alpha_n \beta_n} \exp(-\alpha_n x) \sin(\alpha_n x) \sin(\beta_n (y+1)). \tag{72}$$

The only remaining unknown, $\mathcal{J}$, can finally be determined by imposing that the temperature profile interpolates between T_+ and T_-. By integrating (57) in y, we find

$$T(y) = T - \gamma \int_0^y \mathbf{Z}_{xx}(0, s)\, \mathrm{d}s, \tag{73}$$

where we have identified $T(0) = T = (T^+ + T^-)/2$. By substituting expression (72) into (73) and performing the integral term by term, we obtain

$$T(y) = T + \frac{4\gamma\mathcal{J}}{\omega^2} \sum_{\text{odd}\, n} \frac{\alpha_n}{\beta_n^2} \cos(\beta_n (y+1)). \tag{74}$$

The value of $\mathcal{J}$ is obtained by imposing $T(-1) = T^+$. From (74), it follows that

$$\frac{\Delta T}{2} = 8\mathcal{J} \left(\frac{2\gamma}{\pi^3 \omega^3}\right)^{1/2} \sum_{\text{odd}\, n} n^{-3/2}. \tag{75}$$

Using the formula [22]

$$\sum_{\text{odd}\, n} n^{-3/2} = \frac{\sqrt{8}-1}{\sqrt{8}} \zeta\left(\frac{3}{2}\right), \tag{76}$$

where the Riemann ζ-function has been introduced, we obtain for $\mathcal{J}$

$$\mathcal{J} = \left(\frac{\pi^3 \omega^3}{\gamma}\right)^{1/2} \frac{\Delta T}{8(\sqrt{8}-1)\zeta(3/2)}, \tag{77}$$

which corresponds to expression (20) for the heat flux in the thermodynamic limit. Moreover, by substituting $\mathcal{J}$ into (74), we obtain expression (19) for the temperature profile. Finally, equation (77) allows a unique identification of $\mathbf{Z}$. From (72) we find

$$\mathbf{Z}(x, y) = -\frac{\Delta T}{\omega\sqrt{2}(\sqrt{8}-1)\zeta(3/2)} \sum_{\text{odd}\, n} n^{-3/2}\, \mathrm{e}^{-\alpha_n x} \sin(\alpha_n x) \sin(\beta_n (y+1)). \tag{78}$$

5. Discussion and open problems

Several comments are in order about the analytical results derived in the previous section, starting from expression (20) for the leading term of the heat flux. First, we see that the flux J is proportional to the temperature difference ΔT. This feature not only applies to the leading term, but also is a general property which follows from the harmonic nature of the underlying dynamics. In more general contexts, we expect a nonlinear response regime to exist.

Moreover, J is independent of the strength of the coupling with the baths λ. This can be physically understood by realizing that λ plays the role of the inverse of a contact resistance. In the thermodynamic limit, the overall thermal resistance is the sum of the contact plus the bulk contribution which eventually dominates, no matter how small is λ. Only for $\lambda = 0$, the asymptotic regime cannot be attained (the system is isolated). The coupling λ will presumably manifest itself when accounting for higher order terms.

It is interesting to note the inverse square root dependence of J on the rate γ of internal collisions. The limiting values $\gamma \to 0$ and $\gamma \to \infty$ signal a crossover towards a regime characterized by a slower (faster) decay of J, respectively. This is the case, because $\gamma = 0$

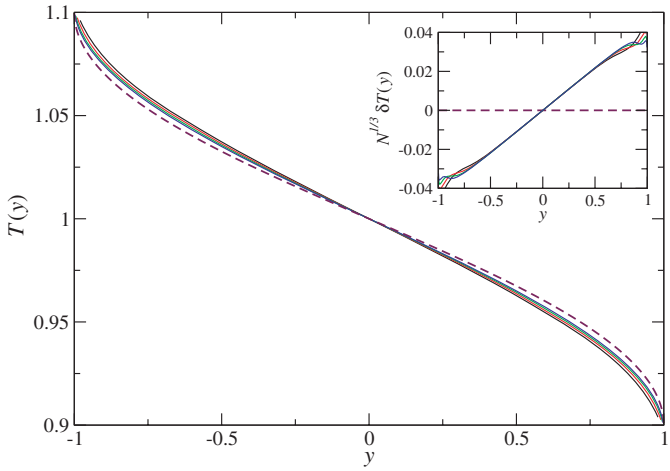

Figure 2. Temperature profile $T(y)$ as given by the analytical expression (18), for $T_+ = 1.1$, $T_- = 0.9$, $\omega = \lambda = \gamma = 1$ (dashed curve). The solid curves correspond to the profile $T_{\rm num}$, obtained from the numerical solution of equations (16*a*)–(16*c*) for $N = 100,\ 200,\ 400$ and 800. The finite-size deviations from (18), $\delta T \equiv T - T_{\rm num}$, rescaled by $N^{1/3}$, are shown in the inset.

corresponds to an integrable dynamics, while for $\gamma = \infty$ the decay of the heat flux is determined by higher-order terms.

