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Fourier's Law for a Microscopic Model of Heat Conduction

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We consider a chain of N harmonic oscillators perturbed by a conservative stochastic dynamics and coupled at the boundaries to two gaussian thermostats at different temperatures. The stochastic perturbation is given by a diffusion process that exchange momentum between nearest neighbor oscillators conserving the total kinetic energy. The resulting total dynamics is a degenerate hypoelliptic diffusion with a smooth stationary state. We prove that the stationary state, in the limit as $N \to \infty$, satisfies Fourier's law and the linear profile for the energy average.

KEY WORDS: Fourier's law; heat conduction; entropy production; non-equilibrium stationary state.

1. INTRODUCTION

In insulating crystals heat is transported by lattice vibrations, and since the pioneering work of Debye, systems of anharmonic oscillators have been used as microscopic models for heat conduction (for a review cf. refs. 12 and 4). These systems are then connected at the extremities to two thermostats at different temperatures. Non-linear effects are extremely important in order to obtain finite conductivity. Enough strong non-linearity causes scattering between phonons and should imply a sufficiently fast decay of correlations for heat currents. In fact it is well known that harmonic chains, because of their infinitely many conserved quantities, have energy transport independent of the lenght of the chain and do not obey

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Fourier's law.[15] On the other hand a rigorous treatment of a non-linear system, even the proof of the existence of the conductivity coefficient, is out of reach of current mathematical techniques.

In the present paper, we study a model of a chain of *harmonic* oscillators where the hamiltonian dynamic is perturbed by a random continuous exchange of kinetic energy between nearest neighbors oscillators. This random exchange conserves the total kinetic energy and destroy all other conservation laws. In this sense it simulates the long time effect of the non-linearities in the deterministic model. This random exchange of kinetic energy is realized by a diffusion on the circle of constant kinetic energy of nearest neighbor oscillators. We expect the same macroscopic behavior and results if this diffusions are replaced by jump processes.

The interaction with the reservoirs are modeled by Ornstein–Uhlenbeck processes at the corresponding temperatures. It results that the total dynamics of the system is a degenerate hypoelliptic diffusion on the phase space. The stationary state is given by the law of independent gaussian variables if and only if the temperatures of the thermostats are equal (equilibrium).

We prove that in the stationary state Fourier's law is valid for the energy flow, that the total energy of the system is proportional to its size, and that the average energy per volume, in the infinite volume limit, is given by the average of the temperatures ad the boundaries. Then we prove a linear profile for the energy. A corresponding law of large number (hydrodynamic limit) should be valid for this system, but at the moment we have not been able to prove this.

The macroscopic evolution of the *dynamical* fluctuation in equilibrium for the corresponding infinite model, have been proven in a companion paper.[7]

With similar motivations other stochastic models have been proposed before. In 1970, Bosterly, Rich and Visscher[2] considered a chain of harmonic oscillators where each oscillator is also connected to an interior bath, modeled, like the boundary terms, by Ornstein–Uhlenbeck processes. The temperature of each bath is then chosen in a self-consistent way. Fourier's law and the linear profile of temperature for this model in the steady state have been proven recently by Bonetto, Lebowitz and Lukkarinen.[3] There are two main difference between this model and ours. In the Bosterly, Rich and Visscher model, energy is not conserved by the bulk dynamics, even though the temperatures of the internal baths are regulated so that the *average* flow of energy between the oscillators and the internal baths is null. In our system the bulk dynamic conserves energy, and only the boundary reservoirs can change the total energy. The second difference is that the dynamic of the Bosterly, Rich and Visscher model is linear, and consequently the stationary state is fully gaussian. Fourier's law, linear profile of temperatures and other result can then be obtained by computing the limit of the 2-point correlations of the stationary state. The stochastic perturbation we consider is intrinsically non-linear and the stationary state is non-gaussian (except in the equilibrium case).

Another model has been introduced in 1982 by Kipnis, Marchioro and Presutti[10] where the energy is microscopically conserved but the hamiltonian part of the dynamics is removed. The dynamics consist only on random exchange of energy between nearest-neighbor *oscillators*, given by properly defined jump processes. The striking duality properties of this process make it explicitly solvable, and in ref. 10 Fourier's law and linear profile of temperature are proven. Recently a deterministic hamiltonian model has been proposed in ref. 8 where it is argued that, in a proper high temperature limit and under a chaoticity assumption, the model of Kipnis, Marchioro and Presutti can be recovered.

The main tool we use in our proof is a bound of the entropy production of the bulk dynamics. This tool has been successful in the analogous problem of Fick's law in some lattice dynamics.[6,11]

One of the main difficulties in proving Fourier's law and hydrodynamic limit is to establish a *fluctuation–dissipation* relation, i.e. a decomposition of the current of the conserved quantity (here the energy) in a dissipative part (a spatial *gradient*) and a fluctuating part (a *time derivative*). Thanks to the stochastic perturbation one can write here an exact fluctuation–dissipation relation (cf. Eq. (28)). Then, in order to obtain Fourier's law, we have to bound (uniformly in the size of the system) the second moment of the positions and velocity at the boundary. In fact we can bound the second moments of all the coordinates, that gives a bound of the expectation of the total energy proportional to the size of the system.

