Journal of Statistical Physics, Vol. 115, Nos. 5/6, June 2004 (© 2004)

Perturbative Analysis of Anharmonic Chains of Oscillators Out of Equilibrium

R. Lefevere[1] **and A. Schenkel**[2]

Received March 8, 2003; accepted December 24, 2003

We compute the first-order correction to the correlation functions of the stationary state of a stochastically forced harmonic chain out of equilibrium when a small on-site anharmonic potential is added. This is achieved by deriving a suitable formula for the covariance matrix of the invariant state. We find that the first-order correction of the heat current does not depend on the size of the system. Second, the temperature profile is linear when the harmonic part of the on-site potential is zero. The sign of the gradient of the profile, however, is opposite to the sign of the temperature difference of the two heat baths.

KEY WORDS: Heat conduction; anharmonic chains; nonequilibrium steady states; Fourier law.

1. INTRODUCTION

The goal of this paper is to begin a perturbative analysis of invariant probability measures arising in the context of nonequilibrium statistical mechanics. As a model at hand, we will consider a Hamiltonian chain of N oscillators interacting through nearest-neighbour interactions, coupled at its boundaries to stochastic heat baths of different temperatures, and that we will perturb by a small anharmonic (quartic) on-site interaction. The covariance of the stationary state in the purely harmonic case has been computed in refs. 11 and 13. For anharmonic cases, almost nothing is known about the physical content of the stationary state, except results about the positivity of entropy production and validity of linear response theory.[7] In this paper, we consider the model of ref. 13 with an additional

[1] Institut de Physique Théorique, Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium; e-mail: lefevere@fyma.ucl.ac.be

[2] Department of Mathematics, Helsinki University, P.O. Box 4, 00014 Helsinki, Finland.

0022-4715/04/0600-1389/0

quartic on-site potential, as described in section 4. This model has been numerically studied in refs. 1 and 9 and shown to satisfy Fourier law. It is to be contrasted with the so-called FPU model in one dimension where the nonlinearity is included in the interaction between nearest-neighbours. In that case, Fourier law is not observed.

It is a natural idea to attempt to understand the physical properties of the stationary state by performing a perturbative analysis. Such an approach, based on the phonon picture, has been exploited by physicists to tackle the Fourier law, see ref. 2 for a classical exposition. In particular, the Peierls theory seems successful in computing the thermal conductivity and its thermal and dimensional dependence. The Peierls approach assumes from the beginning the existence of an infinite nonequilibrium state where local temperature equilibrium is expected to hold. It is also based on several implicit assumptions, such as the validity of a Boltzmann equation for phonons. In this paper, we adopt a different approach and begin a rigorous perturbative analysis of a finite (although taking N large will have some simplifying features) anharmonic chain. Our starting point is a formula for the correlation functions of the stationary measure. This formula allows us to derive (matrix) equations for the first-order correction. The relationship between our approach by stationary nonequilibrium states (SNS) and the Peierls approach is, at this stage, far from clear. A first interesting step would be to achieve some understanding of the equivalence of the definition of the thermal conductivity by the Green–Kubo formula and its definition in the SNS approach as, roughly speaking, the ratio of the heat current and the temperature gradient.

The main obstacle to developing a perturbation expansion of SNS's is that, in contrast to the equilibrium case, no explicit formula for the invariant density is known. Moreover, the fact that the relevant models are degenerate in a stochastic sense makes it laborious to obtain a systematic perturbation expansion starting from the equations of motion. We will derive and use a formula for the two-point correlation functions of invariant states, which holds under the assumption of L^1-convergence of the finite-time correlation functions to those of the (unique) invariant measure. We emphasize that the validity of the formula is not restricted to the concrete problem of the anharmonic chain considered here. It may prove useful whenever the invariant measure is not explicitly known, in particular in the context of transport phenomena modelized by hypoelliptic stochastic processes. We also remark that the form of the formula for the covariance is very similar to, and provides a lower bound on, the expectation of the Malliavin matrix.

Our main result concerning the heat current is that its first-order correction remains uniformly bounded as the number of oscillators goes to infinity. Regarding the significance of this result, we recall that the heat current in the harmonic case is independent of the length of the chain.[11, 13] On the other hand, it is expected to be inversely proportional to the length of the chain in the anharmonic case, as it should if Fourier law holds, which numerical studies strongly suggest, see, e.g., refs. 1 and 9. One thus expects the heat current in the harmonic limit to develop a singularity as the length of the chain increases. In this respect, our result shows that such a singularity does not manifest itself in a first-order perturbative analysis. Our second result concerns the first-order correction to the temperature profile. It is exponentially decaying in the bulk of the chain, with a decay rate that depends on the strength of the harmonic part of the on-site potential. When this strength vanishes, the correction to the temperature profile is linear. However, the sign is "wrong," in the sense that the linear profile has the *lowest* temperature near the *hottest* bath and the *highest* temperature near the *coldest* bath. This is analogous to the result of ref. 13, where the temperature profile is also oriented in the "wrong" direction. The main difference is of course that in ref. 13, the temperature profile is exponentially decaying. Although we have no satisfactory explanation for this surprising behaviour, we briefly comment on this point in the concluding section. Another feature of our solution is that the temperature profile is shifted downwards, in the sense that the temperature at the middle point of the chain is lower than the arithmetic mean of the temperatures of the heat baths.

The remainder of this paper is organized as follows. In Section 2, we specify the basic set-up for the type of anharmonic chains we will consider. Section 3 is devoted to the derivation of our basic formula for the covariance. In Section 4, we derive the matrix equations for the first-order corrections to the harmonic case. Sections 5 and 6 are devoted to the resolution of these equations. This is done by generalizing the methods of refs. 11 and 13. Finally, some concluding comments are collected in Section 7.

2. A MODEL FOR HEAT CONDUCTION

In order to explain the behaviour of the thermal conductivity in crystalline solids, one often modelizes the solid by a chain (or lattice in higher dimension) whose ends are coupled to heat baths maintained at different temperatures. The coupling can be taken stochastic and more precisely of Langevin type. In one dimension, the set-up is as follows. At each site of a lattice $\{1,..., N\}$ is attached a particle of momentum p_i and position q_i. The dynamics is Hamiltonian in the bulk and stochastic through the

Langevin coupling to heat baths at the boundaries. The Hamiltonian is of the form,

$$H(\underline{p}, \underline{q}) = \sum_{i=1}^{N} \left(\tfrac{1}{2} p_i^2 + V(q_i)\right) + \sum_{i=2}^{N} U(q_i - q_{i-1}) + U(q_1) + U(q_N). \tag{2.1}$$

Specific choices for the potentials U and V will be specified below. The equations of motions are given by,

$$dq_i = p_i\, dt, \qquad i = 1,\dots, N, \tag{2.2}$$

$$dp_i = -\frac{\partial H}{\partial q_i}(\underline{p}, \underline{q})\, dt, \qquad i = 2,\dots, N-1, \tag{2.3}$$

and,

$$dp_1 = -\frac{\partial H}{\partial q_1}(\underline{p}, \underline{q})\, dt - \gamma p_1\, dt + \sqrt{2\gamma k T_1}\, dw_l, \tag{2.4}$$

$$dp_N = -\frac{\partial H}{\partial q_N}(\underline{p}, \underline{q})\, dt - \gamma p_N\, dt + \sqrt{2\gamma k T_N}\, dw_r. \tag{2.5}$$

T_1 and T_N stand for the temperature of the left and right reservoirs, respectively, whereas w_l and w_r are two independent standard Wiener processes.

It is an easy fact to check that when $T_1 = T_N = T = \beta^{-1}$, the measure on the configuration space $\mathbf{R}^{2N}$ whose density with respect to the Lebesgue measure is given by

$$\rho(\underline{p}, \underline{q}) = Z^{-1} e^{-\beta H(\underline{p}, \underline{q})} \tag{2.6}$$

is invariant (stationary) for the stochastic dynamics defined above. Explicitly, one can check that for L the generator of the dynamics and any function f in its domain,

$$\int Lf\, \rho(\underline{p}, \underline{q})\, d\underline{p}\, d\underline{q} = 0. \tag{2.7}$$

In the case of two different temperatures, existence, uniqueness and exponential convergence to an unique invariant state has been established under fairly general conditions on the potentials U and V.[4, 6, 7, 12] In the case of harmonic coupling, the covariance of the stationary state has been exactly computed in refs. 11 and 13.

An essential ingredient of the proof of the uniqueness is the fact that the system satisfies the so-called Hörmander condition. This condition implies that the noise spreads in a sufficiently good way through the system, so that the transition probabilities have smooth densities. This property is encapsulated in the non-degeneracy of the Malliavin matrix associated to the stochastic system under study. As the noise represents the injection of energy into the system, it is natural to enquire about the relationship between the Malliavin matrix and the correlation functions of the stationary state. This might provide a way to tackle the description of the stationary state when its density is not explicitly known. Indeed, from a physical point of view, the central question, once uniqueness has been established, is to compute the energy spectrum and correlation functions of the stationary state and ultimately, to establish the validity of the Fourier law. As mentioned above, the case of a harmonic chain has been completely and explicitly solved. The main feature of the solution is a flat temperature profile and an associated infinite thermal conductivity.

The basic idea in order to perform a perturbation theory of the non-equilibrium stationary state is to write the two-point correlation function of the stationary measure under a "Malliavin" form, similar to the form derived by Nakazawa in the Gaussian harmonic case.[11]

3. THE MALLIAVIN MATRIX AND THE COVARIANCE MATRIX OF THE STATIONARY MEASURE

We consider now a general system of stochastic equations. Denote by $x_t \in \mathbf{R}^d$ the solution of the stochastic differential equation,

$$dx_t = X_0(x_t)\,dt + \sum_{k=1}^{n} X_k(x_t)\,dw_k(t) \tag{3.1}$$

with initial condition $x_0 = x$, where the w_k's are n independent one-dimensional Brownian motions and X_l, $l = 0,..., n$, are $\mathscr{C}^\infty$ vector fields over $\mathbf{R}^d$ satisfying for any multi-index α,

$$\|\partial^\alpha X_l(x)\| \leqslant C(1 + \|x\|^{K_\alpha}) \tag{3.2}$$

for some $K_\alpha > 0$. We note that solutions to such equations are in general not ensured to exist globally. In the sequel, we restrict ourselves to the following situations.

