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► **To cite this version:**

Stefano Olla, Marielle Simon. Microscopic derivation of an adiabatic thermodynamic transformation. Brazilian Journal of Probability and Statistics, 2015, pp.23. 10.1214/14-BJPS275 . hal-01067091v2

HAL Id: hal-01067091

<https://hal.science/hal-01067091v2>

Submitted on 10 Dec 2014

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MICROSCOPIC DERIVATION OF AN ADIABATIC THERMODYNAMIC TRANSFORMATION

STEFANO OLLA AND MARIELLE SIMON

ABSTRACT. We obtain macroscopic adiabatic thermodynamic transformations by space-time scalings of a microscopic Hamiltonian dynamics subject to random collisions with the environment. The microscopic dynamics is given by a chain of oscillators subject to a varying tension (external force) and to collisions with external independent particles of “infinite mass”. The effect of each collision is to change the sign of the velocity without changing the modulus. This way the energy is conserved by the resulting dynamics. After a diffusive space-time scaling and coarse-graining, the profiles of volume and energy converge to the solution of a deterministic diffusive system of equations with boundary conditions given by the applied tension. This defines an irreversible thermodynamic transformation from an initial equilibrium to a new equilibrium given by the final tension applied. Quasi-static reversible adiabatic transformations are then obtained by a further time scaling. Then we prove that the relations between the limit work, internal energy and thermodynamic entropy agree with the first and second principle of thermodynamics.

1. INTRODUCTION

In classical thermodynamics, adiabatic transformations are defined as those processes that change the state of the system from an equilibrium to another only by the action of an external force. This means that the system is isolated, not in contact with any *heat bath*, and that the change in its internal energy U is only due to the work done by the applied external force. The second law of thermodynamics states that the only possible adiabatic transformations are those that do not decrease the thermodynamic entropy S of the system. Irreversible adiabatic transformations assume a strict increase of the entropy, while if entropy remains constant the transformation is called reversible or quasi-static.

When connecting this transformation to the microscopic dynamics of the atoms constituting the system, we understand this thermodynamic behaviour as the macroscopic *deterministic* change of the observables that characterize the thermodynamic equilibria (in the case studied in this article, the energy and the volume, or the temperature and the tension). We intend *macroscopic* in the sense that we would like to recover this behaviour in a large space and time scale: the thermodynamic system is composed by a huge number of atoms and we look

This work has been partially supported by the European Advanced Grant *Macroscopic Laws and Dynamical Systems* (MALADY) (ERC AdG 246953), by the fellowship L’Oreal France-UNESCO *Pour les femmes et la science*, and by the CAPES and CNPq program *Science Without Borders*.

at a very large time scale with respect to the typical frequency of atoms vibration. Mathematically this means a space-time scaling limit procedure.

We study these adiabatic transformations in a one dimensional model of a wire. Macroscopically the equilibrium states are characterized by the length L and the energy U (as extensive quantities), or by the temperature $T = \beta^{-1}$ and the tension τ . Microscopically we model this wire by a Hamiltonian system constituted by a chain of springs attached at one extreme to a point, while at the other extreme a force $\bar{\tau}$ acts on the last particle. The Hamiltonian dynamics of the chain is perturbed by independent random changes of the sign of velocities. This random perturbation can be seen as the effect of collisions with *environment* particles of infinite mass moving independently, in orthogonal direction to the wire. Notice that these random collisions conserve the energy of particles, so that the dynamics is still adiabatic.

The first effect of these random perturbations is to ensure that the only parameters characterizing the macroscopic equilibrium states are the energy and the length, i.e. that the system obeys the so called 0th law of thermodynamics. In fact these random perturbations select the Gibbs probability measures on the configurations, parametrized by the conserved quantities, as the only stationary measures for the corresponding infinite dynamics (for details see [5, 3]).