2. THE MODEL

Atoms are labeled by $x \in \{1, \dots, N-1\}$. Atom 1 and $N-1$ are in contact with two separate heat reservoirs at two different temperatures T_l and T_r. The interaction between the reservoirs is modeled by two Ornstein–Uhlenbeck processes at the corresponding temperatures. The moments of the atoms are denoted by $p_1, \dots, p_{N-1}$ and the positions by $q_1, \dots, q_{N-1}$. The distances between the positions are denoted by $r_1, \dots, r_{N-2}$, where $r_x = q_{x+1} - q_x$. The hamiltonian of the system that represents the total energy inside the system is given by

$$\mathcal{H}_N = \sum_{x=1}^{N-1} e_x, \quad e_x = \frac{\left(p_x^2 + (r_x - \rho)^2\right)}{2} \qquad x = 1, \dots, N-2; \quad e_{N-1} = \frac{p_{N-1}^2}{2}. \tag{1}$$

The dynamics is described by the following system of stochastic differential equations:

$$
\begin{aligned}
dr_x &= (p_{x+1} - p_x)dt, \qquad x = 1, \dots, N-2 \\
dp_x &= (r_x - r_{x-1})dt - \gamma p_x dt + \sqrt{\gamma}\left(p_{x-1} dw_{x-1,x} - p_{x+1} dw_{x,x+1}\right), \\
&\quad x = 2, \dots, N-2 \\
dp_1 &= (r_1 - \rho)dt - \frac{1+\gamma}{2} p_1 dt - \sqrt{\gamma} p_2 dw_{1,2} + \sqrt{T_l} dw_{0,1}, \\
dp_{N-1} &= -(r_{N-2} - \rho)dt - \frac{1+\gamma}{2} p_{N-1} dt + \sqrt{\gamma} p_{N-2} dw_{N-2,N-1} \\
&\quad + \sqrt{T_r} dw_{N-1,N},
\end{aligned}
\tag{2}
$$

Here $w_{x,x+1}(t), x = 0, \dots, N-1$, are independent standard brownian motions (with 0 average and diffusion equal to 1). The parameter $\gamma > 0$ regulates the strength of the random exchange of momenta between the nearest neighbor particles.

Observe that by translating r_x in $r_x - \rho$ one has the same equations for the new coordinate but with $\rho = 0$. So we set $\rho = 0$ without any loss of generality.

The generator of the evolution has the form

$$
\begin{aligned}
L_N &= \sum_{x=1}^{N-2} (p_{x+1} - p_x)\partial_{r_x} + \sum_{x=2}^{N-2} (r_x - r_{x-1})\partial_{p_x} + r_1 \partial_{p_1} - r_{N-2}\partial_{p_{N-1}} \\
&\quad + \frac{\gamma}{2} \sum_{x=1}^{N-2} X_{x,x+1}^2 + \frac{1}{2}\left(T_l \partial_{p_1}^2 - p_1 \partial_{p_1}\right) + \frac{1}{2}\left(T_r \partial_{p_{N-1}}^2 - p_{N-1}\partial_{p_{N-1}}\right),
\end{aligned}
\tag{3}
$$

where

$$
X_{x,x+1} = p_{x+1}\partial_{p_x} - p_x \partial_{p_{x+1}}. \tag{4}
$$

One can check easily that the Lie algebra generated by these vector fields and the hamiltonian part of L_N has full rank at every point of the state space $\mathbb{R}^{N-1} \times \mathbb{R}^{N-2}$. By Hörmander theorem it follows that this operator is hypoelliptic (cf. theorem 22.2.1 in ref. 9), so the stationary measure has a smooth density. We denote with $\langle \cdot \rangle$ the expectation with respect to the stationary measure. In the appendix at the end of the paper we give a proof of the existence and uniqueness of the stationary measure.

Energy is conserved by the bulk part of the dynamics and we have

$$L_N e_x = j_{x-1,x} - j_{x,x+1} \tag{5}$$

with

$$\begin{aligned} j_{x,x+1} &= -r_x p_{x+1} - \frac{\gamma}{2}(p_{x+1}^2 - p_x^2), \quad x = 1, \dots, N-2 \\ j_{0,1} &= \frac{1}{2}(T_l - p_1^2), \qquad j_{N-1,N} = -\frac{1}{2}(T_r - p_{N-1}^2). \end{aligned} \tag{6}$$

Consequently $j_{x,x+1}$ is called instantaneous current of energy. Because of stationarity, for any $x = 1, N-1$ we have

$$\langle j_{x,x+1} \rangle = \langle j_{0,1} \rangle = \langle j_{N-1,N} \rangle \tag{7}$$

The following theorems are the main results of this paper.