Assumption 3.1. For all $x \in \mathbf{R}^d$, Eq. (3.1) has a unique strong solution x_t, $t > 0$. This solution has finite moments of all order: for all

$p \geqslant 1$, $T < \infty$, and $x \in \mathbf{R}^d$, there exists a constant $C = C(x, p, T) < \infty$ such that for $0 \leqslant t \leqslant T$,

$$\mathbf{E}_x(\|x_t\|^p) \leqslant C. \tag{3.3}$$

When in need of emphasizing the dependence of the solution to (3.1) on the initial condition x and the realization of the d-dimensional Brownian motion w in the interval $[0, t]$, we shall write it as $x_t(x, w([0, t]))$. We denote by $\mathscr{P}^t$ the associated semigroup,

$$\mathscr{P}^t f(x) = \mathbf{E}_x(f(x_t)) \equiv \int f(x_t(x, w([0, t]))) \, \mathbf{dP}(w([0, t]), \tag{3.4}$$

where $\mathbf{P}$ is the d-dimensional Wiener measure, by $\mathscr{A}$ the generator of the semigroup, and by L the associated second order differential operator,

$$L = \sum_{i=1}^{d} X_0^i \, \partial_i + \sum_{i, j=1}^{d} a_{ij} \, \partial_i \partial_j, \tag{3.5}$$

where, with $\otimes$ denoting the tensor product,

$$a = \tfrac{1}{2} \sum_{k=1}^{n} X_k \otimes X_k. \tag{3.6}$$

From Assumption 3.1 on the process solution x_t and the bounds (3.2) for the vector fields X_l, it follows that for each t and $w[0, t]$, the map $x \mapsto x_t(x, w[0, t])$ is $\mathscr{C}^\infty$ on $\mathbf{R}^d$ with derivatives of all orders satisfying the stochastic differential equation obtained from (3.1) by formal differentiation. Furthermore, for all multi-index α, $p \geqslant 1$, and $t \geqslant 0$,

$$\mathbf{E}(\|\partial^\alpha x_t(x, \cdot)\|^p) < \infty. \tag{3.7}$$

In the sequel, we will denote $U_t(x, w[0, t]) = Dx_t(x, w[0, t])$, where DX denotes the Jacobian matrix of a vector field X on $\mathbf{R}^d$. The matrix U_t is the linearized flow and it solves the equation, with initial condition $U_0 = \mathbf{1}$,

$$dU_t = DX_0(x_t) \, U_t \, dt + \sum_{k=1}^{n} DX_k(x_t) \, U_t \, dw_k(t). \tag{3.8}$$

Below, $\mathbf{E}_x U_t$ denotes $\int U_t(x, w[0, t]) \, \mathbf{dP}(w[0, t])$.

Let us now assume the existence of an invariant probability measure μ for the process solution x_t of (3.1) and consider the covariance matrix at time t,

$$C_t(x) \equiv \mathbf{E}_x(x_t \otimes x_t) - \mathbf{E}_x x_t \otimes \mathbf{E}_x x_t. \tag{3.9}$$

The following result is the starting point of the perturbative analysis performed in subsequent sections. It provides an expression for $\mu(C_t)$ in terms of the linearized flow U_t, where $\mu(f)$ is a shorthand notation for $\int_{\mathbf{R}^d} f(x)\,d\mu(x)$.

Proposition 3.2. Suppose that the bounds (3.2) and Assumption 3.1 are satisfied. Suppose in addition that the invariant measure μ for the process solution x_t of (3.1) is such that the functions $x \mapsto \mathbf{E}_x x_s^i$, $x \mapsto L\mathbf{E}_x x_s^i$, and $x \mapsto a_{ij}(x)\,\mathbf{E}_x U_s^{jl}$, belong to $L^2(\mathbf{R}^d, d\mu)$ for all i, j, l, and $s \leqslant t$. Then,

$$\mu(C_t) = \int_0^t ds \sum_{k=1}^n \mu(\mathbf{E}_. U_s X_k(.) \otimes \mathbf{E}_. U_s X_k(.)). \tag{3.10}$$

Proof. We will show below that the map $s \mapsto \mu(\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s)$ is differentiable, with

$$\frac{d}{ds}\mu(\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s) = -\sum_{k=1}^n \mu(\mathbf{E}_. U_s X_k(.) \otimes \mathbf{E}_. U_s X_k(.)). \tag{3.11}$$

Identity (3.10) thus follows from the invariance of the measure μ, since

$$\mu(C_t) = \mu(\mathbf{E}_.(x_t \otimes x_t)) - \mu(\mathbf{E}_. x_t \otimes \mathbf{E}_. x_t) \tag{3.12}$$

$$= \mu(x \otimes x) - \mu(\mathbf{E}_. x_t \otimes \mathbf{E}_. x_t) \tag{3.13}$$

$$= -\int_0^t ds \frac{d}{ds}\mu(\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s). \tag{3.14}$$

To obtain (3.11), we first note that (3.3) implies that any function $f \in \mathscr{C}^2(\mathbf{R}^d)$ with first derivatives of at most polynomial growth is in the domain of the generator $\mathscr{A}$ with $\mathscr{A}f = Lf$. Similarly, one easily checks that for such f, (3.7) implies $\mathscr{A}(\mathscr{P}_t f) = L(\mathscr{P}_t f)$. Therefore, Kolmogorov equation yields $\frac{d}{ds}(\mathbf{E}_x x_s \otimes \mathbf{E}_x x_s) = L\mathbf{E}_x x_s \otimes \mathbf{E}_x x_s + \mathbf{E}_x x_s \otimes L\mathbf{E}_x x_s$, which, by Hölder inequality and our assumptions, belongs to $L^1(\mathbf{R}^d, d\mu)$. Thus,

$$\frac{d}{ds}\mu(\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s) = \mu(L\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s + \mathbf{E}_. x_s \otimes L\mathbf{E}_. x_s). \tag{3.15}$$

Let us next define for $f, g \in \mathscr{C}^2(\mathbf{R}^d)$,

$$\Gamma(f, g) \equiv L(fg) - fLg - gLf, \tag{3.16}$$

which reads

$$\Gamma(f,g)=2\sum_{i,j=1}^{d} a_{ij}\,\partial_i f\,\partial_j g. \tag{3.17}$$

Since it follows from (3.7) that $\partial_i \mathbf{E}_x x_s^j = \mathbf{E}_x U_s^{ji}$, our assumptions imply as above that $\Gamma(\mathbf{E}_. x_s^i, \mathbf{E}_. x_s^j) \in L^1(\mathbf{R}^d, d\mu)$ for all i, j. It follows in particular that $L(\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s) \in L^1(\mathbf{R}^d, d\mu)$. Because of the invariance of μ (which implies $\mu(Lf)=0$), we are thus free to subtract from the μ-expectation on the right hand side of (3.15) a term $L(\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s)$, so that

$$\frac{d}{ds}\mu((\mathbf{E}_. x_s \otimes \mathbf{E}_. x_s)_{ij}) = -\mu(\Gamma(\mathbf{E}_. x_s^i, \mathbf{E}_. x_s^j)). \tag{3.18}$$

Formula (3.11) finally follows from the computation, recalling (3.6),

$$\Gamma(\mathbf{E}_. x_s^i, \mathbf{E}_. x_s^j)(x) = \sum_{k=1}^{n} (\mathbf{E}_x U_s X_k(x) \otimes \mathbf{E}_x U_s X_k(x))_{ij}. \tag{3.19}$$

This concludes the proof of Proposition 3.2.

Proposition 3.2 immediately implies the

Corollary 3.3. Suppose that the hypothesis of Proposition 3.2 are satisfied for all $t \geqslant 0$. Suppose in addition that

$$\lim_{t\to\infty} C_t = \mu(x\otimes x) - \mu(x)\otimes\mu(x) \equiv \Phi, \tag{3.20}$$

in $L^1(\mathbf{R}^d, d\mu)$. Then,

$$\Phi = \int_0^\infty ds \sum_{k=1}^{n} \mu(\mathbf{E}_. U_s X_k(.) \otimes \mathbf{E}_. U_s X_k(.)). \tag{3.21}$$

Expression (3.21) for the covariance matrix of a stationary state is the basic formula that we shall use to develop a perturbation expansion in the next section. Since both sides of (3.21) involve an averaging with respect to μ, it is not clear at first sight how informations on μ can be extracted from (3.21). We observe, however, that in the case of a linear drift X_0 and constant vector fields X_k, $k=1,\ldots,n$, all expectations may be dropped and (3.21) becomes

$$\Phi_{\text{linear}} = \int_0^\infty ds\, U_s \left(\sum_{k=1}^{n} X_k \otimes X_k\right) U_s^{\mathrm{T}}. \tag{3.22}$$

One thus recovers the standard formula for the covariance of the stationary state of a linear stochastic equation with constant diffusion coefficients. As we shall see in the next section, it is possible to iterate this simple observation in order to begin a perturbation expansion.

Another feature of formula (3.10) is to provide a link between the covariance matrix C_t and the so-called Malliavin matrix. The Malliavin matrix associated to Eq. (3.1) at time t reads, in the normalization of ref. 10,

$$M_t = \int_0^t ds \sum_{k=1}^n U_t V_s X_k(x_s) \otimes U_t V_s X_k(x_s), \tag{3.23}$$

where V_s is the inverse matrix of U_s. An easy computation reveals that $\mu(\mathbf{E}_. M_t)$ can be expressed in a form closely related to (3.10), namely,

$$\mu(\mathbf{E}_. M_t) = \int_0^t ds \sum_{k=1}^n \mu(\mathbf{E}_.(U_s X_k(.) \otimes U_s X_k(.))). \tag{3.24}$$

Indeed, we first observe that for $s \geqslant 0$ fixed, $Y_s^t \equiv U_t V_s$ satisfies $Y_s^s = \mathbf{1}$ and

$$dY_s^t = DX_0(x_t)\, Y_s^t\, dt + \sum_{k=1}^n DX_k(x_t)\, Y_s^t\, dw_k(t) \tag{3.25}$$

for $t \geqslant s$. Comparing with (3.8) yields that $Y_s^t = Y_s^t(x_s(x, w[0,s]), w[s,t])$ has the same $\mathbf{P}$-distributions as $U_{t-s}(x_s(x, w[0,s]), \bar{w}[s,t])$, where $\bar{w}(\tau) = w(\tau) - w(s)$ for $\tau \geqslant s$. Furthermore, for x fixed the map $w \mapsto Y_s^t(x, w[s,t])$ is $w[0,s]$-independent. Since $(x, w) \mapsto Y_s^t(x, w)\, X_k(x) \otimes Y_s^t(x, w)\, X_k(x)$ is measurable, one therefore may use the Markov property of x_t to write,

$$\begin{aligned} &\mathbf{E}_x(Y_s^t(x_s)\, X_k(x_s) \otimes Y_s^t(x_s)\, X_k(x_s)) \\ &\quad = \mathbf{E}_x(\mathbf{E}_{y=x_s}(U_{t-s}(y)\, X_k(y) \otimes U_{t-s}(y)\, X_k(y))). \end{aligned} \tag{3.26}$$

Identity (3.24) then follows by using the invariance of the measure μ and changing variables in the integral over s in (3.23). As a consequence, Proposition 3.2 provides a lower bound on the expectation of the Malliavin matrix.[3]

Corollary 3.4. One has

$$\mu(C_t) \leqslant \mu(\mathbf{E}_. M_t). \tag{3.27}$$

[3] The order relation is defined in the following way. For two matrices X_1, X_2, we say that $X_1 \geqslant X_2$ whenever $X_1 - X_2$ is a positive definite matrix.

Proof. The inequality simply follows from (3.10), (3.24), and the matrix

$$\mathbf{E}_x[(U_s X_k(x) - \mathbf{E}_x U_s X_k(x)) \otimes (U_s X_k(x) - \mathbf{E}_x U_s X_k(x))] \tag{3.28}$$

being positive definite.

