On the Conversion of Work into Heat: Microscopic Models and Macroscopic Equations

Tomasz Komorowski, Joel L. Lebowitz, Stefano Olla, Marielle Simon

SOCIEDADE BRASILEIRA DE MATEMÁTICA

ENSAIOS MATEMÁTICOS
20XX, Volume **XX**, 55–71
XXX

On the Conversion of Work into Heat: Microscopic Models and Macroscopic Equations

Tomasz Komorowski, Joel L. Lebowitz, Stefano Olla and Marielle Simon

Abstract. We summarize and extend some of the results obtained recently for the microscopic and macroscopic behavior of a pinned harmonic chain, with random velocity flips at Poissonian times, acted on by a periodic force at one end and in contact with a heat bath at the other end. Here we consider the case where the system is in contact with two heat baths at different temperatures and a periodic force is applied at any position. This leads in the hydrodynamic limit to a heat equation for the temperature profile with a discontinuous slope at the position where the force acts. Higher dimensional systems, unpinned cases and anharmonic interactions are also considered.

Dedicated to Errico Presutti for his 80th birthday!

Keywords. harmonic chain, periodic force, heat equation for the macroscopic temperature, Dirichlet-Neumann type boundary conditions, work into heat.

2020 Mathematics Subject Classification: 80A19,82C22,82C70,60K35.

1 Introduction

Nature has a hierarchical structure with macroscopic behavior arising from the dynamics of atoms and molecules. The connection between different levels of the hierarchy is however not always straightforward, as seen in the emergent phenomena, such as phase transitions and heat convection. Establishing in a mathematical precise way the connection between the different levels is the central problem of rigorous statistical mechanics.

The derivation of macroscopic behavior from microscopic models by suitable scaling of space and time is a field of science to which Errico has made seminal contributions both for equilibrium and nonequilibrium systems. In this work, which owes a lot to what we have learned from him, we study the transition from microscopic to macroscopic systems in the context of the conversion of work to heat. The conversion of mechanical energy into heat was demostrated by Joule's famous experiment in the 1840's. Joule dropped weights turning a paddle wheel immersed in water. The friction generated heat which he could measure and quantify.

In some recent works on this subject we carried out a rigorous mathematical analysis of a simple microscopic model for this common phenomena. In articles [6, 7], we considered a pinned harmonic chain on which work is done at the right end by an external periodic force. This work is converted into heat via an energy current flowing into a heat reservoir at the left end of the chain. In order to make this system mirror realistic physical systems with a finite heat conductivity we added to the bulk dynamics a random reversal of the velocity of each particle at a rate γ (the pure harmonic crystal is well known to have an infinite heat conductivity, see e.g. [10]). The precise description of the model is given in Section 2. Starting with an initial distribution on the phase space, we have shown that the system approaches a unique periodic state at long times. We have also obtained, in the hydrodynamical diffusive scaling limit, a heat equation for the temperature profile of the chain.

As a consequence of the presence of the periodic forcing, a constant energy flux, equal to the work done by the force, emerges on the macroscopic scale, as well as a boundary condition on the derivative of the temperature profile (Neumann boundary condition), such that Fourier law is satisfied with respect to this energy flux. In 3 we review these results and we present a generalization where the periodic force is applied at any position inside the system, generating Neumann type of boundary conditions in the bulk. We should mention the pioneering work by Errico and collaborators [5] where *current reservoirs* are attached to the boundary of an open symmetric simple exclusion dynamics, that originate non-linear Dirichlet boundary conditions.

In Section 4 we review a work in preparation about the unpinned dynamics [8]. In this situation there are two locally conserved quantities, energy and volume stretch, and the macroscopic evolution is governed by a coupled system of two diffusive equations, see (46) below. In the absence of periodic forcing this problem was previously studied in [9]. In Section 5 we review the generalization to higher dimension, also a work in preparation, as the proof is not a straightforward generalization of the one-dimensional case. In Section 6 we describe few results and some conjectures about the anharmonic case.

Acknowledgements. The work of J.L.L. was supported in part by the A.F.O.S.R. He thanks the Institute for Advanced Studies for its hospitality. T.K. acknowledges the support of the NCN grant 2020/37/B/ST1/00426. This project is partially supported by the ANR grant MICMOV (ANR-19-CE40-0012) of the French National Research Agency (ANR), and by the European Union with the program Fonds européen de développement régional.

2 Description of the model

We consider a pinned chain of $n+1$ harmonic oscillators in contact with a Langevin heat bath at temperature T_- on the left and another Langevin heat bath at temperature T_+ on the right. In addition there is a periodic force acting on the particle labeled by $[n\overline{u}]$, where $\overline{u} \in [0,1]$ and $[a]$ denotes the integer part of a positive real number a. The configuration of particle positions and momenta is described by

$$(\mathbf{q},\mathbf{p}) = (q_0,\dots,q_n,p_0,\dots,p_n) \in \mathbb{R}^{n+1} \times \mathbb{R}^{n+1}. \tag{1}$$

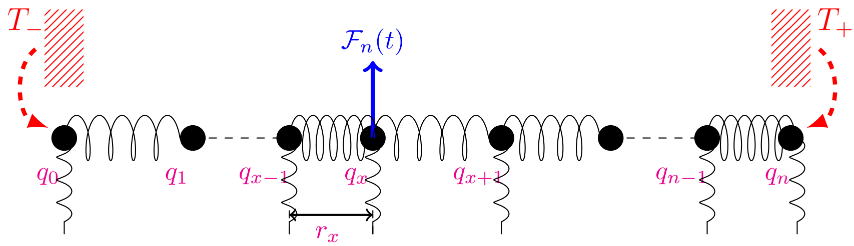
The total energy of the chain is given by the Hamiltonian: $\mathcal{H}_n(\mathbf{q},\mathbf{p}) := \sum_{x=0}^{n} \mathcal{E}_x(\mathbf{q},\mathbf{p})$, where the energy of particle x is defined by

$$\mathcal{E}_x(\mathbf{q},\mathbf{p}) := \frac{p_x^2}{2} + \frac{1}{2}(q_x - q_{x-1})^2 + \frac{\omega_0^2 q_x^2}{2}, \qquad x = 0,\dots,n, \tag{2}$$

where $\omega_0 > 0$ is the pinning strength. We adopt the convention that $q_{-1} := q_0$.