Theorem 1. For any $\gamma > 0$

$$\lim_{N\to\infty} N \langle j_{x,x+1} \rangle = \frac{1}{2}\left(\gamma + \gamma^{-1}\right)(T_l - T_r). \tag{8}$$

Theorem 2. For any $\gamma > 0$

$$\lim_{N\to\infty} \frac{1}{N} \langle \mathcal{H}_N \rangle = \frac{1}{2}(T_l + T_r). \tag{9}$$

It is easy to see that the averages of the total kinetic and potential energy are equal. It follows then, as corollary of theorem 2, that the same result is valid for the kinetic and the potential energies, i.e.

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-1} \left\langle p_x^2 \right\rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-2} \left\langle r_x^2 \right\rangle = \frac{1}{2}(T_l + T_r). \tag{10}$$

Theorem 3. For $\gamma = 1$ and any bounded function $G : [0, 1] \to \mathbb{R}$, we have

$$\lim_{N\to\infty} \left\langle \frac{1}{N} \sum_{x=1}^{N-1} G(x/N) e_x \right\rangle = \int_0^1 G(q) T(q) dq \tag{11}$$

where $T(q) = T_l + (T_r - T_l)q$ is the linear profile interpolating T_l and T_r.

3. ENTROPY PRODUCTION

Denote by $g_{T_r}(p_1, r_1, \ldots, p_{N-2}, r_{N-2}, p_{N-1})$ the density of the product on gaussians with mean 0 and variance T_r. We denote by f_N the density of the stationary measure with respect to g_{T_r}. By hypoellipticity this density is smooth.

By stationarity we have

$$0 = -2\langle L_N \log f_N \rangle = \gamma \sum_{x=1}^{N-2} \int \frac{(X_{x,x+1} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} + T_r \int \frac{(\partial_{p_{N-1}} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} - 2\langle L_l \log f_N \rangle \tag{12}$$

where $L_l = (T_l \partial_{p_1}^2 - p_1 \partial_{p_1})$. Define $h = g_{T_l}/g_{T_r}$, then we can rewrite the last term as

$$\begin{aligned} -2\langle L_l \log f_N \rangle &= -2 \int \frac{f_N}{h} L_l \log\left(\frac{f_N}{h}\right) g_{T_l} d\bar{p}\, d\bar{r} - 2 \int f_N L_l (\log h) g_{T_r} d\bar{p}\, d\bar{r} \\ &= T_l \int \frac{[\partial_{p_1}(f_N/h)]^2}{f_N/h} g_{T_l} d\bar{p}\, d\bar{r} + (T_l^{-1} - T_r^{-1}) \left(T_l - \langle p_1^2 \rangle\right). \end{aligned} \tag{13}$$

So by (30) we have the following bound

$$\gamma \sum_{x=1}^{N-2} \int \frac{(X_{x,x+1} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} + T_r \int \frac{(\partial_{p_{N-1}} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} + T_l \int \frac{[\partial_{p_1}(f_N/h)]^2}{f_N/h} g_{T_l} d\bar{p}\, d\bar{r} = (T_r^{-1} - T_l^{-1}) \left(T_l - \langle p_1^2 \rangle\right) \tag{14}$$

In Section 4, we prove that this last expression is bounded by CN^{-1} for some constant C (cf. Eqs. (30) and (6)). This relation also gives us the right sign for the energy current, i.e. if $T_l < T_r$ we have $\langle j_{x,x+1} \rangle < 0$.

4. SOME BOUNDS

From (6) and (7) we have

$$\langle p_1^2 \rangle + \langle p_{N-1}^2 \rangle = T_l + T_r \tag{15}$$

Observe that, since $L_N r_1^2 = 2(r_1 p_2 - r_1 p_1)$, we have

$$\langle r_1 p_2 \rangle = \langle r_1 p_1 \rangle \tag{16}$$

Equation (7) for $x = 1$ gives

$$\langle j_{1,2} \rangle = -\langle r_1 p_2 \rangle - \frac{\gamma}{2}\left(\langle p_2^2 \rangle - \langle p_1^2 \rangle\right) \tag{17}$$

Since this last is equal to $\langle j_{0,1} \rangle$, using (16), we obtain

$$\frac{\gamma}{2}\langle p_2^2 \rangle = -\langle r_1 p_1 \rangle + \frac{1}{2}(\gamma + 1)\langle p_1^2 \rangle - \frac{1}{2}T_l \tag{18}$$

Then by Schwarz inequality there exists a constant C, depending only on γ, such that

$$\langle p_2^2 \rangle \leqslant C\left(\langle r_1^2 \rangle + \langle p_1^2 \rangle\right) \tag{19}$$

Analogous computation for the index $x = N - 2$ gives

$$\langle p_{N-2}^2 \rangle \leqslant C\big(\langle p_{N-1}^2 \rangle + \langle r_{N-2}^2 \rangle\big). \tag{20}$$