4. PERTURBATIVE ANALYSIS OF THE NONEQUILIBRIUM ANHARMONIC CHAIN

We shall analyse the effect of adding an anharmonic perturbation to a (slightly) modified version of the model treated by Rieder *et al.*[13] We consider the case of a harmonic chain with fixed ends to which one adds an anharmonic on-site potential, i.e., we set in (2.1),

$$U(x) = \tfrac{1}{2}\,\omega^2 x^2 \qquad \text{and} \qquad V = \tfrac{1}{2}\,\omega^2 \kappa x^2 + \tfrac{1}{4}\,\lambda x^4. \tag{4.1}$$

The model considered in ref. 13 has $\kappa = 0$ but the computation of the covariance of the stationary state is very similar and the result is given below. We write the equations of motions (2.2)–(2.5) under the matrix form,

$$\begin{pmatrix} d\underline{q} \\ d\underline{p} \end{pmatrix} = \mathbf{b} \begin{pmatrix} \underline{q} \\ \underline{p} \end{pmatrix} dt - \lambda \begin{pmatrix} \mathbf{0} \\ \mathcal{N}(\underline{q}) \end{pmatrix} dt + \begin{pmatrix} \mathbf{0} \\ \mathbf{dw} \end{pmatrix} \tag{4.2}$$

with $\mathcal{N}(\underline{q})$ and $\mathbf{dw}$ the vectors in $\mathbf{R}^N$ given by $\mathcal{N}_i(\underline{q}) = q_i^3$ and $\mathbf{dw}_i = \delta_{1i}\sqrt{2\gamma k T_1}\, dw_l + \delta_{Ni}\sqrt{2\gamma k T_N}\, dw_r$, and

$$\mathbf{b} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{g}_\kappa & -\mathbf{a} \end{pmatrix} \tag{4.3}$$

where $\mathbf{g}_\kappa$ and $\mathbf{a}$ are $N \times N$ matrices given by $(\mathbf{g}_\kappa)_{ij} = \omega^2((2+\kappa)\,\delta_{ij} - \delta_{ij+1} - \delta_{ij-1})$ and $\mathbf{a}_{ij} = \gamma\delta_{ij}(\delta_{1j} + \delta_{Nj})$. Above, $\mathbf{1}$ denotes the unit matrix and $\mathbf{0}$ the zero matrix or vector, as is clear from the context. We note that the stochastic terms in (4.2) are given by constant vector fields, namely, in the notation of Section 3,

$$X_k = \begin{pmatrix} \mathbf{0} \\ \mathbf{d}_k \end{pmatrix} \qquad \text{where} \quad (\mathbf{d}_k)_j = \delta_{kj}\sqrt{2\gamma k T_k}, \tag{4.4}$$

for $k=1, N$. In particular, the coefficients a_{ij} involved in the generator L are constant. They are given by

$$\sum_{k=1,N} X_k \otimes X_k = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \Delta \end{pmatrix}, \tag{4.5}$$

where $\Delta_{ij} = 2\gamma k \delta_{ij}(T_1 \delta_{1j} + T_N \delta_{Nj})$. Furthermore, the linearized flow U_t^λ of (4.2) is given by

$$dU_t^\lambda = \mathbf{b} U_t^\lambda \, dt - 3\lambda C^\lambda(t) \, U_t^\lambda \, dt, \tag{4.6}$$

where

$$C^\lambda(t) = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{v}^\lambda(t) & \mathbf{0} \end{pmatrix}, \tag{4.7}$$

with $\mathbf{v}_{ij}^\lambda(t) = \delta_{ij} q_i^2(t)$ and $q_i(t)$ the q_i-component of the solution of (4.2) at time t. Finally, we note that the matrix $\mathbf{b}$ in (4.2) has the property that all its eigenvalues have strictly negative real part. A proof of this fact can be found in ref. 11 modulo obvious modifications.

In order to study perturbatively the SNS of our chain, we would like to use the identity (3.21). However, some of the hypothesis of Corollary 3.3 related to the invariant measure are not known to hold for Eq. (4.2) when $\lambda > 0$. (The case $\lambda = 0$ has been covered in ref. 13.) Although from a mathematical point of view, this is not a mere technical problem, we will assume that these hypothesis hold, see Assumption 4.1 below and the remark that follows. On the other hand, Assumption 3.1, i.e., the existence of strong solutions and their moments, follows from standard techniques and we briefly discuss it now. We first note that for $\lambda > 0$, the function $\widetilde{H}(\underline{q}, \underline{p}) = 2N + H(\underline{q}, \underline{p})$, with H the Hamiltonian given by (2.1) and (4.1), satisfies

$$\widetilde{H}(\underline{q}, \underline{p}) \geqslant C(1 + \|\underline{q}\|^2 + \|\underline{p}\|^2), \tag{4.8}$$

for some $C > 0$ and all $(\underline{q}, \underline{p}) \in \mathbf{R}^{2N}$. Thus, $\widetilde{H}$ is a $\mathscr{C}^2(\mathbf{R}^{2N})$ confining function. Furthermore, one computes

$$(L\widetilde{H})(\underline{q}, \underline{p}) = -\gamma(p_1^2 + p_N^2) + 2\gamma k(T_1 + T_N), \tag{4.9}$$

which implies that $L\widetilde{H}$ is uniformly bounded by above. A classical result, see, e.g., ref. 8, Theorem 4.1, then ensures for all initial conditions $(\underline{q}, \underline{p}) \in \mathbf{R}^{2N}$ the existence of a unique global strong solution to (4.2).

Regarding the bounds (3.3), they are an immediate consequence of the following *a priori* bound. For any $\theta \leqslant (2k \max\{T_1, T_N\})^{-1}$, one has

$$\mathbf{E}_{(\underline{q}, \underline{p})}[e^{\theta H(\underline{q}_t, \underline{p}_t)}] \leqslant e^{2\gamma k \theta (T_1 + T_N)\, t}\, e^{\theta H(\underline{q}, \underline{p})}. \tag{4.10}$$

Bound (4.10) can be obtained in a similar way as in the proof of Lemma 3.5 in ref. 12. However, the existence of a unique invariant measure for (4.2) is still an open problem. We thus introduce the following

Assumption 4.1. The finite time truncated two-point correlation function of the process defined by (4.2) converges to the covariance matrix of a unique stationary measure μ^λ in $L^1(\mathbf{R}^{2N}, d\mu^\lambda)$-norm. Furthermore, the decay properties of μ^λ are such that $\mathbf{E}_{(\underline{q}, \underline{p})}[(\underline{q}_t, \underline{p}_t)]$, $L\mathbf{E}_{(\underline{q}, \underline{p})}[(\underline{q}_t, \underline{p}_t)]$, and $\mathbf{E}_{(\underline{q}, \underline{p})}[U_t^\lambda]$ belong to $L^2(\mathbf{R}^{2N}, d\mu^\lambda)$.

Remark. The uniqueness of the invariant measure is proved in refs. 4 and 12 for a large class of anharmonic chains. The invariant measure has a smooth density with exponential decay and is shown to be mixing.[4] An important restriction is that the potential U must not grow asymptotically slower than V, and thus Eq. (4.2) does not fall into the class covered in refs. 4 and 12. However, as is argued in ref. 12, the fact that the on-site potential grows faster than the nearest-neighbour interaction and the existence of breathers for the deterministic dynamics should not affect the ergodic properties of the measure except for the rate of convergence. Although we could consider a similar anharmonic chain with an additional quartic term in the nearest-neighbour interaction, the equations that one then needs to solve, see below, are computationally more involved. Furthermore, restricting to (4.2) will allow us to compare our results to the usual $\lambda\phi^4$ expansion when the temperatures of the two baths are equal.

Provided Assumption 4.1 holds, let Φ^λ denote the covariance matrix of the unique stationary state of Eq. (4.2) and express it according to (3.21) as

$$\Phi^\lambda = \int_0^\infty dt \sum_{k=1, N} \mu^\lambda(\mathbf{E}_{.} U_t^\lambda X_k \otimes \mathbf{E}_{.} U_t^\lambda X_k). \tag{4.11}$$

We first briefly review the harmonic case $\lambda = 0$. As mentioned in Section 3, one obtains from (4.11)

$$\Phi^0 = \int_0^\infty dt\, e^{\mathbf{b}t} \mathbf{D} e^{\mathbf{b}^{\mathrm{T}} t}, \tag{4.12}$$

[4] In ref. 12, the result is actually stronger. The convergence to the unique invariant measure is shown to be exponential.

where

$$\mathbf{D} = \sum_{k=1,N} X_k \otimes X_k = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \Delta \end{pmatrix}, \tag{4.13}$$

with $\Delta_{ij} = 2\gamma k \delta_{ij}(T_1 \delta_{1j} + T_N \delta_{Nj})$. Since the eigenvalues of $\mathbf{b}$ have strictly negative real part, the integral in (4.12) is convergent and it follows from integrating by parts in $\mathbf{b}\Phi^0$ that Φ^0 must satisfy the equation

$$\mathbf{b}\Phi^0 + \Phi^0 \mathbf{b}^{\mathrm{T}} = -\mathbf{D}. \tag{4.14}$$

The unique solution of this equation has been explicitly derived in ref. 13. It is given by

$$\Phi^0 = \begin{pmatrix} \Phi_x^0 & \Phi_z^0 \\ -\Phi_z^0 & \Phi_y^0 \end{pmatrix} \tag{4.15}$$

where, denoting $T = \frac{T_1 + T_N}{2}$, $\eta = \frac{T_1 - T_N}{2T}$, and $\mathbf{G}_\kappa = \omega^{-2} \mathbf{g}_\kappa$,

$$\Phi_x^0 = \frac{kT}{\omega^2} (\mathbf{G}_\kappa^{-1} + \eta \mathbf{X}^0), \tag{4.16}$$

$$\Phi_y^0 = kT(\mathbf{1} + \eta \mathbf{Y}^0), \tag{4.17}$$

$$\Phi_z^0 = \frac{kT}{\gamma} \eta \mathbf{Z}^0, \tag{4.18}$$

and

$$\mathbf{X}^0 = \begin{pmatrix} \phi_1 & \phi_2 & & \phi_{N-2} & \phi_{N-1} & 0 \\ \phi_2 & \iddots & \iddots & \iddots & \iddots & -\phi_{N-1} \\ \phi_3 & \iddots & \iddots & \iddots & \iddots & \\ & \iddots & \iddots & \iddots & \iddots & \\ & & \iddots & \iddots & \iddots & \\ \phi_{N-1} & & & \iddots & \iddots & -\phi_2 \\ 0 & -\phi_{N-1} & & & -\phi_2 & -\phi_1 \end{pmatrix}, \tag{4.19}$$

$$\mathbf{Y}_{ij}^0 = \delta_{ij}(\delta_{i1} - \delta_{iN}) - \nu \mathbf{X}_{ij}^0, \tag{4.20}$$

$$\mathbf{Z}^0 = \begin{pmatrix} 0 & \phi_1 & \phi_2 & & \phi_{N-2} & \phi_{N-1} \\ -\phi_1 & \ddots & \ddots & \ddots & & \phi_{N-2} \\ -\phi_2 & \ddots & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \phi_2 \\ & & & \ddots & \ddots & \phi_1 \\ -\phi_{N-1} & & & -\phi_2 & -\phi_1 & 0 \end{pmatrix}. \tag{4.21}$$

Above, $\nu = \frac{\omega^2}{\gamma^2}$ and the quantities ϕ_j, $1 \leqslant j \leqslant N-1$, satisfy the equation

$$\sum_{j=1}^{N-1} (\mathbf{G}_{\nu+\kappa}^{(N-1)})_{ij}\, \phi_j = \delta_{1i}, \tag{4.22}$$

where $\mathbf{G}_{\nu+\kappa}^{(k)}$ denotes the k-square matrix given by $(\mathbf{G}_{\nu+\kappa}^{(k)})_{ij} = (2+\nu+\kappa)\,\delta_{ij} - \delta_{i,\,j+1} - \delta_{i,\,j-1}$. The solution of (4.22) is given by

$$\phi_j = \frac{\sinh(N-j)\,\alpha}{\sinh N\alpha}, \tag{4.23}$$

with α defined by $\cosh\alpha = 1 + (\nu+\kappa)/2$. Hence, one has for large N and fixed j the asymptotic formula $\phi_j = e^{-\alpha j}$. In the context of SNS, one usually defines the temperature to be the average kinetic energy, i.e., in our case,

$$T_i = (\Phi_y^0)_{ii}. \tag{4.24}$$

It is easy to see that the above solution yields an exponentially flat profile in the bulk of the chain.