The microscopic dynamics of the process $\{(\mathbf{q}(t),\mathbf{p}(t))\}_{t\geqslant 0}$ describing the total chain is given in the bulk by

$$\begin{aligned} &\dot{q}_x(t) = p_x(t), \qquad x \in \{0,\dots,n\}, \\ &\mathrm{d}p_x(t) = \left(\Delta_N q_x - \omega_0^2 q_x\right)\mathrm{d}t - 2p_x(t-)\mathrm{d}N_x(\gamma t) + \delta_{x,[n\overline{u}]}\mathcal{F}_n(t)\mathrm{d}t, \end{aligned} \tag{3}$$



for $x \in \{1, \dots, n-1\}$, and at the boundaries the equations are

$$\mathrm{d}p_0(t) = \Big(q_1(t) - q_0(t) - \omega_0^2 q_0(t)\Big)\mathrm{d}t - 2\gamma_- p_0(t)\mathrm{d}t + \sqrt{4\gamma_- T_-}\mathrm{d}\widetilde{w}_-(t) \tag{4}$$

$$\mathrm{d}p_n(t) = \Big(q_{n-1}(t) - q_n(t) - \omega_0^2 q_n(t)\Big)\mathrm{d}t - 2\gamma_+ p_n(t)\mathrm{d}t + \sqrt{4\gamma_+ T_+}\mathrm{d}\widetilde{w}_+(t).$$

Here $\Delta_N q_x = q_{x+1} + q_{x-1} - 2q_x$ is the Neumann discrete Laplacian, corresponding to the choice of the boundary conditions $q_{n+1} := q_n$ and $q_{-1} := q_0$. Processes $\{N_x(t), x = 1, \dots, n-1\}$ are independent Poisson processes of intensity 1, while $\widetilde{w}_\pm(t)$ are two independent standard Wiener processes, independent of the Poisson processes. Parameters $\gamma > 0, \gamma_\pm \geqslant 0$ regulate the intensity of the random perturbations and the Langevin thermostats.

Finally, we assume that the forcing $\mathcal{F}_n(t)$ is θ_n-periodic, with the period $\theta_n = n^b\theta$, and the amplitude n^{-a}, i.e.

$$\mathcal{F}_n(t) = \frac{1}{n^a}\mathcal{F}\left(\frac{t}{n^b\theta}\right) + \overline{F} \tag{5}$$

where $\mathcal{F}(t)$ is a smooth 1-periodic function such that

$$\int_0^1 \mathcal{F}(t)\mathrm{d}t = 0, \qquad \int_0^1 \mathcal{F}(t)^2\mathrm{d}t > 0. \tag{6}$$

The constant part of the forcing $\overline{F}$ does not influence the macroscopic behavior of energy in the pinned case, but it is important in the unpinned case where tension of the chain is a relevant parameter, as it can be seen in 4 below.

In order to ensure stability of the system in the limit $n \to \infty$ we need to assume that the parameters a, b satisfy

$$a \geqslant 0, \qquad b \geqslant 0, \qquad b + a = \frac{1}{2}. \tag{7}$$

The choice $b = 0$ corresponds to a fixed period θ independent of n, i.e. the periodic forcing acts on a microscopic time, then we need to set $a = \frac{1}{2}$ in order to have an average work done of order $\frac{1}{n}$ (see (11) for the definition). In fact the maximum of energy current the system can hold without exploding should be of order $\frac{1}{n}$, and the work done has to be of the same order. With the choice $0 < b < \frac{1}{2}$, the periodic forcing is acting on mesoscopic time scales and in order to keep the average work done of order $\frac{1}{n}$ we need to choose $a = \frac{1}{2} - b$.

3 The pinned dynamics: $\omega_0 > 0$

In the presence of the pinning force, $\omega_0 > 0$, the system is not translation invariant and the only conserved quantity in the bulk is the energy.

The microscopic energy currents are given by

$$\frac{d}{dt}\mathcal{E}_x(t) = j_{x-1,x}(t) - j_{x,x+1}(t) + \delta_{x,[n\overline{u}]}\mathcal{F}_n(t)p_x(t), \tag{8}$$

with

$$j_{x,x+1}(t) := -p_x(t)(q_{x+1}(t) - q_x(t)), \qquad \text{if} \quad x \in \{0, ..., n-1\} \tag{9}$$

and at the boundaries

$$j_{-1,0}(t) := 2\gamma_- \left(T_- - p_0^2(t)\right), \qquad j_{n,n+1}(t) := -2\gamma_+ \left(T_+ - p_n^2(t)\right). \tag{10}$$

The work done up to time t by the periodic force is given by

$$W_n(t) = \int_0^t \mathcal{F}_n(s)p_{[nu]}(s)\mathrm{d}s, \tag{11}$$

where we adopt the usual sign convention that positive work means energy going into the system.

Consider an initial configuration given by $(\mathbf{q}, \mathbf{p})$, and denote by $\mathbb{E} = \mathbb{E}_{\mathbf{q},\mathbf{p}}$ the expectation of the process with this initial configuration. Thanks to the assumption (7) we expect that, for large n, the average work per unit time is of order $1/n$. In fact, the limit can be computed explicitly and for diffusive times n^2t equals:

$$\lim_{n\to\infty} \frac{1}{n}\mathbb{E}_{\mathbf{q},\mathbf{p}}\left(W_n(n^2t)\right) = t\mathbb{W}, \quad t > 0, \tag{12}$$

where $\mathbb{W}$ is independent of $\mathbf{q}, \mathbf{p}$, n and t. More precisely it is given by (cf. [7, Theorem 2.1 and Remark 2.3]):

$$\mathbb{W} = \left(\frac{2\pi}{\theta}\right)^2 \sum_{\ell\in\mathbb{Z}} \ell^2 \mathcal{Q}(\ell), \tag{13}$$