Observe now that

$$L_N(r_1 p_1) = p_1(p_2 - p_1) + r_1^2 - \frac{\gamma + 1}{2} p_1 r_1 \tag{21}$$

so we have the relation

$$\langle r_1^2 \rangle = \langle p_1^2 \rangle - \langle p_1 p_2 \rangle + \frac{\gamma + 1}{2}\langle p_1 r_1 \rangle \tag{22}$$

and by use of (18)

$$\langle r_1^2 \rangle = \langle p_1^2 \rangle - \langle p_1 p_2 \rangle + \left(\frac{\gamma + 1}{2}\right)^2 \langle p_1^2 \rangle - \frac{\gamma(\gamma + 1)}{4}\langle p_2^2 \rangle - \frac{\gamma + 1}{4} T_l \tag{23}$$

and by Schwarz inequality, for any $\alpha > 0$

$$\langle r_1^2 \rangle \leqslant \left(1 + \left(\frac{\gamma + 1}{2}\right)^2 + \frac{1}{2\alpha}\right)\langle p_1^2 \rangle + \left(\frac{\alpha}{2} - \frac{\gamma(\gamma + 1)}{4}\right)\langle p_2^2 \rangle \tag{24}$$

choosing properly α one obtains a constant C depending only on γ, such that

$$\langle r_1^2 \rangle \leqslant C \langle p_1^2 \rangle \tag{25}$$

and an analogous bound is obtained for $\langle r_{N-2}^2 \rangle$.

Putting all together we have obtained the following lemma:

Lemma 1. There exists a constant C depending only on γ and linearly on T_l and T_r such that

$$\langle r_1^2 \rangle + \langle p_1^2 \rangle + \langle p_2^2 \rangle + \langle r_{N-2}^2 \rangle + \langle p_{N-1}^2 \rangle + \langle p_{N-2}^2 \rangle \leqslant C(T_l + T_r) \tag{26}$$

The bulk dynamics is only apparently non-gradient since defining

$$h_x = \frac{1}{2\gamma} p_{x+1}(r_x + r_{x+1}) + \frac{1}{4} p_{x+1}^2, \quad x = 1, \ldots, N-3 \tag{27}$$

permits to rewrite

$$\begin{aligned} j_{x,x+1} &= -\nabla \left(\frac{1}{2\gamma} r_x^2 + \frac{\gamma}{2} p_x^2 + \frac{1}{2\gamma} p_x p_{x+1} + \frac{\gamma}{4} \nabla (p_x^2) \right) + L h_x, \\ & x = 1, \ldots, N-3. \end{aligned} \tag{28}$$

where the discrete gradient ∇ of a discrete function w is defined by $(\nabla w)(x) = w(x+1) - w(x)$. Using again (7) we have

$$\begin{aligned} \langle j_{0,1} \rangle &= \frac{1}{N-3} \sum_{x=1}^{N-3} \langle j_{x,x+1} \rangle \\ &= -\frac{1}{N-3} \left(\frac{1}{2\gamma} \langle r_{N-2}^2 \rangle + \frac{\gamma}{2} \langle p_{N-2}^2 \rangle + \frac{1}{2\gamma} \langle p_{N-2} p_{N-1} \rangle \right. \\ &\quad + \frac{\gamma}{4} \left(\langle p_{N-1}^2 \rangle - \langle p_{N-2}^2 \rangle \right) - \frac{1}{2\gamma} \langle r_1^2 \rangle - \frac{\gamma}{2} \langle p_1^2 \rangle \\ &\quad \left. - \frac{1}{2\gamma} \langle p_2 p_1 \rangle - \frac{\gamma}{4} \left(\langle p_2^2 \rangle - \langle p_1^2 \rangle \right) \right) \end{aligned} \tag{29}$$

and by (26) we obtain that there exists a constant C depending only on T_l, T_r and γ such that

$$|\langle j_{x,x+1} \rangle| \leqslant \frac{C}{N}, \qquad x = 0, \ldots, N-1. \tag{30}$$

5. FOURIER'S LAW

Proposition 1. For $x = 1$ and $N - 2$ we have

$$\lim_{N\to\infty} \langle p_x p_{x+1} \rangle = 0 \tag{31a}$$

$$\lim_{N\to\infty} \langle r_x p_{x+1} \rangle = 0 \tag{31b}$$

$$\lim_{N\to\infty} \langle (p_x^2 - p_{x+1}^2) \rangle = 0 \tag{31c}$$

Proof. Let us prove the case $x = 1$, for $x = N - 2$ the proof is similar. By (14), (30) and (26)

$$\begin{aligned}\langle r_1 p_2 \rangle = \langle r_1 p_1 \rangle &= \int r_1 p_1 (f_N/h) g_{T_l} d\bar{p}\, d\bar{r} = T_l \int r_1 \partial_{p_1} (f_N/h) g_{T_l} d\bar{p}\, d\bar{r} \\ &\leqslant T_l \langle r_1^2 \rangle^{1/2} \left(\int \frac{[\partial_{p_1}(f_N/h)]^2}{f_N/h} g_{T_l} \right)^{1/2} d\bar{p}\, d\bar{r} \leqslant \frac{C}{\sqrt{N}}\end{aligned} \tag{32}$$

The proof for $\langle p_1 p_2 \rangle$ is similar.