We now turn to the first-order perturbation of the anharmonic chain. Below, all derivatives with respect to λ at $\lambda = 0$ are to be understood as derivative from the right. We first introduce our second assumption on the process solution of (4.2).

Assumption 4.2. The invariant measure μ^λ is absolutely continuous with respect to the Lebesgue measure. As a function of λ, its density $\rho^\lambda(x)$ is C^∞ in an interval $[0, \lambda_+)$ for all x and some $\lambda_+ > 0$.

Remark. At least in cases where uniqueness of the invariant measure has been established, the proof of Assumption 4.2 should follow from an analysis similar to the ones developed in refs. 5 or 15 to prove smoothness of the probability transitions in a parameter of the related stochastic differential equations. We postpone the proof of this fact to a future publication.

To derive an expression for $\Phi^1 \equiv \frac{d}{d\lambda} \Phi^\lambda|_{\lambda=0}$, we compute from (4.11)

$$\Phi^1 = \frac{d}{d\lambda} \Phi^\lambda|_{\lambda=0} \tag{4.25}$$

$$= \mu^1 \left(\int_0^\infty dt \sum_{i=1,N} \mathbf{E}_. U_t^0 X_i(.) \otimes \mathbf{E}_. U_t^0 X_i(.) \right)$$

$$+ \mu^0 \left(\int_0^\infty dt \sum_{i=1,N} \mathbf{E}_. \frac{d}{d\lambda} U_t^\lambda|_{\lambda=0} X_i(.) \otimes \mathbf{E}_. U_t^0 X_i(.) \right) + \text{tr.}, \tag{4.26}$$

and observe that the first term vanishes because $\mu^1 \equiv \frac{d}{d\lambda} \mu^\lambda|_{\lambda=0}$ integrates constants to zero. In order to compute the last terms, we first evaluate $W_t \equiv \frac{d}{d\lambda} U_t^\lambda|_{\lambda=0}$. Deriving with respect to λ on both sides of Eq. (4.6), we get

$$dW_t = \mathbf{b} W_t \, dt - 3C^0(t) \, U_t^0 \, dt, \tag{4.27}$$

from which it follows that, since $W_0 = 0$,

$$W_t = -3 \int_0^t ds \, e^{\mathbf{b}(t-s)} C^0(s) \, e^{\mathbf{b}s}. \tag{4.28}$$

Inserting (4.28) in (4.26), we obtain, using in addition the invariance of μ^0,

$$\Phi^1 = -3 \int_0^\infty dt \int_0^t ds \sum_{i=1,N} e^{\mathbf{b}(t-s)} \mathbf{N} e^{\mathbf{b}s} X_i \otimes e^{\mathbf{b}t} X_i + \text{tr.}, \tag{4.29}$$

$$= -3 \int_0^\infty dt \int_0^t ds \, e^{\mathbf{b}(t-s)} \, \mathbf{N} e^{\mathbf{b}s} \, \mathbf{D} e^{\mathbf{b}^{\mathrm{T}} t} + \text{tr.}, \tag{4.30}$$

where $\mathbf{D}$ is given by (4.13) and

$$\mathbf{N} = \mu^0(C^0(0)) = \begin{pmatrix} 0 & 0 \\ \operatorname{diag}(\Phi_x^0) & 0 \end{pmatrix}. \tag{4.31}$$

Exchanging the integrations over t and s and changing variables leads to

$$\Phi^1 = -3 \int_0^\infty dt \, e^{\mathbf{b}t} \mathbf{N} \left(\int_0^\infty ds \, e^{\mathbf{b}s} \mathbf{D} e^{\mathbf{b}^{\mathrm{T}} s} \right) e^{\mathbf{b}^{\mathrm{T}} t} + \text{tr.}, \tag{4.32}$$

which, with (4.12), finally yields,

$$\Phi^1 = -3 \int_0^\infty dt \, e^{\mathbf{b}t} (\mathbf{N} \Phi^0 + \Phi^0 \mathbf{N}^{\mathrm{T}}) \, e^{\mathbf{b}^{\mathrm{T}} t}. \tag{4.33}$$

The method used to derive the above equation will also provide the equations for the next orders of the perturbation expansion. However, obtaining them concretely requires some more work and we reserve that part and the general Feynman rules for a further publication. We note that integrating by parts in (4.33) yields the equation for Φ^1

$$\mathbf{b}\Phi^1+\Phi^1\mathbf{b}^{\mathrm{T}}=3(\mathbf{N}\Phi^0+\Phi^0\mathbf{N}^{\mathrm{T}}). \tag{4.34}$$

In Section 6, we will derive an explicit expression for Φ^1 and thus for the first order correction to the heat current and temperature profile. It turns out to be easier to do so by solving Eq. (4.34) rather than by using (4.33). In the next section, we first make a few preliminary remarks about equations of the form (4.34).

5. SOLVING THE EQUATION FOR THE FIRST ORDER

The symmetry properties of the inhomogeneous term in Eq. (4.34) will play a special role. We will need to consider symmetry properties both with respect to the diagonal and to the cross-diagonal.

Notation. For a K-square matrix $\mathbf{M}$, we denote by $\mathbf{M}^{\mathrm{C}}$ the transpose of $\mathbf{M}$ with respect to the cross-diagonal, namely, $(\mathbf{M}^{\mathrm{C}})_{ij}=\mathbf{M}_{K+1-j,\,K+1-i}$.

Definition. We call a square matrix $\mathbf{M}$ c-symmetric or c-antisymmetric if $\mathbf{M}^{\mathrm{C}}=\mathbf{M}$ or, respectively, $\mathbf{M}^{\mathrm{C}}=-\mathbf{M}$. Denoting

$$\mathbf{J}=\begin{pmatrix}\mathbf{0} & \mathbf{1}\\ \mathbf{1} & \mathbf{0}\end{pmatrix}, \tag{5.1}$$

we call a $2N$-square matrix $\mathbf{M}$ CT-symmetric or CT-antisymmetric if $\mathbf{M}^{\mathrm{C}}=\mathbf{JMJ}$ or, respectively, $\mathbf{M}^{\mathrm{C}}=-\mathbf{JMJ}$.

We first list a few properties of equations of the form (4.34).

Lemma 5.1. Let $\mathbf{b}$ as above and $\mathbf{H}$ a $2N$-square matrix. One has:

(a) The unique solution of the equation

$$\mathbf{b}\Phi+\Phi\mathbf{b}^{\mathrm{T}}=\mathbf{H} \tag{5.2}$$

is given by

$$\Phi=-\int_0^{\infty} dt\, e^{\mathbf{b}t}\mathbf{H}e^{\mathbf{b}^{\mathrm{T}}t}. \tag{5.3}$$

(b) If $\mathbf{H}$ is CT-symmetric or CT-antisymmetric, then Φ is CT-symmetric or, respectively, CT-antisymmetric.

(c) If $\mathbf{H}$ is of the form

$$\mathbf{H}=\begin{pmatrix} \mathbf{0} & * \\ * & * \end{pmatrix}, \tag{5.4}$$

then the solution of (5.2) is of the form

$$\Phi=\begin{pmatrix} \mathbf{X} & \mathbf{Z} \\ -\mathbf{Z} & \mathbf{Y} \end{pmatrix}. \tag{5.5}$$

Proof. Point (a) follows from the matrix $\mathbf{b}$ having all its eigenvalues with strictly negative real part. Indeed, this property implies that the operator $\Phi \mapsto \mathbf{b}\Phi+\Phi\mathbf{b}^{\mathrm{T}}$ is invertible, and integrating by part in $\mathbf{b}\Phi$ reveals that (5.3) is the unique solution of (5.2). Point (c) is obvious, whereas (b) follows from the identity $\mathbf{J}\mathbf{b}^{\mathrm{C}}\mathbf{J}=\mathbf{b}^{\mathrm{T}}$ and uniqueness of the solution of (5.2).

Lemma 5.1 implies in particular that Φ^1 is the unique solution of (4.34) and is of the form

$$\Phi^1=\begin{pmatrix} \Phi_x^1 & \Phi_z^1 \\ -\Phi_z^1 & \Phi_y^1 \end{pmatrix}. \tag{5.6}$$

In particular, it follows from (5.6) and Φ^1 being symmetric that Φ_z^1 is antisymmetric. In order to find an expression for the solution of Eq. (4.34), we decompose the inhomogeneous term on the RHS of (4.34) into powers of η and solve the equation separately for each case. One has

$$3(\mathbf{N}\Phi^0+\Phi^0\mathbf{N}^{\mathrm{T}})=\frac{3k^2T^2}{\omega^4}(\mathbf{H}_0+\eta\mathbf{H}_1+\eta^2\mathbf{H}_2), \tag{5.7}$$

where, cf. (4.15)–(4.18) and (4.31),

$$\mathbf{H}_0=\begin{pmatrix} \mathbf{0} & \mathbf{G}_\kappa^{-1}\mathbf{V}_0 \\ \mathbf{V}_0\mathbf{G}_\kappa^{-1} & \mathbf{0} \end{pmatrix}, \tag{5.8}$$

$$\mathbf{H}_1=\begin{pmatrix} \mathbf{0} & \mathbf{X}^0\mathbf{V}_0+\mathbf{G}_\kappa^{-1}\mathbf{V}_1 \\ \mathbf{V}_1\mathbf{G}_\kappa^{-1}+\mathbf{V}_0\mathbf{X}^0 & \gamma\nu[\mathbf{V}_0,\mathbf{Z}^0] \end{pmatrix}, \tag{5.9}$$

$$\mathbf{H}_2=\begin{pmatrix} \mathbf{0} & \mathbf{X}^0\mathbf{V}_1 \\ \mathbf{V}_1\mathbf{X}^0 & \gamma\nu[\mathbf{V}_1,\mathbf{Z}^0] \end{pmatrix}, \tag{5.10}$$

with

$$\mathbf{V}_0 \equiv \operatorname{diag}(\mathbf{G}_\kappa^{-1}), \qquad \mathbf{V}_1 \equiv \operatorname{diag}(\mathbf{X}^0). \tag{5.11}$$

In the sequel, we will denote $(\mathbf{V}_0)_{ij} = \delta_{ij} g_i$, where $g_i = (\mathbf{G}_\kappa^{-1})_{ii}$ read

$$g_i = \frac{\sinh i\bar{\alpha}}{\sinh \bar{\alpha}} \frac{\sinh(N+1-i)\,\bar{\alpha}}{\sinh(N+1)\,\bar{\alpha}}, \tag{5.12}$$

with $\bar{\alpha}$ defined by $\cosh \bar{\alpha} = 1+\kappa/2$. Writing

$$\Phi^1 = \frac{3k^2T^2}{\omega^4}\,(\Phi_0^1 + \eta\Phi_1^1 + \eta^2\Phi_2^1), \tag{5.13}$$

one thus obtains that Φ_l^1, $l = 0, 1, 2$, is the unique solution of

$$\mathbf{b}\Phi_l^1 + \Phi_l^1\mathbf{b}^{\mathrm{T}} = \mathbf{H}_l. \tag{5.14}$$