where $\mathcal{Q}(\ell)$ is explicit: if $b=0$ (and $a=\frac{1}{2}$) then

$$\mathcal{Q}(\ell) = 4\gamma|\widehat{\mathcal{F}}(\ell)|^2 \int_0^1 \cos^2\left(\frac{\pi z}{2}\right) \times \left\{\left[4\sin^2\left(\frac{\pi z}{2}\right) + \omega_0^2 - \left(\frac{2\pi\ell}{\theta}\right)^2\right]^2 + \left(\frac{4\gamma\pi\ell}{\theta}\right)^2\right\}^{-1} \mathrm{d}z \tag{14}$$

while if $b>0$ then

$$\mathcal{Q}(\ell) = 4\gamma|\widehat{\mathcal{F}}(\ell)|^2 \int_0^1 \cos^2\left(\frac{\pi z}{2}\right)\left[4\sin^2\left(\frac{\pi z}{2}\right) + \omega_0^2\right]^{-2} \mathrm{d}z. \tag{15}$$

Note that the latter case corresponds to (14) with $\lim_{n\to+\infty}\theta_n = +\infty$. Here

$$\widehat{\mathcal{F}}(\ell) = \int_0^1 e^{-2\pi i\ell t}\mathcal{F}(t)\mathrm{d}t, \quad \ell\in\mathbb{Z}. \tag{16}$$

Note that by (6) we have $\widehat{\mathcal{F}}(0)=0$. We moreover assume that

$$\sum_\ell |\widehat{\mathcal{F}}(\ell)| < \infty. \tag{17}$$

Notice that $\mathbb{W}>0$ if $\sum_{\ell\neq 0}|\widehat{\mathcal{F}}(\ell)|>0$ and it does not depend on $T_\pm$ nor on $\overline{u}$.

In [7] we have studied the macroscopic evolution of the temperature profile in the diffusive space-time scaling in the case $\gamma_+ = 0$ and the periodic force acting on the last particle (i.e. $\overline{u}=1$). We have assumed that the initial configuration of the particles is random with a distribution satisfying an entropy bound. More precisely, define the Gibbs measure

$$\nu_{T_-}(\mathrm{d}\mathbf{q},\mathrm{d}\mathbf{p}) := \frac{1}{Z}\prod_{x=0}^n \exp\left\{-\frac{\mathcal{E}_x(\mathbf{q},\mathbf{p})}{T_-}\right\}\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}, \tag{18}$$

where Z is the normalizing constant. Let $\mu_n(t)$ be the probability law of $(\mathbf{q}(n^2t),\mathbf{p}(n^2t))$. We suppose that the initial distribution $\mu_n(0)$ has a density $f_n(0)$ with respect to ν_{T_-} that belongs to $C^2(\mathbb{R}^{2(n+1)})$ – the space of functions with two continuous derivatives. By the standard regularity theory for SDEs then $\mu_n(t)$ possesses a C^2 regular density $f_n(t,\mathbf{q},\mathbf{p})$ with respect to ν_{T_-}. We then denote by

$$\mathbf{H}_{n,T_-}(t) := \int_{\Omega_n} f_n(t,\mathbf{q},\mathbf{p})\log f_n(t,\mathbf{q},\mathbf{p})\nu_{T_-}(\mathrm{d}\mathbf{q},\mathrm{d}\mathbf{p}) \tag{19}$$

the relative entropy of $\mu_n(t)$ w.r.t. ν_{T_-}. We assume that there exists a constant $C > 0$ such that the relative entropy satisfies

$$\mathbf{H}_{n,T_-}(0) \leqslant Cn \quad \text{for all } n \geqslant 1. \tag{20}$$

Furthermore we suppose that there exists a continuous function $T_0 : [0,1] \to (0,+\infty)$ such that

$$\lim_{n\to\infty} \frac{1}{n+1} \sum_x \varphi\left(\frac{x}{n+1}\right) \mathbb{E}\big(\mathcal{E}_x(0)\big) = \int_0^1 \varphi(u) T_0(u) \mathrm{d}u, \tag{21}$$

for any $\varphi \in C[0,1]$ – the space of continuous functions on $[0,1]$. Here and in the following we denote $\mathcal{E}_x(t) = \mathcal{E}_x(\mathbf{q}(t), \mathbf{p}(t))$. Following the same argument as in [7], and assuming that $\gamma_+ > 0, \gamma_- > 0$ (both heat bath are present), we find that

$$\lim_{n\to\infty} \frac{1}{n+1} \sum_x \varphi\left(\frac{x}{n+1}\right) \mathbb{E}\left(\mathcal{E}_x(n^2 t)\right) = \int_0^1 \varphi(u) T(t,u) \mathrm{d}u, \tag{22}$$

where $T(t,u)$ is the solution of the heat equation

$$\partial_t T = D_\gamma \partial_u^2 T, \quad u \in (0,1), \tag{23}$$

with $T(0,u) = T_0(u)$ and with the following boundary conditions:

- if $\overline{u} \in (0,1)$

$$\begin{aligned} &T(t,0) = T_-, \quad T(t,1) = T_+, \\ &\partial_u T(t,\overline{u}^-) - \partial_u T(t,\overline{u}^+) = \frac{\mathbb{W}}{D_\gamma}, \end{aligned} \tag{24}$$

- if $\overline{u} = 0$ or 1, then the force does not influence the hydrodynamic limit, since all the energy generated by the work flows into the corresponding heat bath, and the boundary conditions are only given by

$$T(t,0) = T_-, \; T(t,1) = T_+.$$

Moreover, in the case one thermostat is absent, say $\gamma_+ = 0$, the boundary conditions become the following:

- if $\overline{u} \in (0,1)$

$$\begin{aligned} &T(t,0) = T_-, \quad \partial_u T(t,1) = 0, \\ &\partial_u T(t,\overline{u}^-) - \partial_u T(t,\overline{u}^+) = \frac{\mathbb{W}}{D_\gamma}, \end{aligned} \tag{25}$$

- if, for instance, $\overline{u} = 1$ then we have

$$T(t,0) = T_-, \quad \partial_u T(t,1) = \frac{\mathbb{W}}{D_\gamma}. \tag{26}$$

This last case (26) is proven in [7], while the boundary conditions (24) and (25) can be proved by a very similar argument.