Another important consequence of these collisions is the suppression of momentum conservation, so that there is no ballistic transport on a macroscopic scale. Thus, we expect a diffusive behaviour of the energy and the volume stretch caused by a change of the exterior tension $\bar{\tau}$, before attaining the new equilibrium. Consequently the correct space-time macroscopic rescaling is diffusive. The change of the external force $\bar{\tau}$ should happen on the macroscopic time scale, i.e. very slowly with respect to the typical time scale of the dynamics of the atoms.

We expect that, under a diffusive space-time scale, the empirical profiles of the stretch and the energy, due to a change of the applied tension $\bar{\tau}$, evolve deterministically following the diffusive system of partial differential equations (2.7). The solution of this system eventually will converge to a new equilibrium state. This deterministic evolution of the profiles describes an irreversible adiabatic transformation, and, as shown in section 4, it increases the thermodynamic entropy of the system. The reversible or quasi-static transformations are then obtained by a further rescaling of time, see subsection 4.2, similar as proposed in [1, 2, 10]. It should be possible to obtain these quasi-static transformation in a direct limit at a larger (subdiffusive) time scale, this will be object of further investigation.

The scaling limit for the non-linear system is still out of the known mathematical techniques, as it requires to deal with the *non-gradient* energy current in the energy conservation law. Even though the convergence of the Green-Kubo formula defining the energy diffusivity is proven in [4], the actual proof of the macroscopic equation requires a fluctuation-dissipation decomposition of the energy current (cf. [11] for such decomposition in a non-linear dynamics conserving only energy). In the linear case (harmonic oscillators), there is an explicit fluctuation-dissipation decomposition of the energy current and it is possible to

perform the scaling limit. This was done in [12] for the periodic boundary conditions case. We adapt here that proof for the case of mixed boundary conditions with slowly changing external tension.

In [8], the macroscopic limit was studied in the same model, for non-linear springs, but with a stochastic exchange of momentum between nearest neighbour particles. This dynamics also conserves the momentum, besides the energy and the volume. For that system the macroscopic space-time scale is hyperbolic, and the macroscopic equations are given by the Euler system of conservation laws. Notice that in the harmonic case these are just linear wave equations, and the corresponding macroscopic equation will not bring the system to a new equilibrium state, that can be reached only at a super-diffusive space-time scale [6]. In the non-linear case we need a better understanding of the entropy production of the shock waves that appear in the solution to Euler equations.

Isothermal transformations in this model have been deduced in [10] in the non-linear case, where the heat bath is modelled by Langevin thermostats. In this evolution only the volume evolves macroscopically. In [10] these heat baths act on the bulk of the chain, at every point. If we want to make them act only at the boundaries of the chain, then we should obtain the same macroscopic equations as in the present article, but with boundary conditions corresponding to the thermostat temperature (this will be object of further investigation).

With the result contained in the present article we complete the deduction of the macroscopic Carnot cycle from the microscopic dynamics.

2. ADIABATIC MICROSCOPIC DYNAMICS

We consider a chain of n coupled oscillators in one dimension. Each particle has the same mass that we set equal to 1. The position of atom i is denoted by $q_i \in \mathbb{R}$, while its momentum is denoted by $p_i \in \mathbb{R}$. Thus the configuration space is $(\mathbb{R} \times \mathbb{R})^n$. We assume that an extra particle 0 is attached to a fixed point and does not move, i.e. $(q_0, p_0) \equiv (0, 0)$, while on particle n we apply a force $\bar{\tau}(t)$ depending on time. Observe that only the particle 0 is constrained to not move, and that q_i can assume also negative values.