In order to scale out the constants in $\mathbf{b}$, we denote for $l = 0, 1, 2$,

$$\Phi_l^1 = \begin{pmatrix} \frac{1}{\omega^2}\mathbf{X}_l & \frac{1}{\gamma}\mathbf{Z}_l \\ -\frac{1}{\gamma}\mathbf{Z}_l & \mathbf{Y}_l \end{pmatrix}, \tag{5.15}$$

together with

$$\mathbf{R} = \gamma^{-1}\mathbf{a}, \qquad \mathbf{G}_\kappa = \omega^{-2}\mathbf{g}_\kappa, \tag{5.16}$$

namely, $\mathbf{R}_{ij} = \delta_{ij}(\delta_{1j} + \delta_{Nj})$ and $(\mathbf{G}_\kappa)_{ij} = (2+\kappa)\,\delta_{ij} - \delta_{ij+1} - \delta_{ij-1}$. The zero order term in (5.13) is just the first-order perturbation of the anharmonic chain at the equilibrium $T_1 = T_N$. Inserting (5.15) into (5.14) for $l = 0$ yields the equivalent system of equations for $\mathbf{X}_0$, $\mathbf{Y}_0$, and $\mathbf{Z}_0$

$$\mathbf{Y}_0 = \mathbf{X}_0\mathbf{G}_\kappa + \mathbf{Z}_0\mathbf{R} + \mathbf{G}_\kappa^{-1}\mathbf{V}_0, \tag{5.17}$$

$$[\mathbf{G}_\kappa, \mathbf{Z}_0] = -\frac{1}{\nu}\{\mathbf{R}, \mathbf{Y}_0\}, \tag{5.18}$$

with the requirement that $\mathbf{X}_0$, $\mathbf{Y}_0$ are symmetric and $\mathbf{Z}_0$ is antisymmetric. One easily checks that its unique solution is given by

$$\mathbf{X}_0 = -\mathbf{G}_\kappa^{-1}\mathbf{V}_0\mathbf{G}_\kappa^{-1}, \qquad \mathbf{Y}_0 = 0, \qquad \mathbf{Z}_0 = 0, \tag{5.19}$$

thus recovering, as expected, the first-order correction of the $\lambda\phi^4$ model. Proceeding similarly for Φ_1^1 and Φ_2^1, one finds that $\mathbf{X}_1$, $\mathbf{Y}_1$, $\mathbf{Z}_1$ solve

$$\mathbf{Y}_1 = \mathbf{X}_1 \mathbf{G}_\kappa + \mathbf{Z}_1 \mathbf{R} + (\mathbf{X}^0 \mathbf{V}_0 + \mathbf{G}_\kappa^{-1} \mathbf{V}_1), \tag{5.20}$$

$$[\mathbf{G}_\kappa, \mathbf{Z}_1] = -\frac{1}{\nu} \{\mathbf{R}, \mathbf{Y}_1\} + [\mathbf{Z}^0, \mathbf{V}_0], \tag{5.21}$$

whereas $\mathbf{X}_2$, $\mathbf{Y}_2$, $\mathbf{Z}_2$ solve

$$\mathbf{Y}_2 = \mathbf{X}_2 \mathbf{G}_\kappa + \mathbf{Z}_2 \mathbf{R} + \mathbf{X}^0 \mathbf{V}_1, \tag{5.22}$$

$$[\mathbf{G}_\kappa, \mathbf{Z}_2] = -\frac{1}{\nu} \{\mathbf{R}, \mathbf{Y}_2\} + [\mathbf{Z}^0, \mathbf{V}_1]. \tag{5.23}$$

Furthermore, using the c-symmetry properties of the solution $\mathbf{X}^0$ and $\mathbf{Z}^0$ of the harmonic case, cf. (4.19) and (4.21), one easily checks that $\mathbf{H}_1$ is CT-antisymmetric, whereas $\mathbf{H}_2$ is CT-symmetric. This implies that $\mathbf{X}_1$, $\mathbf{Y}_1$ are c-antisymmetric and $\mathbf{Z}_1$ is c-symmetric, whereas $\mathbf{X}_2$, $\mathbf{Y}_2$ are c-symmetric and $\mathbf{Z}_2$ is c-antisymmetric. This simply reflects the fact that changing the sign of η corresponds to interchanging the reservoirs at the ends of the chain.

In the next section, we will derive explicit expressions for the solutions of the above equations. To this end, we will need the following identities. Let $\mathbf{X}$ be a solution of

$$[\mathbf{G}_\kappa, \mathbf{X}] = \mathscr{U}, \tag{5.24}$$

with $\mathscr{U}$ a given matrix. It thus follows from $[\mathbf{G}_\kappa, \mathbf{X}]_{ij} = \mathscr{U}_{ij}$ that

$$\mathbf{X}_{i,j+1} - \mathbf{X}_{i-1,j} = \mathscr{U}_{ij} + (\mathbf{X}_{i+1,j} - \mathbf{X}_{i,j-1}), \tag{5.25}$$

where matrix elements with an index equals to zero or $N+1$ are set to zero. Let us first consider $\mathbf{X}$ antisymmetric. In particular, $\mathbf{X}$ is entirely determined by its elements $\mathbf{X}_{ij}$ with $i<j$ and satisfies $\mathbf{X}_{j+1,i} - \mathbf{X}_{j,i-1} = -(\mathbf{X}_{i,j+1} - \mathbf{X}_{i-1,j})$. For $i \leqslant j$, applying (5.25) recursively $j-i$ times thus leads to

$$\mathbf{X}_{i,j+1} - \mathbf{X}_{i-1,j} = \frac{1}{2} \sum_{l=0}^{j-i} \mathscr{U}_{i+l,j-l}. \tag{5.26}$$

This gives all matrix elements $\mathbf{X}_{1j}$, $1<j \leqslant N$. Applying (5.26) recursively $i-1$ times finally leads to

$$\mathbf{X}_{ij} = \frac{1}{2} \sum_{k=0}^{i-1} \sum_{l=0}^{j-i-1} \mathscr{U}_{i+l-k,j-l-k-1}, \tag{5.27}$$

for i, j such that $i<j$. Proceeding similarly, one obtains for a c-antisymmetric matrix $\mathbf{X}$ satisfying (5.24),

$$\mathbf{X}_{ij}=\frac{1}{2}\sum_{k=0}^{i-1}\sum_{l=0}^{N-i-j}\mathcal{U}_{i+l-k,\,j+l+k+1}, \tag{5.28}$$

for $i+j\leqslant N$. If $\mathbf{X}$ is both antisymmetric and c-antisymmetric, one iterates identity (5.26) $N+1-i-j$ times to obtain

$$\mathbf{X}_{ij}=-\frac{1}{4}\sum_{k=0}^{j-i-1}\sum_{l=0}^{N-i-j}\mathcal{U}_{i+l+k+1,\,j+l-k}, \tag{5.29}$$

for $i<j$ and $i+j\leqslant N$. Finally, proceeding similarly but without assuming any symmetry properties, one derives an expression for $\mathbf{X}$ depending both on $\mathcal{U}$ and the first line of $\mathbf{X}$,

$$\mathbf{X}_{ij}=\sum_{k=1}^{i}\mathbf{X}_{1,\,i+j-2k+1}-\sum_{k=1}^{i-1}\sum_{l=1}^{i-k}\mathcal{U}_{i+1-k-l,\,j-k+l}, \tag{5.30}$$

for $1<i\leqslant j$ and $i+j\leqslant N+1$. Formula (5.30) will be used later for $\mathbf{X}$ symmetric and c-symmetric. It reflects the fact that in such cases, the solution of (5.24) is determined up to a polynomial $P(\mathbf{G})$, that is up to N independent variables which can be supplemented as the first line of $\mathbf{X}$.

6. THE FIRST-ORDER CORRECTION

In this section, we derive an expression for the first-order correction to the heat current and temperature profile.

We find that the part corresponding to the heat current is uniformly bounded in N. Regarding the temperature profile, the part of the solution proportional to η is exponentially decaying in the bulk of the chain whenever $\kappa>0$. The decay rate is slower than in the purely harmonic case. For $\kappa=0$, the profile proportional to η is linear in the bulk of the chain and we compute its slope explicitly. However, as mentioned in the Section 1, the sign is "wrong," namely, the linear profile has the *lowest* temperature close to the *hottest* bath and the *highest* temperature close to the *coldest* bath. The same type of phenomenon is present for $\kappa>0$, in the sense that the profile is not monotonic, see Fig. 1. Moreover, we observe that the part proportional to η^2 gives a significant contribution resulting in a shift of the temperature at the middle point of the chain, see Fig. 2. The temperature at this point is no more the arithmetic mean of the baths temperatures. Although surprising, this phenomenon is observed in numerical studies of certain anharmonic chains, see refs. 1 and 9.

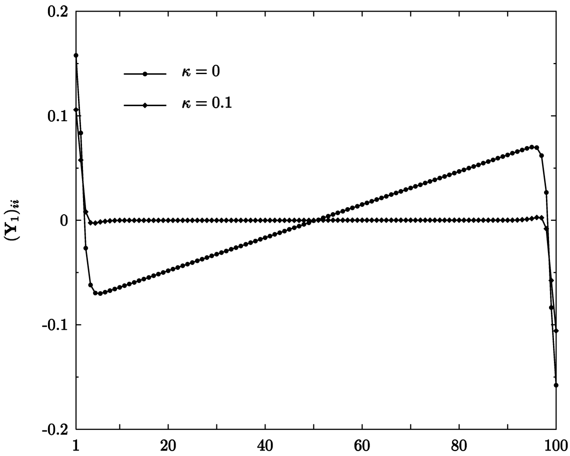

Fig. 1. Contribution of $\mathbf{Y}_1$ to the temperature profile ($\nu=1$, $N=100$).

6.1. First-Order Correction to the Heat Current

In our model, the heat current in the SNS is given by $(\Phi_z^\lambda)_{i,i+1}$. The first-order correction will thus be given in terms of, cf. (5.13) and (5.15),

$$\Phi_z^1 = \frac{3k^2T^2}{\gamma\omega^4}(\mathbf{Z}_0 + \eta\mathbf{Z}_1 + \eta^2\mathbf{Z}_2). \tag{6.1}$$

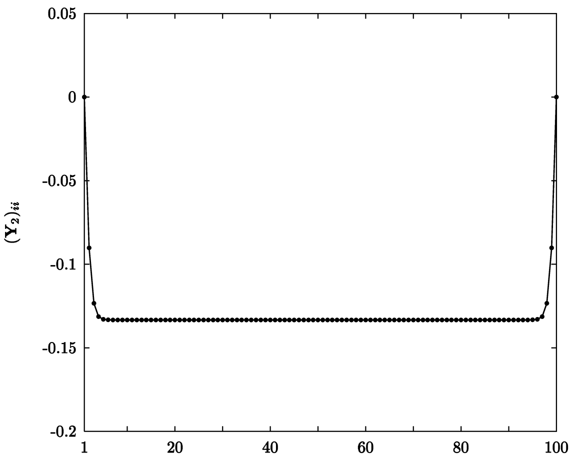

Fig. 2. Contribution of $\mathbf{Y}_2$ to the temperature profile ($\nu=1$, $\kappa=0$, $N=100$).