Now by (30) for $x = 1$ we have

$$\lim_{N\to\infty} \langle (p_1^2 - p_2^2) \rangle = 0 \quad \blacksquare \tag{33}$$

Then by (22) we have

$$\lim_{N\to\infty} \langle r_1^2 \rangle = \lim_{N\to\infty} \langle p_1^2 \rangle = T_l \tag{34}$$

and similarly

$$\lim_{N\to\infty} \langle r_{N-2}^2 \rangle = \lim_{N\to\infty} \langle p_{N-1}^2 \rangle = T_r \tag{35}$$

By (29) it follows that

$$\lim_{N\to\infty} N \langle j_{x,x+1} \rangle = \frac{1}{2} \left(\gamma + \gamma^{-1} \right) (T_l - T_r) \tag{36}$$

i.e. the law of Fourier.

6. AVERAGE ENERGY

We first state the following equipartition result:

Proposition 2.

$$\left\langle \sum_{x=1}^{N-1} p_x^2 \right\rangle = \left\langle \sum_{x=1}^{N-2} r_x^2 \right\rangle \tag{37}$$

Proof. Recall that $r_x = q_{x+1} - q_x$. Then

$$L_N \left(\sum_{x=1}^{N-1} q_x p_x \right) = \sum_{x=1}^{N-1} p_x^2 - \sum_{x=1}^{N-2} r_x^2 - \gamma \sum_{x=2}^{N-2} q_x p_x - \frac{1+\gamma}{2} (q_1 p_1 + q_{N-1} p_{N-1}) \tag{38}$$

Since $L_N q_x^2 = 2 q_x p_x$, (37) follows. ∎

We prove now theorem 2.

Proof. We claim there exists a constant $C > 0$ independent of N such that

$$\left\langle \frac{\mathcal{H}_N}{N} \right\rangle \leqslant C \tag{39}$$

Define

$$\phi(x) = \frac{1}{2\gamma} \langle r_x^2 \rangle + \frac{\gamma}{4} \left(\langle p_x^2 \rangle + \langle p_{x+1}^2 \rangle \right) + \frac{1}{2\gamma} \langle p_x p_{x+1} \rangle. \tag{40}$$

By (5) and (28), we have

$$\Delta \phi(x) = 0, \quad x = 2, \dots, N-3 \tag{41}$$

Here, $(\Delta w)(x) = w(x+1) + w(x-1) - 2w(x)$ is the usual discrete Laplacian of the function $w(x)$. By (26) and the maximum principle, it follows that there exists a constant C independent of N such that

$$|\phi(x)| \leqslant C, \quad x = 1, \dots, N-2 \tag{42}$$

In fact we have furthermore, by the explicit expression of $\phi(x)$ and the result of the previous sections that

$$\lim_{N\to\infty}\frac{1}{N}\sum_{x=1}^{N-2}\phi(x)=\frac{1}{2}(\gamma+\gamma^{-1})(T_r+T_r) \tag{43}$$

By a straightforward calculation we can write, for $x=2,\dots,N-2$,

$$p_x p_{x+1}=-\frac{1}{3\gamma}\nabla\left((r_x+r_{x-1})p_{x-1}\right)-\frac{1}{3\gamma}L_N\left(\frac{1}{2}(r_x+r_{x-1})^2+p_x p_{x+1}-r_x^2\right) \tag{44}$$

Consequently, taking expectation with respect to the stationary state and summing from $x=2$ to $N-2$ we obtain

$$\sum_{x=2}^{N-3}\langle p_x p_{x+1}\rangle=\frac{1}{3\gamma}\left(\langle(r_{N-2}+r_{N-3})p_{N-3}\rangle-\langle(r_2+r_1)p_1\rangle\right) \tag{45}$$

Now we also have that

$$L_N(p_1p_2)=-\frac{5\gamma+1}{2}p_1p_2+r_2p_1+L_N\left(\frac{r_1^2}{2}\right) \tag{46}$$

which implies, by (26),

$$\langle r_2p_1\rangle=\frac{5\gamma+1}{2}\langle p_1p_2\rangle\ \leqslant C \tag{47}$$