The diffusion coefficient D is not influenced by the boundary conditions and it is given in all cases explicitly by the formula

$$D_\gamma = \frac{1}{4\gamma}\omega_0^2\Big(G_{\omega_0}(0) + G_{\omega_0}(1)\Big) = \frac{1}{4\gamma}\frac{2}{2+\omega_0^2+\omega_0\sqrt{\omega_0^2+4}}. \tag{27}$$

Here $G_{\omega_0}(x) = \left(\omega_0^2 - \Delta\right)^{-1}(x)$, where Δ is the standard discrete Laplacian on $\mathbb{Z}$. The thermal diffusion coefficient D_γ can also be expressed by a different formula, that arises from the kinetic limit, related to this model [1]. Namely,

$$D_\gamma = \frac{1}{4\gamma}2\pi^2\int_0^1 \left[\omega'(k)\right]^2 dk, \tag{28}$$

where $\omega(k) = \sqrt{\omega_0^2 + 4\sin^2(\pi k)}$ is the dispersion relation of the nearest neighbor pinned harmonic chain. The expression (28) gives a general formula for the thermal diffusion for more general harmonic chains characterized by the dispersion relation $\omega(k)$.

In [7] it is also proven an equipartition law for both the kinetic and potential energies. It implies in particular that the limit for the temperature profile equals twice the limit of the average of the kinetic energy, i.e.

$$\lim_{n\to\infty}\frac{1}{n+1}\sum_x \varphi\left(\frac{x}{n+1}\right)\mathbb{E}\left(p_x^2(n^2t)\right) = \int_0^1 \varphi(u)T(t,u)\mathrm{d}u, \tag{29}$$

3.1 Clausius inequality

From the evolution of the relative entropy, if $\gamma_+ = 0$ we get the following inequality

$$\frac{1}{n}\left(\mathbf{H}_{n,T_+}(t) - \mathbf{H}_{n,T_+}(0)\right) \leqslant \frac{1}{nT_-}\mathbb{E}\left(W_n(n^2t)\right). \tag{30}$$

By Fourier's law (see (23)) the macroscopic current at the right endpoint equals $-(D/4\gamma)\int_0^t \partial_u T(s,1)\mathrm{d}s$, and we obtain the following inequality in the macroscopic limit:

$$\lim_{n\to+\infty}\frac{1}{n}\left(\mathbf{H}_{n,T_+}(t) - \mathbf{H}_{n,T_+}(0)\right) \leqslant \frac{t\mathbb{W}}{T_-}. \tag{31}$$

3.2 Stationary periodic state

We define a *periodic stationary probability measure* $\{\mu_t^P, t \in [0, +\infty)\}$ for the dynamics of the chain as a solution of the forward equation $\partial_t \mu_t^P = \mathcal{G}_t^* \mu_t^P$ such that $\mu_{t+\theta_n}^P = \mu_t^P$, where $\mathcal{G}_t^*$ is the adjoint of the generator $\mathcal{G}_t$ of the dynamics. This condition is equivalent with

$$\int_0^{\theta_n} \mathrm{d}s \int_{\mathbb{R}^{2(1+n)}} \mathcal{G}_s F(\mathbf{r}, \mathbf{p}) \mu_s^P(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p}) = 0, \tag{32}$$

for any smooth test function F. Using the contraction principle, in a manner similar to the proof of the existence and uniqueness of self-consistent reservoirs for a harmonic crystal (see [3, Theorem 3.1]) one can prove that for a fixed $n \geqslant 1$ there exists a unique θ_n-periodic stationary state $\{\mu_s^P, s \in [0, +\infty)\}$ for the system (3)-(4). The measures μ_s^P are absolutely continuous with respect to the Lebesgue measure $\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}$ and the density $\mu_s^P(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p}) = f_s^P(\mathbf{q}, \mathbf{p})\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}$ is strictly positive. This has been shown in the case $\gamma_+ = 0$ and $\overline{u} = 1$ in [6, Theorem 1.1].

Suppose that $\{(\mathbf{q}(t), \mathbf{p}(t))\}_{t \geqslant 0}$ is the solution of (3)-(4) initially distributed according to μ_0^P. Given a measurable function $F : \mathbb{R}^{2(n+1)} \to \mathbb{R}$ integrable w.r.t. each measure $\{\mu_s^P, s \in [0, +\infty)\}$ we denote

$$\overline{F}(t) := \mathbb{E}_{\mu_0^P}\Big(F\big(\mathbf{q}(t), \mathbf{p}(t)\big)\Big) = \int_{\mathbb{R}^{2(n+1)}} F(\mathbf{q}, \mathbf{p}) \mu_t^P(\mathrm{d}\mathbf{q}, \mathrm{d}\mathbf{p}), \quad t \geqslant 0, \tag{33}$$

where $\mathbb{E}_{\mu_0^P}$ is the expectation corresponding to the initial data distributed according to μ_0^P. The function $\overline{F}(t)$ is θ_n-periodic. We denote its time average by

$$\langle\langle F \rangle\rangle := \frac{1}{\theta_n} \int_0^{\theta_n} \overline{F}(t)\mathrm{d}t. \tag{34}$$

3.3 The macroscopic stationary state

In the general case the stationary temperature profile, corresponding to (23) and (24), is given by

$$\begin{aligned} T_{ss}(u) = &\left[T_- + \left(\frac{\mathbb{W}}{D_\gamma}(1 - \overline{u}) + T_+ - T_-\right) u\right] 1_{u \leqslant \overline{u}} \\ &+ \left[T_+ + \left(\frac{\mathbb{W}}{D_\gamma}\overline{u} - T_+ + T_-\right)(1 - u)\right] 1_{u > \overline{u}}. \end{aligned} \tag{35}$$