As for the temperature profile, we should stress that the equation (19) represents the first example of an analytic expression obtained in the presence of anomalous heat conduction. This is all the way more important, by recalling that, as noticed in [20], the temperature profile of this stochastic model is quite similar to that found in a purely deterministic system such as the purely quartic Fermi–Pasta–Ulam chain. Even more remarkably, $T(y)$ is a parameter-free function. Indeed, once the profile is shifted around the average temperature and the temperature difference is rescaled to unity, the resulting shape $\Theta(y)$ is independent not only of λ but also of γ and ω. This suggests that the temperature profile might be universal (at least in the limit of small temperature differences in truly nonlinear systems). Unfortunately, pure numerics alone is not sufficient to clarify this issue. Finally, we wish to comment on the singularity observed at the two extrema, namely for y close to -1 and 1. From (19), we find that for $y = -1 + \delta y$

$$\delta\Theta(y) \approx \sum_{\text{odd } n}^{1/\delta y} n^{1/2}\delta y^2 \approx \delta y^{1/2}, \tag{79}$$

where the cosine has been approximated with a parabola and the sum has been limited to $n < 1/\delta y$, to prevent that the argument of the cosine becomes larger than O(1). Altogether the above equation tells us that the profile is characterized by a square root singularity.

Although our analysis has allowed us to determine an exact expression for the field $\mathbf{Z}(x, y)$ at leading order in the bulk, and thus for the temperature profile and the heat current in the steady state, the determination of the other fields $\mathbf{V}(x, y)$ and $\mathbf{Y}(x, y)$ requires knowledge of higher-order terms. Indeed, the integration constant $\mathcal{F}(y)$ in (47) that helps determining $\mathbf{V}(x, y)$ and $\mathbf{Y}(x, y)$ cannot be obtained from our analysis. A comparison with numerics [23] suggests that $\mathcal{F}(y) = 0$, but none of the equations we have analysed in the previous section supports this observation. Presumably one should consider some other combinations

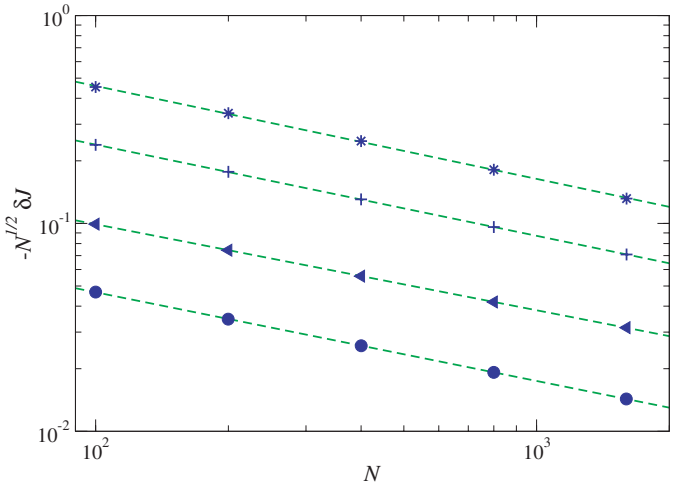

Figure 3. Finite-size deviation of the heat flux $\delta J \equiv J - J_{\rm num}$, rescaled by $N^{1/2}$, as a function of the size of the chain N, for $\gamma = 1$ (circles), 2 (triangles), 5 (pluses) and 10 (stars), other parameters as in the previous figure. The lines correspond to power-law fits, from which we extract that the corrective terms scale as $-\delta J \sim N^{-\alpha}$ with $\alpha = 0.927, 0.914, 0.939$ and 0.947, respectively.

of equations (16*a*)–(16*c*), but the investigation is hindered by the fact that we are not entitled to use any information on the behaviour of higher-order terms.

As a matter of fact, the estimation of the higher-order terms starting from the leading corrections is a highly nontrivial problem, since such terms are likely to be nonanalytic in the smallness parameter ε. This is seen by comparing the analytical results and the numerical solutions for finite chains. The first evidence is presented in figure 2, where we have plotted the analytical profile $T(y)$ and the numerical ones $T_{\rm num}$ computed for chains of different lengths N. From the data in the inset, we deduce that $T - T_{\rm num}$ is approximately proportional to $N^{-1/3}$. While this confirms the correctness of expression (19), it also indicates that the leading correction is of $\mathrm{O}(\varepsilon^{2/3})$. Nonanalytic corrections affect also the heat current. This is illustrated in figure 3, where we plot the difference between the numerical values $J_{\rm num}$ and the leading-order term J, formula (20), for different system sizes N and for various γ values. In all cases, we see a clean power-law convergence to zero but the value of the power is systematically smaller than 1, meaning once again that nonanalytic higher-order terms in ε exist. An appropriate scheme for the treatment of higher-order terms remains an open question.

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