For the other side we have

$$\begin{aligned}&L_N\left(-\frac{1}{2}(r_{N-2}+r_{N-3})^2+p_{N-1}p_{N-2}\right)\\&\quad=r_{N-2}p_{N-2}-p_{N-3}(r_{N-2}+r_{N-3})-\frac{5\gamma+1}{2}p_{N-1}p_{N-2}\end{aligned} \tag{48}$$

so that

$$\langle p_{N-3}(r_{N-2}+r_{N-3})\rangle=-\frac{5\gamma+1}{2}\langle p_{N-1}p_{N-2}\rangle+\langle r_{N-2}p_{N-2}\rangle \tag{49}$$

and again by (26) this quantity is bounded in absolute value by a constant independent of N. So we can conclude that

$$\left|\sum_{x=1}^{N-3} \langle p_x p_{x+1}\rangle\right| \leqslant C \tag{50}$$

with C a constant independent of N. It follows by (50) and (43) that

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-2} \left[\frac{1}{2\gamma}\langle r_x^2\rangle + \frac{\gamma}{4}\left(\langle p_x^2\rangle + \langle p_{x+1}^2\rangle\right)\right] = \frac{1}{2}(\gamma+\gamma^{-1})(T_r+T_r) \tag{51}$$

The by using (37) we finally get (9) and (10). ▮

7. ENERGY PROFILE FOR $\gamma = 1$

From the results of the previous section we have that

$$\lim_{N\to\infty} \phi([Nq]) = \frac{1}{2}(\gamma+\gamma^{-1})T(q) \tag{52}$$

If $\gamma = 1$ we have

$$\begin{aligned}\phi(x) &= \frac{1}{2}\langle r_x^2\rangle + \frac{1}{4}\left(\langle p_{x+1}^2\rangle + \langle p_x^2\rangle\right) + \frac{1}{2}\langle p_x p_{x+1}\rangle \\ &= \langle e_x\rangle + \psi(x)\end{aligned} \tag{53}$$

with

$$\psi(x) = \frac{1}{2}\langle p_x p_{x+1}\rangle + \frac{1}{4}\left(\langle p_{x+1}^2\rangle - \langle p_x^2\rangle\right)$$

for $x = 1,\ldots,N-2$.

Then, in order to prove (11), we are left to prove

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-2} G(x/N)\psi(x) = 0 \tag{54}$$

Because of (44), $\psi(x) = \nabla\xi(x)$ with ξ a bounded function, so (54) follows by summation by part.

8. OPEN PROBLEMS AND OTHER MODELS

We have proven for our stochastic model the Fourier law for any value of the coupling γ and the linear profile of the *energy* for the case $\gamma = 1$. The essential tool used has been a bound on the entropy production. This bound on the entropy production together with a uniform bound on $\langle p_x^{2+\delta} \rangle$ will provide a proof of the linear *temperature* profile and of *local equilibrium* for any value of γ. Unfortunately we have not been able to prove yet such uniform bound of the higher moments of the velocities, but we conjecture that it is certainly satisfied.

The proof we have exposed in the present paper can be adapted for some modification of the model. For example one can add a pinning given by *on site* harmonic potential, adding to the hamiltonian a term $\sum_{x=1}^{N-1} \nu^2 q_x^2/2$. Or adding stochastic reservoirs like in the model of Bolsterli–Rich–Visscher[2,3] with self consistent temperatures, i.e. we can add to the generator a term

$$\lambda \sum_{x=2}^{N-2} \left(T_x \partial_{p_x}^2 - p_x \partial_{p_x} \right)$$

where the temperatures T_x are imposed to be equal to $\langle p_x^2 \rangle$. In this case we find that the self-consistent profile T_x is asymptotically linear and the Fourier law is given by

$$\lim_{N\to\infty} N < j_{x,x+1} >= \left(\frac{1}{2(\gamma+\lambda)} + \frac{\gamma}{2} \right) (T_l - T_r). \qquad (55)$$

which, in the limit as $\gamma \to 0$ is in agreement with the results of Bonetto–Lebowitz–Lukkarinen.[3] The proof of (55) is very close to the one exposed in Sections 3, 4, 5. In fact one has the decomposition of the current in the form

$$\nabla \tilde{\phi}_x + L_N h_x - \frac{\lambda}{2}(p_{x+1}^2 - T_{x+1})$$

with the function h_x given by

$$h_x = \frac{1}{2(\gamma+\lambda)} p_{x+1}(r_x + r_{x+1}) + \frac{1}{4} p_{x+1}^2, \quad x = 1, \ldots, N-3 \qquad (56)$$

Observe that this works also in the case $\gamma = 0$ if $\lambda > 0$.

In this last model one can also prove local equilibrium by proper use of the entropy production bound, similarly as done in ref. 13. In the case $\gamma = 0$ and in presence of pinning, local equilibrium is proved in ref. 3.

A. APPENDIX

In this section, we prove existence and uniqueness of the stationary measure $\langle\cdot\rangle$ for any left temperature T_l and right temperature T_r. Recently, refs. 5 and 14 proved existence and uniqueness of the stationary measure for a non-harmonic chain with reservoirs at the boundaries.

A.1. Existence

Let us denote by $\Omega=\{\omega=(p_1,\dots,p_{N-1},r_1,\dots,r_{N-2})\in\mathbb{R}^{2N-3}\}$ the configuration space and by $(\omega_s)_{s\geqslant 0}$ the Markov process with generator (3).