By (5.19), $\mathbf{Z}_0$ does not contribute and one easily checks that for $1 \leqslant i \leqslant N-1$,

$$(\mathbf{Z}_2)_{i,\, i+1} = 0. \tag{6.2}$$

That is, $\mathbf{Z}_2$ does not contribute to the current either. Indeed, recall that $\mathbf{Z}_2$ is antisymmetric and satisfies Eq. (5.23). Since $\{\mathbf{R}, \mathbf{Y}_2\}$ is a bordered matrix and $[\mathbf{Z}^0, \mathbf{V}_1]$ is zero on the diagonal, one obtains by using formula (5.27) that

$$-\frac{1}{\nu}(\mathbf{Y}_2)_{11} = (\mathbf{Z}_2)_{12} = (\mathbf{Z}_2)_{23} = \cdots = (\mathbf{Z}_2)_{N-1,\, N}. \tag{6.3}$$

This leads to (6.2), since $(\mathbf{Z}_2)_{12} = -(\mathbf{Z}_2)_{N-1,\, N}$ by c-antisymmetry of $\mathbf{Z}_2$. We note for later use that this also implies

$$(\mathbf{Y}_2)_{11} = 0. \tag{6.4}$$

It thus remains to consider the contribution of $\mathbf{Z}_1$. Since $\mathbf{Z}_1$ is antisymmetric, one obtains from (5.21) that

$$\mathbf{Z}_1 = \mathbf{Z} + \mathscr{Z}, \tag{6.5}$$

where $\mathbf{Z}$ and $\mathscr{Z}$ are given by formula (5.27) with $\mathscr{U}$ replaced by $-\frac{1}{\nu}\{\mathbf{R}, \mathbf{Y}_1\}$ and, respectively, $[\mathbf{Z}^0, \mathbf{V}_0]$. We first observe that $\{\mathbf{R}, \mathbf{Y}_1\}$ is a bordered symmetric matrix, so that formula (5.27) yields

$$\mathbf{Z} = \begin{pmatrix} 0 & \varphi_1 & \varphi_2 & & \varphi_{N-2} & \varphi_{N-1} \\ -\varphi_1 & \ddots & \ddots & \ddots & & \varphi_{N-2} \\ -\varphi_2 & \ddots & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \varphi_2 \\ & & & \ddots & \ddots & \varphi_1 \\ -\varphi_{N-1} & & & -\varphi_2 & -\varphi_1 & 0 \end{pmatrix}, \tag{6.6}$$

where the quantities $\varphi_1, \ldots, \varphi_{N-1}$ are related to the first line of $\mathbf{Y}_1$, namely, for $j = 1, \ldots, N-1$,

$$\nu \varphi_j = -(\mathbf{Y}_1)_{1j}. \tag{6.7}$$

Furthermore, $[\mathbf{Z}^0, \mathbf{V}_0]$ having zero diagonal implies that $\mathscr{Z}_{i,\, i+1} = 0$. One therefore obtains

$$(\mathbf{Z}_1)_{i,\, i+1} = \mathbf{Z}_{i,\, i+1} = \varphi_1. \tag{6.8}$$

In order to compute the vector $\varphi \in \mathbf{R}^{N-1}$, one considers the first line of Eq. (5.20) for $\mathbf{Y}_1$ into which one substitutes identity (6.7). We first need to compute $\mathbf{X}_1$. Equation (5.20) and the symmetry properties of $\mathbf{X}_1$, $\mathbf{Y}_1$ and $\mathbf{Z}_1$ imply that $\mathbf{X}_1$ satisfies

$$[\mathbf{G}_\kappa, \mathbf{X}_1] = \{\mathbf{R}, \mathbf{Z}_1\} + ([\mathbf{X}^0, \mathbf{V}_0] + [\mathbf{G}_\kappa^{-1}, \mathbf{V}_1]) \tag{6.9}$$

$$= \{\mathbf{R}, \mathbf{Z}\} + \{\mathbf{R}, \mathscr{Z}\} + ([\mathbf{X}^0, \mathbf{V}_0] + [\mathbf{G}_\kappa^{-1}, \mathbf{V}_1]). \tag{6.10}$$

Since $\mathbf{X}_1$ is c-antisymmetric, it follows from (6.10) that

$$\mathbf{X}_1 = \mathbf{X} + \mathscr{X}, \tag{6.11}$$

where $\mathbf{X}$ and $\mathscr{X}$ are given by formula (5.28) with $\mathscr{U}$ replaced by $\{\mathbf{R}, \mathbf{Z}\}$ and, respectively, $\{\mathbf{R}, \mathscr{Z}\} + ([\mathbf{X}^0, \mathbf{V}_0] + [\mathbf{G}_\kappa^{-1}, \mathbf{V}_1])$. Using that $\{\mathbf{R}, \mathbf{Z}\}$ is a bordered antisymmetric matrix, one obtains from (5.28) and (6.6) that

$$\mathbf{X} = \begin{pmatrix}
\varphi_1 & \varphi_2 & \varphi_3 & & \varphi_{N-1} & 0 \\
\varphi_2 & \iddots & \iddots & \iddots & \iddots & -\varphi_{N-1} \\
\varphi_3 & \iddots & \iddots & \iddots & \iddots & \\
 & \iddots & \iddots & \iddots & \iddots & \\
\varphi_{N-1} & & & \iddots & \iddots & -\varphi_2 \\
0 & -\varphi_{N-1} & & & -\varphi_2 & -\varphi_1
\end{pmatrix}. \tag{6.12}$$

Equation (5.20) now reads

$$\mathbf{Y}_1 = \mathbf{X}\mathbf{G}_\kappa + \mathbf{Z}\mathbf{R} + \mathbf{W}, \tag{6.13}$$

with

$$\mathbf{W} = \mathscr{X}\mathbf{G}_\kappa + \mathscr{Z}\mathbf{R} + (\mathbf{X}^0\mathbf{V}_0 + \mathbf{G}_\kappa^{-1}\mathbf{V}_1), \tag{6.14}$$

and since $(\mathbf{X}\mathbf{G}_\kappa + \mathbf{Z}\mathbf{R})_{1j} = (\mathbf{G}_\kappa \mathbf{X}_{1\cdot})_j = (\mathbf{G}_\kappa^{(N-1)}\varphi)_j$ for $j = 1, \ldots, N-1$, where $\mathbf{G}_\kappa^{(k)}$ denotes the k-square version of $\mathbf{G}_\kappa$, it follows from (6.7) that

$$\mathbf{G}_{\nu+\kappa}^{(N-1)}\varphi = -\mathbf{w}, \tag{6.15}$$

where $\mathbf{w} \in \mathbf{R}^{N-1}$ is given by $\mathbf{w}_j = \mathbf{W}_{1j}$, $j = 1, \ldots, N-1$. Therefore, one finally obtains, recalling that $\eta = \frac{T_1 - T_N}{2T}$,

$$(\Phi_z^1)_{i,i+1} = \frac{3k^2 T (T_1 - T_N)}{2\gamma\omega^4}\varphi_1, \tag{6.16}$$

with φ given by $\varphi = -[\mathbf{G}_{\nu+\kappa}^{(N-1)}]^{-1}\,\mathbf{w}$. As $(\Phi_z^1)_{i,\,i+1}$ represent the first-order correction to the current, it is consistent to see that they are all equal to each other.

Before turning to the first-order correction of the temperature profile, we study the behaviour of φ_1 with N. We first note that $\mathbf{X}$ solves the equation $[\mathbf{G}_\kappa, \mathbf{X}] = \{\mathbf{R}, \mathbf{Z}\}$, as is easily checked from (6.6) and (6.12). This implies that $\mathscr{X}$ solves, cf. (6.10) and (6.11),

$$[\mathbf{G}_\kappa, \mathscr{X}] = \{\mathbf{R}, \mathbf{Z}\} + ([\mathbf{X}^0, \mathbf{V}_0] + [\mathbf{G}_\kappa^{-1}, \mathbf{V}_1]), \tag{6.17}$$

which in turn implies, by using in addition the symmetry properties of the matrices involved in (6.14), that $\mathbf{W}$ is c-antisymmetric and satisfies the equation

$$[\mathbf{G}_\kappa, \mathbf{W}] = \mathbf{G}_\kappa \mathscr{Z}\mathbf{R} + \mathbf{R}\mathscr{Z}\mathbf{G}_\kappa + (\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_0 - \mathbf{V}_0 \mathbf{X}^0 \mathbf{G}_\kappa). \tag{6.18}$$

Hence, $\mathbf{W}_{1N} = 0$ and it follows from formula (5.28) that

$$\mathbf{w} = \mathbf{w}^{(1)} + \mathbf{w}^{(2)}, \tag{6.19}$$

where, for $1 \leqslant j \leqslant N-1$,

$$\mathbf{w}_j^{(1)} = \frac{1}{2} \sum_{l=1}^{N-j} (\mathbf{G}_\kappa \mathscr{Z}\mathbf{R} + \mathbf{R}\mathscr{Z}\mathbf{G}_\kappa)_{l,\,l+j}, \tag{6.20}$$

$$\mathbf{w}_j^{(2)} = \frac{1}{2} \sum_{l=1}^{N-j} (\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_0 - \mathbf{V}_0 \mathbf{X}^0 \mathbf{G}_\kappa)_{l,\,l+j}. \tag{6.21}$$

We first consider $\mathbf{w}^{(1)}$. We note that $\mathbf{G}_\kappa \mathscr{Z}\mathbf{R} + \mathbf{R}\mathscr{Z}\mathbf{G}_\kappa$ is a bordered c-symmetric matrix and that $\mathscr{Z}$ is c-symmetric since both $\mathbf{Z}_1$ and $\mathbf{Z}$ are c-symmetric. One thus obtains from (6.20)

$$\mathbf{w}^{(1)} = \mathbf{G}_\kappa^{(N-1)}\, \widetilde{\mathscr{Z}}, \tag{6.22}$$

where, for $1 \leqslant j \leqslant N-1$,

$$\widetilde{\mathscr{Z}}_j = \mathscr{Z}_{1,\,j+1}. \tag{6.23}$$

In order to compute $\widetilde{\mathscr{Z}}$, we note that $\mathbf{Z}$ solves the equation $[\mathbf{G}_\kappa, \mathbf{Z}] = -\frac{1}{\nu}\{\mathbf{R}, \mathbf{Y}_1\}$, as is easily checked from (6.6) and (6.7). Therefore, $\mathscr{Z}$ solves, cf. (5.21) and (6.5),

$$[\mathbf{G}_\kappa, \mathscr{Z}] = [\mathbf{Z}^0, \mathbf{V}_0], \tag{6.24}$$

and since $\mathscr{Z}$ is antisymmetric, as both $\mathbf{Z}_1$ and $\mathbf{Z}$ are, it follows from (4.21), $(\mathbf{V}_0)_{ij} = \delta_{ij} g_i$, and formula (5.27), that for $2 \leqslant j \leqslant N$,

$$\mathscr{Z}_{1j} = \frac{1}{2} \sum_{l=1}^{j-1} (g_{j-l} - g_l)\, \phi_{j-2l}, \tag{6.25}$$

with the convention $\phi_{-k} = -\phi_k$, $0 \leqslant k \leqslant N-1$. Thus, $\mathbf{w}^{(1)}$ is given by (6.22) with $\widetilde{\mathscr{Z}} \in \mathbf{R}^{N-1}$ given by

$$\widetilde{\mathscr{Z}}_j = \frac{1}{2} \sum_{l=1}^{j} (g_{j+1-l} - g_l)\, \phi_{j+1-2l}. \tag{6.26}$$

We next consider $\mathbf{w}^{(2)}$. We first note that

$$\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_0 - \mathbf{V}_0 \mathbf{X}^0 \mathbf{G}_\kappa = (\mathbf{G}_{\nu+\kappa} \mathbf{X}^0 \mathbf{V}_0 - \mathbf{V}_0 \mathbf{X}^0 \mathbf{G}_{\nu+\kappa}) + \nu(\mathbf{V}_0 \mathbf{X}^0 - \mathbf{X}^0 \mathbf{V}_0), \tag{6.27}$$

and compute, using (4.19), (4.22), and $(\mathbf{V}_0)_{ij} = \delta_{ij} g_i$, that for $i \leqslant j$,

$$(\mathbf{G}_{\nu+\kappa} \mathbf{X}^0 \mathbf{V}_0 - \mathbf{V}_0 \mathbf{X}^0 \mathbf{G}_{\nu+\kappa})_{ij} = \delta_{1i}\, g_j \phi_{j-1} + \delta_{Nj}\, g_i \phi_{N-i}. \tag{6.28}$$

Therefore,

$$(\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_0 - \mathbf{V}_0 \mathbf{X}^0 \mathbf{G}_\kappa)_{ij} = \delta_{i1}\, g_j \phi_{j-1} + \delta_{jN}\, g_i \phi_{N-i} + \nu(g_i - g_j)\, \phi_{i+j-1}, \tag{6.29}$$

with the convention $\phi_{N+k} = -\phi_{N-k}$, $0 \leqslant k \leqslant N$. One thus finally obtains for $\mathbf{w}^{(2)} \in \mathbf{R}^{N-1}$, using in addition that $g_{N-j} = g_{j+1}$,

$$\mathbf{w}^{(2)}_j = g_{j+1} \phi_j + \frac{\nu}{2} \sum_{l=1}^{N-j} (g_l - g_{j+l})\, \phi_{j-1+2l}. \tag{6.30}$$

Using (6.15), (6.19), (6.22), (6.26), (6.30), and the fact that the ϕ_j's decay exponentially, it is easy to see that φ_1 is uniformly bounded in N.