If the right heat bath is absent, i.e. $\gamma_+ = 0$ (then the boundary condition (25) holds), then

$$T_{ss}(u) = \left[T_- + \frac{\mathbb{W}}{D_\gamma} u\right] 1_{u \leqslant \overline{u}} + \left[T_- + \frac{\mathbb{W}}{D_\gamma}\overline{u}\right] 1_{u > \overline{u}}. \tag{36}$$

Finally, if $\gamma_+ = 0$ and $\overline{u} = 1$ corresponding to the boundary condition (26), then it has been proved in [6, Theorem 3.3] that for any $\varphi \in C[0,1]$:

$$\begin{aligned}\lim_{n\to\infty} \frac{1}{n+1}\sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right)\langle\langle p_x^2\rangle\rangle &= \lim_{n\to\infty} \frac{1}{n+1}\sum_{x=0}^{n} \varphi\left(\frac{x}{n+1}\right)\langle\langle \mathcal{E}_x\rangle\rangle \\ &= \int_0^1 \varphi(u) T_{ss}(u)\mathrm{d}u,\end{aligned} \tag{37}$$

with the stationary profile given by

$$T_{ss}(u) = T_- + \frac{\mathbb{W}}{D_\gamma} u. \tag{38}$$

Notice that when $\gamma \to 0$ we have that $T_{ss}(u) \to T_-$ in (36) and (38), while $T_{ss}(u) \to (T_+ - T_-)u + T_-$ in (35). This does not correspond to the stationary situation with $\gamma = 0$, cf. [10] for the case in absence of periodic forcing.

Furthermore, in [6, Theorem 9.1], we prove that in the case when the period of the force is of a fixed microscopic size (i.e. $b = 0$ and $a = -1/2$) the fluctuations of the kinetic energy functional vanish, i.e. there exists a constant $C > 0$ such that

$$\sum_{x=0}^{n} \int_0^\theta \left(\overline{p_x^2}(t) - \langle\langle p_x^2\rangle\rangle\right)^2 \mathrm{d}t \leqslant \frac{C}{n^2}, \quad n = 1, 2, \dots \tag{39}$$

4 The unpinned dynamics: $\omega_0 = 0$

When the system is unpinned, i.e. $\omega_0 = 0$, it is translational invariant and one should consider only the relative distance between the particles. We introduce the variables

$$r_x := q_x - q_{x-1}, \qquad x = 1, \dots, n, \tag{40}$$

sometimes referred to as the *volume stretch*. In this situation there are two conserved quantities in the bulk: the energy $\mathcal{E}_x = \frac{1}{2}(p_x^2 + r_x^2)$ and the volume r_x. The hydrodynamic limit for this unpinned dynamics with Langevin heat bath at both endpoints has been studied in [9]. In [8] we consider the situation when the force is applied at the right endpoint of the chain and the only heat bath is located at its left endpoint. The microscopic dynamics of the process $\{(\mathbf{r}(t), \mathbf{p}(t))\}_{t\geqslant 0}$ describing the total chain is given by

$$\begin{aligned}&\dot{r}_x(t) = p_x(t) - p_{x-1}(t)\\ &\mathrm{d}p_x(t) = (r_{x+1}(t) - r_x(t))\mathrm{d}t - 2p_x(t^-)\mathrm{d}N_x(\gamma t) + \delta_{x,n}\mathcal{F}_n(t)\mathrm{d}t,\end{aligned} \tag{41}$$

for $x = 1, \ldots, n$ and at the left boundary

$$\mathrm{d}p_0(t) = r_1 \mathrm{d}t - 2\gamma_- p_0(t)\mathrm{d}t + \sqrt{4\gamma_- T_-}\mathrm{d}w_-(t). \tag{42}$$

Here the force is given by (5). We use the convention $r_0 = r_{n+1} := 0$. One can immmediately see, from the first equation of (41), that r_x is a second (locally) conserved quantity besides the energy.

The energy currents are again given by (9) and (10). The work performed by the force is again given by (11). We have

$$\lim_{n\to\infty} \frac{1}{n}\mathbb{E}_{\mathbf{r},\mathbf{p}}\left(W_n(n^2 t)\right) = t\mathbb{W} \tag{43}$$

where $\mathbb{W}$ is independent of t and $(\mathbf{r}, \mathbf{p})$ – the initial configuration of stretches and momenta. In the case $a = 1/2$ and $b = 0$ it is given by (see [8] in preparation):

$$\mathbb{W} = \mathbb{W}_{\mathrm{mech}} + \mathbb{W}_{\mathrm{Q}}, \tag{44}$$

where

$$\mathbb{W}_{\mathrm{mech}} := \frac{\overline{F}^2}{2\gamma}, \qquad \mathbb{W}_{\mathrm{Q}} := \sum_{\ell\in\mathbb{Z}} \left(\frac{2\pi\ell}{\theta}\right)^2 \mathcal{Q}(\ell),$$

correspond to the mechanical and thermal parts of the work performed on the system. Here $\mathcal{Q}(\ell)$ is given by (14), setting $\omega_0 = 0$. In the case $b > 0$, we have $a + b/4 = 1/2$ and $\mathbb{W}$ is given by (44) with the same formula for $\mathbb{W}_{\mathrm{mech}}$ and

$$\mathbb{W}_{\mathrm{Q}} := 2\sum_{\ell\in\mathbb{Z}} \left(\frac{\pi|\ell|}{\gamma\theta}\right)^{1/2} |\widehat{\mathcal{F}}(\ell)|^2.$$

To formulate the hydrodynamic limit we assume, besides (20) and (21), that for any test function $\varphi \in C[0, 1]$ we have

$$\begin{aligned}
\lim_{n\to+\infty} \frac{1}{n+1}\sum_{x=0}^{n} \mathbb{E}\big(p_x^2(0)\big)\varphi\left(\frac{x}{n+1}\right) &= \int_0^1 T_0(u)\varphi(u)\mathrm{d}u, \\
\lim_{n\to+\infty} \frac{1}{n+1}\sum_{x=0}^{n} \mathbb{E}\big(r_x(0)\big)\varphi\left(\frac{x}{n+1}\right) &= \int_0^1 r_0(u)\varphi(u)\mathrm{d}u.
\end{aligned} \tag{45}$$