Denote $\mathbf{q} := (q_1, \dots, q_n)$ and $\mathbf{p} := (p_1, \dots, p_n)$. The interaction between two particles i and $i - 1$ is described by the potential energy $V(q_i - q_{i-1})$ of an anharmonic spring relying the particles. We assume $V(r)$ to be a positive smooth function which for large r grows faster than linear but at most quadratic, that means that there exists a constant $C > 0$ such that

$$\lim_{|r| \rightarrow \infty} \frac{V(r)}{|r|} = \infty,$$

$$\limsup_{|r| \rightarrow \infty} V''(r) \leq C < \infty.$$

Energy is defined by the following Hamiltonian:

$$\sum_{i=1}^n \left(\frac{p_i^2}{2} + V(q_i - q_{i-1}) \right).$$

Since we focus on a nearest neighbor interaction, we may define the distance between particles by

$$r_i = q_i - q_{i-1}, \quad i = 1, \dots, n.$$

The particles are subject to an interaction with the environment that does not change the energy: each particle has an independent Poissonian clock and its momentum changes sign when it rings. The equations of motion are given by

$$\begin{cases} dr_i(t) = n^2(p_i(t) - p_{i-1}(t)) dt \\ dp_i(t) = n^2(V'(r_{i+1}(t)) - V'(r_i(t))) dt - 2p_i(t^-) d\mathcal{N}_i(\gamma n^2 t), \quad i = 1, \dots, n-1, \\ dp_n(t) = n^2(\bar{\tau}(t) - V'(r_n(t))) dt - 2p_n(t^-) d\mathcal{N}_n(\gamma n^2 t). \end{cases}$$

Here $\{\mathcal{N}_i(t)\}_i$ are n -independent Poisson processes of intensity 1, the constant γ is strictly positive, and p_0 is set identically to 0. We have already rescaled time according to the diffusive space-time scaling. Notice that $\bar{\tau}(t)$ changes at this macroscopic time scale. The generator of this diffusion is given by

$$\mathcal{L}_n^{\bar{\tau}(t)} := n^2 A_n^{\bar{\tau}(t)} + n^2 \gamma S_n.$$

Here the Liouville operator A_n^{τ} is given by

$$A_n^{\tau} = \sum_{i=1}^n (p_i - p_{i-1}) \frac{\partial}{\partial r_i} + \sum_{i=1}^{n-1} (V'(r_{i+1}) - V'(r_i)) \frac{\partial}{\partial p_i} + (\tau - V'(r_n)) \frac{\partial}{\partial p_n},$$

while, for $f : (\mathbb{R} \times \mathbb{R})^n \rightarrow \mathbb{R}$,

$$S_n f(\mathbf{r}, \mathbf{p}) = \sum_{i=1}^n (f(\mathbf{r}, \mathbf{p}^i) - f(\mathbf{r}, \mathbf{p}))$$

where $(\mathbf{p}^i)_j = p_j$ if $j \neq i$ and $(\mathbf{p}^i)_i = -p_i$. For $\bar{\tau}(t) = \tau$ constant, the system has a family of stationary measures given by the canonical Gibbs distributions

$$d\mu_{\tau, T}^n = \prod_{i=1}^n e^{-\frac{1}{T}(\mathcal{E}_i - \tau r_i) - \mathcal{G}_{\tau, T}} dr_i dp_i, \quad T > 0, \quad (2.1)$$

where we denote

$$\mathcal{E}_i = \frac{p_i^2}{2} + V(r_i),$$

the energy that we attribute to the particle i , and

$$\mathcal{G}_{\tau, T} = \log \left[\sqrt{2\pi T} \int e^{-\frac{1}{T}(V(r) - \tau r)} dr \right]. \quad (2.2)$$

Observe that the function $\mathbf{r}(\tau, T) = T \partial_{\tau} \mathcal{G}_{\tau, T}$ gives the average equilibrium length in function of the tension τ , and

$$\mathbf{u}(\tau, T) = \tau \mathbf{r}(\tau, T) + T^2 \partial_T \mathcal{G}_{\tau, T}$$

is the corresponding thermodynamic internal energy function. We denote the inverse of the average length \mathfrak{r} by $\boldsymbol{\tau}(\mathfrak{r}, \mathbf{u})$. Thermodynamic entropy $S(\mathfrak{r}, \mathbf{u})$ is defined as