6.2. First-Order Correction to the Temperature Profile

We now analyse the first-order correction to the temperature profile. It is given by $(\Phi^1_y)_{ii}$ where, cf. (5.13) and (5.15),

$$\Phi^1_y = \frac{3k^2 T^2}{\omega^4} (\mathbf{Y}_0 + \eta \mathbf{Y}_1 + \eta^2 \mathbf{Y}_2). \tag{6.31}$$

By (5.19), $\mathbf{Y}_0$ does not contribute to Φ^1_y. In order to compute the diagonal of $\mathbf{Y}_1$, we use the fact that $\mathbf{Y}_1$ is c-antisymmetric and satisfies the equation, as a consequence of (5.20),

$$[\mathbf{G}_\kappa, \mathbf{Y}_1] = \mathbf{G}_\kappa \mathbf{Z}_1 \mathbf{R} + \mathbf{R} \mathbf{Z}_1 \mathbf{G}_\kappa + (\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_0 - \mathbf{V}_0 \mathbf{X}^0 \mathbf{G}_\kappa). \tag{6.32}$$

Using (5.28), (6.29), and the fact that $g_{2i} = g_{N-2i+1}$, one thus obtains for $1 \leqslant i \leqslant [N/2]$, where $[x]$ denotes the largest integer smaller or equal to x,

$$(\mathbf{Y}_1)_{ii} = (\mathbf{G}_\kappa^{(N-1)} \tilde{\mathbf{Z}}_1)_{2i-1} + \left(g_{2i} \phi_{2i-1} + \frac{\nu}{2} \sum_{l=i}^{N-i} \phi_{2l} \sum_{k=0}^{i-1} (g_{l-k} - g_{l+k+1}) \right), \tag{6.33}$$

where $\tilde{\mathbf{Z}}_1 \in \mathbf{R}^{N-1}$ is given by $(\tilde{\mathbf{Z}}_1)_j = (\mathbf{Z}_1)_{1,j+1}$. Since the ϕ_j decay exponentially fast with rate α, see (4.23), it follows that all terms but the first give an exponentially flat contribution to $(\mathbf{Y}_1)_{ii}$. We thus write, and will adopt a similar notation in the sequel,

$$(\mathbf{Y}_1)_{ii} = (\mathbf{G}_\kappa^{(N-1)} \tilde{\mathbf{Z}}_1)_{2i-1} + \mathcal{O}(e^{-\alpha j}). \tag{6.34}$$

In order to compute the dominant term in the above expression, we first use that $\tilde{\mathbf{Z}}_1 = \varphi + \tilde{\mathscr{Z}}$ where $\tilde{\mathscr{Z}}$ is given by (6.26), and $\mathbf{G}_{\nu+\kappa}^{(N-1)} \varphi = -\mathbf{w}$ where $\mathbf{w} = \mathbf{G}_\kappa^{(N-1)} \tilde{\mathscr{Z}} + \mathbf{w}^{(2)}$ with $\mathbf{w}^{(2)}$ given by (6.30), to obtain $\tilde{\mathbf{Z}}_1 = (\mathbf{G}_{\nu+\kappa}^{(N-1)})^{-1} \times (\nu \tilde{\mathscr{Z}} - \mathbf{w}^{(2)})$ and thus

$$(\mathbf{Y}_1)_{ii} = ((\mathbf{G}_{\nu+\kappa}^{(N-1)})^{-1} \mathbf{G}_\kappa^{(N-1)} (\nu \tilde{\mathscr{Z}} - \mathbf{w}^{(2)}))_{2i-1} + \mathcal{O}(e^{-\alpha j}). \tag{6.35}$$

It follows from the expression (6.21) for $\mathbf{w}^{(2)}$ and properties of $\mathbf{G}_\kappa^{(N-1)}$, $\mathbf{G}_{\nu+\kappa}^{(N-1)}$, and their inverse, that the second term gives an exponentially flat contribution to the temperature profile. To compute the remaining term $y \equiv \nu (\mathbf{G}_{\nu+\kappa}^{(N-1)})^{-1} \mathbf{G}_\kappa^{(N-1)} \tilde{\mathscr{Z}}$, we first note that it satisfies

$$\mathbf{G}_{\nu+\kappa}^{(N-1)} y = \nu \mathbf{G}_\kappa^{(N-1)} \tilde{\mathscr{Z}}. \tag{6.36}$$

We next compute $\mathbf{G}_\kappa^{(N-1)} \tilde{\mathscr{Z}}$. In the expression (6.26) for $\tilde{\mathscr{Z}}$, changing the summation index to k with $2k = j+1-2l$ if j is odd and $2k = j-2l$ if j is even, one obtains, using in addition the symmetry properties of g_i, that for $j \geqslant 2$

$$\tilde{\mathscr{Z}}_j = \begin{cases} \displaystyle\sum_{k=1}^{\frac{j-1}{2}} (g_{\frac{j+1}{2}+k} - g_{\frac{j+1}{2}-k})\, \phi_{2k} & \text{if } j \text{ is odd,} \\ \displaystyle\sum_{k=1}^{\frac{j}{2}} (g_{\frac{j}{2}+k} - g_{\frac{j}{2}+1-k})\, \phi_{2k-1} & \text{if } j \text{ is even.} \end{cases} \tag{6.37}$$

For $j=1$, $\tilde{\mathscr{Z}}_1=0$. Computing the differences of g's arising in the above expression leads to

$$\tilde{\mathscr{Z}}_j=\frac{\sinh(N-j)\,\bar{\alpha}}{\sinh(N+1)\,\bar{\alpha}}\sum_{k=1}^{\frac{j-1+\bar{j}}{2}}\frac{\sinh(2k-\bar{j})\,\bar{\alpha}}{\sinh\bar{\alpha}}\,\phi_{2k-\bar{j}},\tag{6.38}$$

where $\bar{j}=0$ if j is odd and $\bar{j}=1$ if j is even. Hence, $\tilde{\mathscr{Z}}$ can be rewritten as

$$\tilde{\mathscr{Z}}_j=\rho_{\bar{j}}\,\frac{\sinh(N-j)\,\bar{\alpha}}{\sinh(N+1)\,\bar{\alpha}}+\mathscr{O}(e^{-\alpha j}),\tag{6.39}$$

where the constants ρ_0 and ρ_1 are given by

$$\rho_\sigma=\sum_{k=1}^{[N/2]}\frac{\sinh(2k-\sigma)\,\bar{\alpha}}{\sinh\bar{\alpha}}\,\phi_{2k-\sigma},\qquad \sigma=0,1.\tag{6.40}$$

A straightforward computation finally leads to, recalling that $\cosh\bar{\alpha}=1+\kappa/2$,

$$(\mathbf{G}_\kappa^{(N-1)}\tilde{\mathscr{Z}})_j=(-1)^{\bar{j}+1}\,(2+\kappa)(\rho_1-\rho_0)\,\frac{\sinh(N-j)\,\bar{\alpha}}{\sinh(N+1)\,\bar{\alpha}}+C_1\delta_{1j}+\mathscr{O}(e^{-\alpha j}),\tag{6.41}$$

where C_1 is a constant that depends on N and $\bar{\alpha}$ only. It thus remains to compute the vector y given by Eq. (6.36). To this end, we note that a vector of the form (6.41) is almost an eigenvector of $\mathbf{G}_{\nu+\kappa}^{(N-1)}$. More precisely, one has for v with $v_j=(-1)^{\bar{j}+1}\sinh(N-j)\,\bar{\alpha}$,

$$(\mathbf{G}_{\nu+\kappa}^{(N-1)}v)_j=(4+\nu+2\kappa)\,v_j+\delta_{1j}\sinh N\bar{\alpha}.\tag{6.42}$$

Therefore, writing

$$y_j=(-1)^{\bar{j}+1}\,\frac{\nu(2+\kappa)(\rho_1-\rho_0)}{(4+\nu+2\kappa)}\,\frac{\sinh(N-j)\,\bar{\alpha}}{\sinh(N+1)\,\bar{\alpha}}+r_j,\tag{6.43}$$

and inserting in (6.36) yield for r the equation $(\mathbf{G}_{\nu+\kappa}^{(N-1)}r)_j=C_2\delta_{1j}+\mathscr{O}(e^{-\alpha j})$ with C_2 a constant depending on N and $\bar{\alpha}$, cf. (6.41) and (6.42), whose solution reads, by using (4.22),

$$r_j=C_2\phi_j+\mathscr{O}(e^{-\alpha j}).\tag{6.44}$$

Hence, r is an exponentially decaying correction to y as given by (6.43). Finally, since $(\mathbf{Y}_1)_{ii} = y_{2i-1}$ for $1 \leqslant i \leqslant [N/2]$, we obtain from (6.43),

$$(\mathbf{Y}_1)_{ii} = -\frac{\nu(2+\kappa)(\rho_1-\rho_0)}{(4+\nu+2\kappa)} \frac{\sinh(N+1-2i)\,\bar{\alpha}}{\sinh(N+1)\,\bar{\alpha}} + \mathcal{O}(e^{-2\alpha i}). \tag{6.45}$$

Since $\mathbf{Y}_1$ is c-antisymmetry, (6.45) also gives the elements $(\mathbf{Y}_1)_{ii}$ for $[N/2]+1 \leqslant i \leqslant N$. In particular, since $\cosh \bar{\alpha} = 1+\kappa/2$, it follows that the contribution of $\mathbf{Y}_1$ to the temperature profile is exponentially flat in the bulk of the chain whenever $\kappa > 0$. When $\kappa = 0$, on the other hand, $\bar{\alpha} = 0$ and $\mathbf{Y}_1$ gives a linear profile. In the limit $N \to \infty$, it is straightforward to compute that for $\kappa = 0$, ρ_1 and ρ_0 are given by

$$\rho_0 = \frac{1}{2\sinh^2 \alpha} \qquad \text{and} \qquad \rho_1 = \frac{\cosh \alpha}{2\sinh^2 \alpha}, \tag{6.46}$$

with α defined by $\cosh \alpha = 1+\nu/2$. One thus has $\rho_1 - \rho_0 = 1/(4+\nu)$ and the temperature profile for $\kappa = 0$ is given by

$$(\mathbf{Y}_1)_{ii} = \frac{2\nu}{(4+\nu)^2}\left(\frac{2i}{N+1} - 1\right) + \mathcal{O}(e^{-2\alpha i}). \tag{6.47}$$

The temperature profile is linear, but oriented in the "wrong" direction. Indeed, if for instance $T_1 > T_N$, then one obtains from (6.31), which involves a multiplication by $\eta = (T_1 - T_N)/(T_1 + T_N)$, that the slope is positive.