In addition, if we assume that $a = 1/2$ and $b = 0$, then

$$\Big(\mathbb{E}\big(p_x^2(n^2 t)\big), \mathbb{E}\big(r_x(n^2 t)\big)\Big)_{x=0,\ldots,n}$$

converge weakly, cf. (37), to $(T(t,u), r(t,u))$, the unique solution of the following system

$$\begin{aligned} \partial_t T(t,u) &= \frac{1}{4\gamma}\partial_{uu} T(t,u) + \frac{1}{2\gamma}(\partial_u r(t,u))^2 \\ \partial_t r(t,u) &= \frac{1}{2\gamma}\partial_{uu} r(t,u), \qquad (t,u) \in \mathbb{R}_+ \times (0,1), \end{aligned} \tag{46}$$

with the boundary and initial conditions:

$$\begin{aligned} &r(t,0) = 0, \qquad r(t,1) = \overline{F}, \\ &T(t,0) = T_-, \quad \partial_u T(1) = 4\gamma \mathbb{W}_Q \\ &T(0,u) = T_0(u), \quad r(0,u) = r_0(u). \end{aligned} \tag{47}$$

This result will be shown in [8].

Notice that the thermal energy, i.e. the temperature $T(t,u)$, is not a conserved quantity in the bulk. This is given instead by the total energy $\mathcal{E}(t,u) = T(t,u) + \frac{1}{2}r(t,u)^2$ that satisfies the equation

$$\partial_t \mathcal{E}(t,u) = \frac{1}{4\gamma}\partial_{uu}\left(\mathcal{E}(t,u) + \frac{1}{2}r(t,u)^2\right) \tag{48}$$

that is equivalent to (46). Consequently we understand that the term $\frac{1}{2\gamma}(\partial_u r(t,u))^2$ is the rate of transfer of mechanical energy to thermal energy in the bulk. Of course we also have that $\mathbb{E}\big(\mathcal{E}_x(n^2 t)\big)$ converges weakly to $\mathcal{E}(t,u)$.

In the case the forcing is done on a point $[n\overline{u}]$ in the bulk of the system, and a heat bath is present on the right hand side ($\gamma_+ > 0$), then the boundary conditions we expect are the following:

$$\begin{aligned} &r(t,0) = 0, \quad \partial_u r(t,\overline{u}^+) = \partial_u r(t,\overline{u}^-), \\ &r(t,\overline{u}^-) - r(t,\overline{u}^+) = \overline{F}, \quad r(t,1) = 0, \\ &T(t,0) = T_-, \quad \partial_u T(\overline{u}^-) - \partial_u T(\overline{u}^+) = 4\gamma \mathbb{W}_Q, \qquad T(t,1) = T_+. \end{aligned} \tag{49}$$

As in the pinned case, the macroscopic stationary temperature profiles can be computed. In the case of the stationary state corresponding to (46) the elongation stationary profile is given by

$$r_{ss}(u) = \overline{F}u, \qquad u \in [0,1] \tag{50}$$

and the temperature stationary profile is given by

$$T_{ss}(u) = \overline{F}^2 u(1-u) + (\overline{F}^2 + 4\gamma \mathbb{W}_Q)u + T_-, \qquad u \in [0,1]. \tag{51}$$

Note that, contrary to the pinned case, the temperature profile is not linear (see (38)) but parabolic.

In the case the forcing is in the bulk and the thermostats are present at both endpoints, the stationary solution with boundary conditions (49) is given by

$$\begin{aligned} r_{ss}(u) &= \overline{F}\left(u - 1_{u \geqslant \overline{u}}\right), \\ T_{ss}(u) &= \left[T_- + \left(4\gamma \mathbb{W}_Q (1-\overline{u}) + T_+ - T_-\right) u\right] 1_{u \leqslant \overline{u}} \\ &\qquad + \left[T_+ + \left(4\gamma \mathbb{W}_Q \overline{u} - T_+ + T_-\right)(1-u)\right] 1_{u > \overline{u}} + \overline{F}^2 u(1-u). \end{aligned} \tag{52}$$

5 Higher dimension

We can consider the discrete lattice

$$\Xi_{d,n} = \{\mathbf{x} = \{x_1, \ldots, x_d\}, x_j = 0, \ldots, n, x_j = x_{j+n} \text{ if } j \neq 1\},$$

and the configuration of positions and momenta are described by

$$(\mathbf{q}, \mathbf{p}) = (q_{\mathbf{x}}, p_{\mathbf{x}}) \in \mathbb{R}^{\Xi_{d,n}} \times \mathbb{R}^{\Xi_{d,n}}.$$

The microscopic dynamics of the process $\{(\mathbf{q}(t), \mathbf{p}(t))\}_{t \geqslant 0}$ describing the total chain is now given in the bulk by

$$\begin{aligned} \dot{q}_{\mathbf{x}}(t) &= p_{\mathbf{x}}(t), \qquad \mathbf{x} \in \Xi_{d,n}, \\ \mathrm{d}p_{\mathbf{x}}(t) &= \left(\Delta_N q_{\mathbf{x}} - \omega_0^2 q_{\mathbf{x}}\right) \mathrm{d}t - 2p_{\mathbf{x}}(t-)\mathrm{d}N_{\mathbf{x}}(\gamma t) + \mathcal{F}_{n,\mathbf{x}}(t)\mathrm{d}t, \end{aligned} \tag{53}$$

for $x_1 \in \{1, \ldots, n-1\}$, and at the boundaries by

$$\begin{aligned} \mathrm{d}p_{\mathbf{x}}(t) &= \left(\Delta_N q_{\mathbf{x}} - \omega_0^2 q_{\mathbf{x}}(t)\right)\mathrm{d}t - 2\gamma_- p_{\mathbf{x}}(t)\mathrm{d}t + \sqrt{4\gamma_- T_-}\,\mathrm{d}\widetilde{w}_{\mathbf{x}}(t), x_1 = 0 \\ \mathrm{d}p_{\mathbf{x}}(t) &= \left(\Delta_N q_{\mathbf{x}} - \omega_0^2 q_{\mathbf{x}}(t)\right)\mathrm{d}t - 2\gamma_+ p_{\mathbf{x}}(t)\mathrm{d}t + \sqrt{4\gamma_+ T_+}\,\mathrm{d}\widetilde{w}_{\mathbf{x}}(t), x_1 = n. \end{aligned} \tag{54}$$