$$S(\mathfrak{r}, \mathbf{u}) = \frac{1}{T} (\mathbf{u} - \boldsymbol{\tau}\mathfrak{r}) + \mathcal{G}_{\boldsymbol{\tau}, T} \quad (2.3)$$

so that $\partial_{\mathbf{u}}S = T^{-1}$ and $\partial_{\mathfrak{r}}S = -T^{-1}\boldsymbol{\tau}$. From now on, we reindex notations by using the inverse temperature $\beta := T^{-1}$. In the following we will need to consider local Gibbs measures (non homogeneous product), corresponding to profiles of tension and temperature $\{\tau(x), \beta^{-1}(x), x \in [0, 1]\}$:

$$d\mu_{\boldsymbol{\tau}(\cdot), \beta(\cdot)}^n = \prod_{i=1}^n e^{-\beta(i/n)(\mathcal{E}_i - \tau(i/n)r_i) - \mathcal{G}_{\boldsymbol{\tau}(i/n), \beta(i/n)}} dr_i dp_i. \quad (2.4)$$

Given an initial profile of tension $\tau(0, x)$ and temperature $\beta^{-1}(0, x)$, we assume that the initial probability state is given by the corresponding $\mu_{\boldsymbol{\tau}(0, \cdot), \beta(0, \cdot)}^n$. This implies the following convergence in probability with respect to the initial distribution:

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n G(i/n)r_i(0) &\longrightarrow \int_0^1 G(x)\mathfrak{r}(\tau(0, x), \beta(0, x)) dx \\ \frac{1}{n} \sum_{i=1}^n G(i/n)\mathcal{E}_i(0) &\longrightarrow \int_0^1 G(x)\mathbf{u}(\tau(0, x), \beta(0, x)) dx \end{aligned} \quad (2.5)$$

for any continuous compactly supported test function $G \in \mathcal{C}_0(\mathbb{R})$. We expect the same convergence to happen at the macroscopic time t :

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n G(i/n)r_i(t) &\longrightarrow \int_0^1 G(x)r(t, x) dx \\ \frac{1}{n} \sum_{i=1}^n G(i/n)\mathcal{E}_i(t) &\longrightarrow \int_0^1 G(x)u(t, x) dx \end{aligned} \quad (2.6)$$

and the macroscopic evolution for the volume and energy profiles should follow the system of equations, for $(t, x) \in \mathbb{R}_+ \times [0, 1]$

$$\begin{aligned} \partial_t r(t, x) &= \frac{1}{2\gamma} \partial_{xx} [\boldsymbol{\tau}(r, u)] \\ \partial_t u(t, x) &= \partial_x [\mathcal{D}(r, u) \partial_x [\beta^{-1}(r, u)]] + \frac{1}{4\gamma} \partial_{xx} [\boldsymbol{\tau}^2(r, u)] \end{aligned} \quad (2.7)$$

with the following boundary conditions:

$$\begin{cases} \partial_x [\boldsymbol{\tau}(r, u)](t, 0) = 0 \\ \partial_x [\beta^{-1}(r, u)](t, 0) = 0 \end{cases} \quad \begin{cases} \boldsymbol{\tau}(r(t, 1), u(t, 1)) = \bar{\boldsymbol{\tau}}(t) \\ \partial_x [\beta^{-1}(r, u)](t, 1) = 0 \end{cases}$$

and initial conditions

$$\begin{cases} r(0, x) = \mathfrak{r}(\tau(0, x), \beta(0, x)) \\ u(0, x) = \mathbf{u}(\tau(0, x), \beta(0, x)). \end{cases}$$

Equation (2.7) can be deduced by linear response theory (cf. [4]) and the thermal diffusivity \mathcal{D} is defined by the corresponding Green-Kubo formulas. The convergence of the corresponding Green-Kubo expression is proved in [4]. Still a proof of the hydrodynamic limit (2.5) is out of reach with the known techniques.