We next consider the contribution of $\mathbf{Y}_2$ to the temperature profile. Since $\mathbf{Y}_2$ is c-symmetric, it will introduce, if nonzero, a global shift in the temperature profile. As we shall see, this is indeed the case. To compute the diagonal $(\mathbf{Y}_2)_{ii}$, we proceed as for $\mathbf{Y}_1$. We first recall that $(\mathbf{Y}_2)_{11} = 0$, cf. (6.4), and note that $\mathbf{Y}_2$ also satisfies,

$$[\mathbf{G}_\kappa, \mathbf{Y}_2] = \mathbf{G}_\kappa \mathbf{Z}_2 \mathbf{R} + \mathbf{R} \mathbf{Z}_2 \mathbf{G}_\kappa + (\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_1 - \mathbf{V}_1 \mathbf{X}^0 \mathbf{G}_\kappa). \tag{6.48}$$

Denoting by ψ the first line of $\mathbf{Y}_2$, i.e.,

$$\psi_i \equiv (\mathbf{Y}_2)_{1i}, \tag{6.49}$$

one uses (5.30) to obtain from (6.48) the following expression, for $i \geqslant 2$ and $2i \leqslant N+1$,

$$(\mathbf{Y}_2)_{ii} = \sum_{k=1}^{i-1} \psi_{2k+1} - \sum_{k=1}^{i-1} \sum_{l=1}^{k} \mathbf{U}_{k-l+1,\,k+l}, \tag{6.50}$$

where $\psi_1 = (\mathbf{Y}_2)_{11} = 0$ has been used, and

$$\mathbf{U} = \mathbf{G}_\kappa \mathbf{Z}_2 \mathbf{R} + \mathbf{R}\mathbf{Z}_2 \mathbf{G}_\kappa + (\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_1 - \mathbf{V}_1 \mathbf{X}^0 \mathbf{G}_\kappa). \tag{6.51}$$

Since $\mathbf{Y}_2$ is c-symmetric, (6.50) determines all diagonal elements $(\mathbf{Y}_2)_{ii}$, $2 \leqslant i \leqslant N-1$. The first term on the RHS of (6.48) is a bordered matrix and a straightforward computation yields

$$\sum_{l=1}^{k} (\mathbf{G}_\kappa \mathbf{Z}_2 \mathbf{R} + \mathbf{R}\mathbf{Z}_2 \mathbf{G}_\kappa)_{k-l+1,\, k+l} = (\mathbf{G}_\kappa \zeta)_{2k}, \tag{6.52}$$

where ζ denotes the first line of $\mathbf{Z}_2$, i.e.,

$$\zeta_i = (\mathbf{Z}_2)_{1i}. \tag{6.53}$$

The second term on the RHS of (6.51) is identical to the corresponding term appearing in (6.18), with $\mathbf{V}_0$ replaced by the diagonal matrix $(\mathbf{V}_1)_{ij} = \delta_{ij}\phi_{2i-1}$. For $1 \leqslant i \leqslant j \leqslant N$, it is thus given by, cf. (6.29),

$$\begin{aligned}(\mathbf{G}_\kappa \mathbf{X}^0 \mathbf{V}_1 &- \mathbf{V}_1 \mathbf{X}^0 \mathbf{G}_\kappa)_{ij} \\ &= \nu(\phi_{2i-1} - \phi_{2j-1})\, \phi_{i+j-1} + \delta_{i1}\phi_{2j-1}\phi_{j-1} + \delta_{jN}\phi_{2i-1}\phi_{N-i},\end{aligned} \tag{6.54}$$

with the convention $\phi_{N+k} = -\phi_{N-k}$, $0 \leqslant k \leqslant N$. Inserting (6.52) and (6.54) into (6.50) leads to

$$(\mathbf{Y}_2)_{ii} = \sum_{k=1}^{i-1} \Delta_k \tag{6.55}$$

where, for $k \geqslant 1$ and $2k \leqslant N-1$,

$$\Delta_k = \psi_{2k+1} - (\mathbf{G}_\kappa \zeta)_{2k} - \left(\phi_{2k-1}\phi_{4k-1} + \nu\phi_{2k} \sum_{l=1}^{k} (\phi_{2(k-l)+1} - \phi_{2(k+l)-1}) \right). \tag{6.56}$$

One checks that $|\Delta_k|$ decays exponentially. First, recalling (4.23) and our convention $\phi_{N+k} = -\phi_{N-k}$, $0 \leqslant k \leqslant N$, this is clearly true of the last two terms in (6.56). Next, an expression for the first line of $\mathbf{Y}_2$ can be obtained from Eq. (5.23) by using that $\mathbf{Z}_2$ is c-antisymmetric. Formula (5.28) and $(\mathbf{Z}_2)_{k,\, k+1} = 0$, cf. (6.2), imply that for $1 \leqslant k \leqslant [(N-1)/2]$,

$$\frac{1}{\nu} \psi_{2k+1} = \frac{1}{2} \sum_{n=1}^{k} \phi_{2n} \sum_{l=k}^{N-k-1} (\phi_{2(l+n)+1} - \phi_{2(l-n)+1}), \tag{6.57}$$

with the convention $\phi_{N+k}=-\phi_{N-k}$, $0\leqslant k\leqslant N$. In particular, ψ_{2k+1} decays exponentially. We finally compute ζ, the first line of $\mathbf{Z}_2$. One has $\zeta_1=\zeta_N=0$ by antisymmetry and c-antisymmetry of $\mathbf{Z}_2$, and applying formula (5.29) to Eq. (5.23) yields for $2\leqslant j\leqslant N-1$

$$\zeta_j=\frac{1}{4}\sum_{n=1}^{j-1}\phi_{j-2n}\sum_{l=1}^{N-j}(\phi_{2(l+n)-1}-\phi_{2(j+l-n)-1}), \tag{6.58}$$

with the conventions $\phi_{-k}=-\phi_k$ and $\phi_{N+k}=-\phi_{N-k}$, $0\leqslant k\leqslant N$. Therefore, one has for $2\leqslant i\leqslant[(N+1)/2]$,

$$(\mathbf{Y}_2)_{ii}=h+\mathcal{O}(e^{-\alpha i}), \tag{6.59}$$

where the constant h is given by

$$h=h_1+\nu h_2, \tag{6.60}$$

with

$$h_1=\sum_{k=1}^{[\frac{N-1}{2}]}(2\zeta_{2k+1}-(2+\kappa)\,\zeta_{2k}-\phi_{2k-1}\phi_{4k-1}), \tag{6.61}$$

$$h_2=\sum_{k=1}^{[\frac{N-1}{2}]}\left(\frac{1}{\nu}\psi_{2k+1}-\phi_{2k}\sum_{l=1}^{k}(\phi_{2(k-l)+1}-\phi_{2(k+l)-1})\right). \tag{6.62}$$

A straightforward, but lengthy, computation yields the following asymptotic formulas for large N,

$$h_1=\frac{\cosh\alpha(\cosh\alpha-1-\kappa/2)}{2e^{\alpha}\sinh^2\alpha\sinh 3\alpha}, \tag{6.63}$$

$$h_2=-\frac{1}{4\sinh^2\alpha}\left(\frac{1}{\cosh\alpha}+\frac{\cosh\alpha}{e^{\alpha}\sinh 3\alpha}\right). \tag{6.64}$$

Recalling that $\cosh\alpha=1+(\nu+\kappa)/2$, one obtains

$$h=-\frac{2\nu}{(\nu+\kappa)(2+\nu+\kappa)(4+\nu+\kappa)}. \tag{6.65}$$

7. CONCLUSIONS

In the preceding sections, we have computed the first-order corrections to the heat current and temperature profile in a weakly anharmonic chain of oscillators out of equilibrium. The main feature of the model we considered is that it satisfies Fourier law, according to various numerical studies. In particular, the heat current decreases with the size of the system as $1/N$. This implies that for large N, the heat current is very different from its value in the harmonic case, which is finite and independent of N.[13] If Fourier law does hold whenever the anharmonicity parameter λ is strictly positive, one thus expects the heat current to develop a singularity at $\lambda = 0$ when $N \to \infty$. Our result shows that such a singularity does not manifest itself in a first-order perturbative analysis. The computation of the second-order correction to the current, which we reserve for a future publication, displays a divergence proportional to N when $\kappa = 0$. In the massive case $\kappa > 0$, no such divergence seems to occur. In this respect, we note that to our knowledge, no numerical simulations have been performed for very long chains in a regime of weak anharmonicity. The question of whether Fourier law holds for arbitrarily small values of λ or in regimes of very small temperature is at this point unclear, at least when $\kappa > 0$, see, e.g., ref. 14.

On the other hand, all derivatives of the heat current at $\lambda = 0$ remaining bounded in N would of course not preclude the chain from satisfying Fourier law for finite λ. The question of how much can be captured by a perturbative analysis regarding the behaviour of the heat current as N increases is delicate and concerns the convergence of the perturbation expansion. At $\lambda = 0$, the heat current is not analytic. However, we believe that the perturbation expansion may be Borel summable. Indeed, for the model considered here, it is very reminiscent of the usual $\lambda\phi^4$ expansion, in particular at equilibrium. Nevertheless, due to the singularity mentioned above, one expects at best the radius of convergence to decrease as the length of the chain increases.

Regarding the temperature profile, this issue is more delicate and it is *a priori* conceivable that the physically expected profile would be given by a perturbation expansion in λ. In any case, the smoothness of the invariant measure for a chain of finite length raises the question of how to interpret our result, which displays a counterintuitive orientation for the profile at first-order. There is indeed *a priori* no reason why the coldest oscillator should be closer to the hottest bath and vice-versa. Besides, the temperature profile obtained by the numerical simulations of refs. 1 and 9 is as expected, i.e., roughly linear and correctly oriented. Although those studies have been performed with heat baths modelized by Nose–Hover thermostats, whereas we consider Langevin couplings, it is doubtful that a particular choice of heat bath model would have such drastic consequences.

We note that the surprising behaviour we observe at first-order already occurs in the harmonic case of the chain considered here, in the weaker sense that the exponentially flat profile is non-monotonic.[13] As in ref. 13, we are at present unable to provide a satisfactory physical explanation for this phenomenon. However, we believe it might be related to the boundary conditions that are imposed on the chain and to the way it is coupled to the heat baths. In ref. 11, Nakazawa studied a harmonic chain with free ends (and κ strictly positive in order to ensure existence of the stationary state), as opposed to the fixed ends case considered here. The temperature profile he obtained is not plagued by the "defect" observed in the fixed ends case, namely, it is monotonic (and exponentially decaying). A similar analysis as presented here can be performed for the model studied by Nakazawa. It yields a first-order correction to the temperature profile which is exponentially flat in the bulk of the chain and monotonic, to be compared with the profile for $\kappa = 1/10$ in Fig. 1. This issue can only be clarified by further work involving modifications of the boundary conditions and coupling to the heat baths, in particular perturbative analysis as well as numerical studies in regimes of very weak anharmonicity.

ACKNOWLEDGMENTS

We thank K. Aoki, A. Kupiainen, L. Rey-Bellet, H. Spohn, H. Tasaki, N. Yoshida, and E. Zabey for useful discussions during the preparation of this work. R.L. thanks T. Shiota for his hospitality at Kyoto University. R.L. was supported by the Japan Society for the Promotion of Science and by Les services fédéraux des affaires scientifiques, techniques et culturelles du gouvernement Belge. A.S. was supported by the Swiss National Science Foundation.

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