Lemma 2. If ω_0 is a configuration with finite energy: $\mathcal{H}_N(\omega_0)<+\infty$ then there exists a constant $C>0$ such that

$$\forall t\geqslant 0,\qquad \mathbb{E}_{\omega_0}\left[\frac{1}{t+1}\int_0^t \mathcal{H}_N(\omega_s)ds\right]\leqslant C \tag{A.1}$$

Proof. By (5) and(6), we have

$$L_N\mathcal{H}_N=j_{0,1}-j_{N-1,N} \tag{A.2}$$

It follows that

$$\begin{aligned}&\mathbb{E}_{\omega_0}(\mathcal{H}_N(\omega_t))-\mathcal{H}_N(\omega_0)\\&\quad=\frac{1}{2}\int_0^t \mathbb{E}_{\omega_0}(T_l-p_1^2(s))ds+\frac{1}{2}\int_0^t \mathbb{E}_{\omega_0}(T_r-p_{N-1}^2(s))ds\end{aligned} \tag{A.3}$$

Hence there exists a constant $C>0$ such that

$$\forall t\geqslant 0,\qquad \mathbb{E}_{\omega_0}\left(\frac{\mathcal{H}_N(\omega_t)}{t+1}\right)\leqslant C \tag{A.4}$$

Using the preceding bound, we can repeat the estimates of Section 4 with $\langle.\rangle$ replaced by the average $t^{-1}\int_0^t \mathbb{E}_{\omega_0}$. The only difference is that we have to take in account the boundary terms depending on t. In the sequel, C is a constant independent of t which can change from line to line. By (A.3) and (A.4), we know that

$$\frac{1}{t+1}\int_0^t \mathbb{E}_{\omega_0}(p_1^2(s)+p_{N-1}^2(s))ds\leqslant C \tag{A.5}$$

Since $L_N r_1^2 = 2(r_1 p_2 - r_1 p_1)$, we have

$$\frac{1}{t+1}\left[\mathbb{E}_{\omega_0}(r_1^2(t) - r_1^2(0))\right] = \frac{2}{t+1}\int_0^t \mathbb{E}_{\omega_0}(r_1(s)p_2(s) - r_1(s)p_1(s))ds \tag{A.6}$$

By (A.4), the modulus of the left hand-side is bounded by a constant independent of t. Similarly as what is done in (17) and (18), and using (A.4) to bound the boundary terms, we have

$$\left|\frac{1}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}\left[\frac{\gamma}{2}p_2^2(s) + r_1(s)p_1(s) - \frac{1}{2}(\gamma+1)p_1^2(s)\right]\right| \leqslant C \tag{A.7}$$

By Schwarz's inequality, we conclude

$$\frac{1}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}(p_2^2(s)) \leqslant \frac{C}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}(r_1^2(s) + p_1^2(s)) + C \tag{A.8}$$

This estimate is the equivalent to the estimate (20). In the same way, we can obtain the equivalent of lemma 1, meaning

$$\frac{1}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}(r_1^2(s) + p_1^2(s) + p_2^2(s) + r_{N-2}^2(s) + p_{N-1}^2(s) + p_{N-2}^2(s)) \leqslant C \tag{A.9}$$

Let us now define the function

$$\phi(t,x) = \frac{1}{t+1}\int_0^t \mathbb{E}_{\omega_0}\left[\frac{1}{2\gamma}r_x^2(s) + \frac{\gamma}{4}\left(p_x^2(s) + p_{x+1}^2(s)\right) + \frac{1}{2\gamma}p_x(s)p_{x+1}(s)\right] \tag{A.10}$$

Similarly as Section 6, one can prove there exists functions $(\theta_x)_{x=2,\dots,N-3}$ such that $\theta_x(\omega) \leqslant C\mathcal{H}_N$ and satisfying

$$\Delta\phi(t,x) = \frac{1}{t+1}\mathbb{E}_{\omega_0}(\theta_x(\omega_t)) - \frac{1}{t+1}\theta_x(\omega_0) \tag{A.11}$$

and we obtain

$$|\Delta\phi(t,x)| \leqslant C \tag{A.12}$$

Moreover, by (A.10), $|\phi(t,2)| \leqslant C$, $|\phi(t,N-1)| \leqslant C$. By the maximum principle, it follows that

$$|\phi(t,x)| \leqslant C \tag{A.13}$$

Using Eq. (44) and the bound (A.4), it is easy to show

$$\frac{1}{t+1}\int_0^t \mathbb{E}_{\omega_0}\left[\sum_{x=1}^{N-3} p_x(s)p_{x+1}(s)\right] \leqslant C \tag{A.14}$$

It follows by (A.13) and the preceding inequality that

$$\mathbb{E}_{\omega_0}\left[\frac{1}{t+1}\int_0^t \mathcal{H}_N(\omega_s)ds\right] \leqslant C \quad \blacksquare \tag{A.15}$$

The proof of the existence of the invariant measure is now standard. Let us denote by $(T_t)_{t\geqslant 0}$ the semi-group corresponding to the diffusion (2) and let ω_0 be an arbitrary configuration with finite energy. We consider the following family μ_t of probabilities on Ω:

$$\mu_t = \frac{1}{t}\int_0^t \delta_{\omega_0} T_s\, ds \tag{A.16}$$

where δ_{ω_0} is the Dirac mass on the configuration ω_0. By lemma 2, the sequence of probability measures $(\mu_t)_{t>0}$ is tight. Let μ^* a limit point of the family $(\mu_t)_{t>0}$. A simple checking shows that μ^* is an invariant probability measure of the diffusion (2).