In the harmonic case $V(r) = r^2/2$, Equation (2.5) is proven in [12] with periodic boundary conditions, and we will adapt here that proof in order to deal with the forcing boundary conditions.

3. THE HARMONIC CASE

When the interaction potential is harmonic, explicit computations are available, for instance

$$\mathcal{G}_{\tau,\beta} = \log \left[\frac{\beta}{2\pi} \exp \left(\frac{\tau^2 \beta}{2} \right) \right].$$

The thermodynamic relations between the averaged conserved quantities $\mathfrak{r} \in \mathbb{R}$ and $\mathfrak{u} \in (0, +\infty)$, and the potentials $\tau \in \mathbb{R}$ and $\beta \in (0, +\infty)$ are given by

$$\mathfrak{u}(\tau, \beta) = \frac{1}{\beta} + \frac{\tau^2}{2}, \quad \mathfrak{r}(\tau, \beta) = \tau. \quad (3.1)$$

Furthermore the thermal diffusivity turns out to be equal to $\mathcal{D} = (4\gamma)^{-1}$ (cf. [4]).

Let r_0 and u_0 be two continuous initial profiles on $[0, 1]$, and define the solutions $r(t, \cdot)$ and $u(t, \cdot)$ to the hydrodynamic equation (2.7), rewritten as

$$\begin{aligned} \partial_t r(t, x) &= \frac{1}{2\gamma} \partial_{xx} r(t, x) \\ \partial_t u(t, x) &= \frac{1}{4\gamma} \partial_{xx} \left[u(t, x) + \frac{r^2(t, x)}{2} \right] \end{aligned} \quad (3.2)$$

with the boundary conditions, for $(t, x) \in \mathbb{R}_+ \times [0, 1]$

$$\begin{cases} \partial_x r(t, 0) = 0 \\ r(t, 1) = \bar{\tau}(t) \\ r(0, x) = r_0(x) \end{cases} \quad \begin{cases} \partial_x u(t, 0) = 0 \\ \partial_x u(t, 1) = \bar{\tau}(t) \partial_x r(t, 1) \\ u(0, x) = u_0(x). \end{cases} \quad (3.3)$$

The solutions u, r are smooth when $t > 0$ as soon as the initial condition satisfies $u_0 > r_0^2/2$ (the system of partial differential equations is parabolic).

In this case, the evolution of $r(t, x)$ is autonomous from $u(t, x)$, therefore we can call $R(t) = \int_0^1 r(t, x) dx$ the total length of the chain at time t , that also does not depend on $u(\cdot, \cdot)$, and write the boundary conditions for $u(t, x)$ as

$$\frac{d}{dt} \left[\int_0^1 u(t, x) dx \right] = \bar{\tau}(t) \dot{R}(t) = \frac{d}{dt} L(t) \quad (3.4)$$

where L is the work done by the force $\bar{\tau}$ up to time t .

For a local function ϕ , we denote by $\theta_i \phi$ the shift of the function ϕ : $\theta_i \phi(\mathbf{r}, \mathbf{p}) = \phi(\theta_i \mathbf{r}, \theta_i \mathbf{p})$. This is always well defined for n sufficiently large. The main result is the following:

Theorem 3.1. *We have*

$$\lim_{n \rightarrow \infty} \frac{\mathcal{H}_n(t)}{n} = 0 \quad (3.5)$$

where

$$\mathcal{H}_n(t) = \int f_t^n \log \left(\frac{f_t^n}{\phi_t^n} \right) d\mathbf{r} d\mathbf{p} \quad (3.6)$$

with

- (i) f_t^n the density of the configuration of the system at time t ,
- (ii) ϕ_t^n the density of the “corrected” local Gibbs measure $\nu_{\tau(t,\cdot),\beta(t,\cdot)}^n$ defined as

$$d\nu_{\tau(t,\cdot),\beta(t,\cdot)}^n = \frac{1}{Z(t)} \prod_{i=1}^n e^{-\beta(t,\frac{i}{n})(\mathcal{E}_i - \tau(t,\frac{i}{n})r_i) + \frac{1}{n}F(t,\frac{i}{n})\cdot\theta_i h(\mathbf{r},\mathbf{p})} dr_i dp_i.$$

Above $Z(t)$ is the partition function, and F, h are explicit functions given in (5.5).