Here Δ_N is the discrete laplacian on $\Xi_{d,n}$ with Neumann boundary conditions on the direction 1 and periodic on the others. Processes $\{N_{\mathbf{x}}(t), \mathbf{x} \in \Xi_{d,n}\}$ are independent Poisson of intensity 1, while $\{\widetilde{w}_{\mathbf{x}}(t)\}$ are independent standard Wiener processes, independent of the Poisson processes.

For the pinned model ($\omega_0 \neq 0$) in the absense of forcing ($\mathcal{F}_{n,\mathbf{x}}(t) = 0$ for all $\mathbf{x} \in \Xi_{d,n}$), the macroscopic heat equation is given by

$$\begin{aligned} \partial_t T &= D_\gamma \Delta_u T, \quad u \in (0,1) \times \mathbb{T}^{d-1}, \\ T(t,u) &= \begin{cases} T_- & u_1 = 0, \\ T_+ & u_1 = 1, \end{cases} \end{aligned} \tag{55}$$

where the diffusion coefficient depends on the dimension and is given by

$$D_\gamma = \frac{1}{4\gamma}\frac{1}{2\pi^2}\int_{\mathbb{T}^d} |\nabla\omega(\mathbf{k})|^2\, d\mathbf{k} \tag{56}$$

where $\omega(\mathbf{k}) = \sqrt{\omega_0^2 + 4\sum_{j=1}^d \sin^2(\pi k_j)}$ is the dispersion relation of the harmonic lattice. This coincides with the diffusion coefficient appearing in the self-consistent model, computed in section 7 of [3].

If a driving force is acting in the same way on the right side of the system, i.e. $\mathcal{F}_{n,\mathbf{x}}(t) = \mathcal{F}_n(t)\delta_{x_1,n-1}$, with $\mathcal{F}_n(t)$ satisfying analogous conditions as in dimension 1, and in absence of thermostat on the right, i.e. $\gamma_+ = 0$, then we have the following Neumann type boundary conditions on the right:

$$\nabla T(t,1) = \frac{\mathbb{W}}{D_\gamma}\begin{pmatrix}1\\0\\\vdots\\0\end{pmatrix} \tag{57}$$

where $\mathbb{W}$ is the average work done by the periodic forcing, defined as the limit

$$\mathbb{W} = \frac{1}{t}\lim_{n\to\infty}\frac{1}{n^{d-1}}\sum_{\mathbf{x}}\delta_{x_1,n-1}\mathbb{E}\left(\frac{1}{n}\int_0^{n^2t}\mathcal{F}_n(s)p_{\mathbf{x}}(s)ds\right). \tag{58}$$

More generally, given a smooth $d-1$ dimensional surface $\Gamma \subset (0,1)\times\mathbb{T}^{d-1}$, defining by Γ_n the lattice points $\mathbf{x}$ such that the distance of $\mathbf{x}/n$ from Γ is less that $\frac{1}{2n}$, if $\mathcal{F}_{n,\mathbf{x}}(t) = \mathcal{F}_n(t)\delta_{\mathbf{x},\Gamma_n}$, then we expect the boundary conditions

$$\nabla T(t,u) = \frac{\mathbb{W}}{D_\gamma}\mathbf{n}_\Gamma(u), \qquad u\in\Gamma, \tag{59}$$

where $\mathbf{n}_\Gamma(y)$ is the unit vector normal to Γ in the point u, and $\mathbb{W}$ is a suitable modification of formula (58). For a more general inhomogeneous periodic forcing different macroscopic boundary conditions are expected, and it is a subject of further investigation. The argument used in the one dimensional case in [6, 7] cannot be extended directly to prove (55), (57) or (59). This will be considered in a future work (in preparation).

6 Anharmonic chains

Harmonic chains allow many explicit calculations, in particular we can solve first and second moment equations autonomously, without any need to analyze higher moments. The situation is much more difficult for anharmonic chains, even in presence of the random flip of the velocities sign. Consider the Hamiltonian

$$\mathcal{H}_n(\mathbf{q},\mathbf{p}) := \sum_{x=0}^{n}\left(\frac{p_x^2}{2} + V(q_x - q_{x-1}) + U(q_x)\right), \tag{60}$$

where we set $q_{-1} = 0$. Then consider the stochastic dynamics

$$\begin{aligned} \dot{q}_x(t) &= p_x(t), && x \in \{0,\ldots,n\}, \\ \mathrm{d}p_x(t) &= \partial_{q_x}\mathcal{H}_n \mathrm{d}t - 2p_x(t-)\mathrm{d}N_x(\gamma t), && x \in \{1,\ldots,n-1\}, \end{aligned} \tag{61}$$

and at the boundaries by

$$\begin{aligned} \mathrm{d}p_0(t) =&\ \partial_{q_0}\mathcal{H}_n \mathrm{d}t - 2p_0(t-)\mathrm{d}N_0(\gamma t) - 2\gamma_- p_0(t)\mathrm{d}t + \sqrt{4\gamma_- T_-}\mathrm{d}\widetilde{w}_-(t) \\ \mathrm{d}p_n(t) =&\ \partial_{q_n}\mathcal{H}_n \mathrm{d}t + \mathcal{F}_n(t)\mathrm{d}t - 2p_n(t-)\mathrm{d}N_n(\gamma t) - 2\gamma_+ p_n(t)\mathrm{d}t \\ &+ \sqrt{4\gamma_+ T_+}\mathrm{d}\widetilde{w}_+(t). \end{aligned} \tag{62}$$

The energy currents in the bulk are given by

$$j_{x,x+1}(t) := -p_x(t)V'(q_{x+1}(t) - q_x(t)), \qquad \text{if} \quad x \in \{0,...,n-1\}. \tag{63}$$

The only existing mathematical result is the existence of the thermal diffusivity defined by the Green-Kubo formula (cf. [2]):

$$D_\gamma(T) = \int_0^\infty \mathrm{d}t \sum_{x\in\mathbb{Z}} \mathbb{E}_{\nu_T}\left(j_{x,x+1}(t) j_{0,1}(0)\right), \tag{64}$$

where $\mathbb{E}_{\nu_T}$ is the expectation of the corresponding infinite dynamics in equilibrium at temperature T.