A.2. Uniqueness

Lemma 3. Assume $T_l = T_r = 0$. Then for any initial configuration ω_0 we have

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \mathbb{E}_{\omega_0}\left[\mathcal{H}_N(\omega_s)\right] ds = 0 \tag{A.17}$$

Proof. By (A.3) we have

$$\frac{1}{2t}\int_0^t \mathbb{E}_{\omega_0}\left[(p_1^2(s) + p_{N-1}^2(s))\right] ds \leqslant \frac{\mathcal{H}_N(\omega_0)}{t} \longrightarrow 0 \tag{A.18}$$

as $t \to \infty$. This implies

$$\lim_{t\to\infty} \frac{1}{t}\mathbb{E}_{\omega_0}\left[\mathcal{H}_N(\omega_t)\right] = 0 \tag{A.19}$$

By (5) for $x = N-1$ we have

$$\begin{aligned}\mathbb{E}_{\omega_0}\left[e_{N-1}(t)\right] = e_{N-1}(0) \\ -\int_0^t \left(\mathbb{E}_{\omega_0}\left[r_{N-2}(s)p_{N-1}(s)\right] + \frac{\gamma+1}{2}\mathbb{E}_{\omega_0}\left[p_{N-1}^2(s)\right]\right) ds \\ +\int_0^t \frac{\gamma}{2}\mathbb{E}_{\omega_0}\left[p_{N-2}^2(s)\right] ds\end{aligned} \tag{A.20}$$

Notice that

$$\mathbb{E}_{\omega_0}\left[r_{N-2}(s)^2\right] \leqslant \mathbb{E}_{\omega_0}\left[\mathcal{H}_N(\omega_s)\right] \leqslant \mathbb{E}_{\omega_0}\left[\mathcal{H}_N(\omega_0)\right]. \tag{A.21}$$

Then by Schwarz inequality we obtain

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \mathbb{E}_{\omega_0}\left[p_{N-2}^2(s)\right] ds = 0 \tag{A.22}$$

Iterating this procedure one obtains for any $x = 1, \ldots, N-1$

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \mathbb{E}_{\omega_0}\left[p_x^2(s)\right] ds = 0 \tag{A.23}$$

By integrating in time formula (38) and observing that $\sum_x q_x^2 \leqslant C_N \sum_x r_x^2$ one obtains

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t \mathbb{E}_{\omega_0}\left[\sum_{x=1}^{N-2} r_x^2(s)\right] ds = 0 \quad \blacksquare \tag{A.24}$$

Let μ_1 and μ_2 two invariant probability measures for (2) with temperature on the left T_l and temperature on the right T_r. We consider the following coupling. We note the diffusion satisfying (2) with initial condition distributed according to μ_1 (resp. μ_2) by $(\omega_t^1)_{t\geqslant 0}$ (resp $(\omega_t^2)_{t\geqslant 0}$) and driven by the same Wiener processes $w_{x,x+1}(t), x = 0, \ldots, N-1$. By linearity, the process $(\omega_t^1 - \omega_t^2)_{t\geqslant 0}$ is solution of (2) with $T_l = T_r = 0$.

Let now $F:\Omega\to\mathbb{R}$ be a Lipshitz function:

$$|F(\omega)-F(\tilde{\omega})|\leqslant C\sqrt{\mathcal{H}_N(\omega-\tilde{\omega})} \tag{A.25}$$

We have

$$\begin{aligned}|\mu_1(F)-\mu_2(F)| &=\left|\mathbb{E}\left[\frac{1}{t}\int_0^t F(\omega_s^1)ds\right]-\mathbb{E}\left[\frac{1}{t}\int_0^t F(\omega_s^2)ds\right]\right|\\ &\leqslant C\mathbb{E}\left[\frac{1}{t}\int_0^t \left\{\mathcal{H}_N(\omega_s^1-\omega_s^2)\right\}^{1/2}\right]ds\\ &\leqslant C\sqrt{\mathbb{E}\left[\frac{1}{t}\int_0^t \mathcal{H}_N(\omega_s^1-\omega_s^2)\right]ds}\end{aligned}$$

By (A.17), this last term goes to 0 as t goes to infinity. It follows easily that $\mu_1=\mu_2$.

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