When γ_- and γ_+ are strictly positive we expect the convergence of the temperature profile as in (29) to the solution of

$$\begin{aligned} &\partial_t T = \partial_u\left(D_\gamma(T)\partial_u T\right), \qquad u \in (0,1), \\ &T(t,0) = T_-, \quad T(t,1) = T_+, \\ &T(0,u) = T_0(u). \end{aligned} \tag{65}$$

When $\gamma_+ = 0$, i.e. if only the periodic forcing is acting on the last particle, the boundary condition on $u = 1$ is given by a non-linear Neumann condition:

$$D_\gamma(T(t,1))(\partial_u T)(t,1) = -J(T(t,1)) \tag{66}$$

with a boundary current $J(T)$ depending on the local temperature.

A linear response argument gives the following expression of J as a function of T:

$$\begin{aligned}
-J(T) &= \frac{1}{T}\frac{1}{\theta}\int_0^\theta \mathrm{d}t \int_t^{+\infty} \mathcal{F}\Big(\frac{t}{\theta}\Big)\mathcal{F}\Big(\frac{s}{\theta}\Big)\mathbb{E}^+_{\nu_T}\left(p_0(t)p_0(s)\right)\,\mathrm{d}s \\
&= \frac{1}{T}\int_0^\infty \left(\frac{1}{\theta}\int_0^\theta \mathcal{F}\Big(\frac{t}{\theta}\Big)\mathcal{F}\Big(\frac{t+s}{\theta}\Big)\mathrm{d}t\right)\mathbb{E}^+_{\nu_T}\left(p_0(0)p_0(s)\right)\,\mathrm{d}s,
\end{aligned} \tag{67}$$

where $\mathbb{E}^+_{\nu_T}$ denotes the expectation for the semi-infinite process (i.e. (61) for $x \in \mathbb{Z}_+$, without any forcing or heat bath) in equilibrium at temperature T. As for (64), the integral involved in (67) can be proven convergent by using a similar argument as in [2].

In the harmonic case (67) coincides with (13) with $-J(T) = \mathbb{W}$. In the case of quartic pinning potential U and quadratic V, (66) and (67) have been confirmed recently by numerical simulations [4].

Note also that $-J(T)$ is positive since

$$\begin{aligned}
-J(T) &= \lim_{n\to+\infty}\frac{1}{nT}\int_0^{n\theta}\mathrm{d}t\int_t^{n\theta}\mathcal{F}\left(\frac{t}{\theta}\right)\mathcal{F}\left(\frac{s}{\theta}\right)\mathbb{E}_{\nu_T}\Big[p_n(t)p_n(s)\Big]\mathrm{d}s \\
&= \lim_{n\to+\infty}\frac{1}{2nT}\mathbb{E}_{\nu_T}\left[\left(\int_0^{n\theta}\mathcal{F}\left(\frac{t}{\theta}\right)p_n(t)\mathrm{d}t\right)^2\right] \geqslant 0.
\end{aligned} \tag{68}$$

References

[1] G. Basile, S. Olla, and H. Spohn. Energy transport in stochastically perturbed lattice dynamics. *Arch. Rat. Mech.*, 195(1):171–203, 2009.

[2] C. Bernardin and S. Olla. Transport properties of a chain of anharmonic oscillators with random flip of velocities. *J. Stat. Physics*, 145:1224–1225, 2011.

[3] F. Bonetto, J. L. Lebowitz, and J. Lukkarinen. Fourier's law for a harmonic crystal with self-consistent stochastic reservoirs. *J. Stat. Physics*, 116, 2004.

[4] Shiva Darshan. Private communication. 2023.

[5] A. De Masi, Presutti E., D. Tsagkarogiannis, and M.E. Vares. Current reservoirs in the simple exclusion process. *J Stat Phys*, 144:1151, 2011.

[6] T. Komorowski, J. L. Lebowitz, and S. Olla. Heat flow in a periodically forced, thermostatted chain. *Communications in Mathematical Physics*, 2023.

[7] T. Komorowski, J. L. Lebowitz, and S. Olla. Heat flow in a periodically forced, thermostatted chain II. *J. Stat. Physics*, 190:89, 2023.

[8] T. Komorowski, J. L. Lebowitz, S. Olla, and M. Simon. Heat flow in a periodically forced, thermostatted chain III. the case of an unpinned chain. *in preparation.*

[9] T. Komorowski, S. Olla, and M. Simon. Hydrodynamic limit for a chain with thermal and mechanical boundary forces. *Electronic Journal of Probability*, 26:1–49, 2021.

[10] Z. Rieder, J.L. Lebowitz, and E. Lieb. Properties of harmonic crystal in a stationary non-equilibrium state. *J. Math. Phys.*, 8:1073–1078, 1967.

Tomasz Komorowski
Institute of Mathematics
Polish Academy Of Sciences
Warsaw, Poland.
tkomorowski@impan.pl

Joel L. Lebowitz
Departments of Mathematics and Physics
Rutgers University
lebowitz@math.rutgers.edu

Stefano Olla
CEREMADE
Université Paris Dauphine - PSL Research University
and Institut Universitaire de France
and GSSI, L'Aquila
olla@ceremade.dauphine.fr

Marielle Simon
Université Claude Bernard Lyon 1
CNRS UMR 5208, Institut Camille Jordan
F-69622 Villeurbanne, France
and GSSI, L'Aquila
msimon@math.univ-lyon1.fr