We denote by $\mu[\cdot]$ the expectation with respect to the measure μ . Theorem 3.1 implies the hydrodynamic limits in the following sense:

Corollary 3.2. *Let G be a continuous function on $[0, 1]$ and φ be a local function which satisfies the following property: there exists a finite subset $\Lambda \subset \mathbb{Z}$ and a constant $C > 0$ such that, for all $(\mathbf{r}, \mathbf{p}) \in (\mathbb{R} \times \mathbb{R})^n$, $\varphi(\mathbf{r}, \mathbf{p}) \leq C (1 + \sum_{i \in \Lambda} \mathcal{E}_i)$. Then,*

$$\mu_t^n \left[\left| \frac{1}{n} \sum_i G(i/n) \theta_i \varphi - \int_{[0,1]} G(x) \tilde{\varphi}(u(t,x), r(t,x)) dx \right| \right] \xrightarrow[n \rightarrow \infty]{} 0 \quad (3.7)$$

where $\tilde{\varphi}$ is the grand-canonical expectation of φ : in other words, for any (u, r) ,

$$\tilde{\varphi}(u, r) = \mu_{\tau,\beta}[\varphi] = \int_{(\mathbb{R} \times \mathbb{R})^{\mathbb{Z}}} \varphi(\mathbf{r}, \mathbf{p}) d\mu_{\tau,\beta}(\mathbf{r}, \mathbf{p}). \quad (3.8)$$

We prove Theorem 3.1 in Section 5.

4. THERMODYNAMIC CONSEQUENCES

4.1. Second principle of thermodynamics. Let us first compute the increase of the total thermodynamic entropy, under the macroscopic evolution given by the general equations (2.7):

$$\begin{aligned} \frac{d}{dt} \int_0^1 S(r(t,x), u(t,x)) dx &= \int_0^1 [-\beta \boldsymbol{\tau} \partial_t r + \beta \partial_t u] dx \\ &= \int_0^1 \left[\mathcal{D} \left(\frac{\partial_x \beta}{\beta} \right)^2 + \frac{1}{2\gamma} \beta (\partial_x \boldsymbol{\tau})^2 \right] dx \geq 0. \end{aligned} \quad (4.1)$$

Assume now that we start in equilibrium with a given constant tension τ_0 and constant inverse temperature β_0 . To these values correspond a constant profile of length $r(0,x) = \mathcal{L}_0$ and of energy $u(0,x) = u_0$, that constitute the initial conditions for (2.7). The initial thermodynamic entropy is then $S_0 = S(\mathcal{L}_0, u_0)$.

We now apply a time depending tension $\bar{\tau}(t)$, such that $\bar{\tau}(t) = \tau_1$ for $t \geq \bar{t}$. It is clear that the solution converges as $t \rightarrow \infty$ to a new global equilibrium state, with tension τ_1 . This final equilibrium state has total length \mathcal{L}_1 given by

$$\mathcal{L}_1 = \mathcal{L}_0 + \frac{1}{2\gamma} \int_0^\infty \partial_x [\boldsymbol{\tau}(r, u)](t, 1) dt, \quad (4.2)$$

and energy $u_1 = u_0 + W$, where W is the mechanical work done by the tension $\bar{\tau}(t)$. The total work W can be computed by:

$$W = \frac{1}{2\gamma} \int_0^\infty \bar{\tau}(t) \partial_x [\boldsymbol{\tau}(r, u)](t, 1) dt. \quad (4.3)$$

Consequently the thermodynamic entropy of the final equilibrium state equals

$$S_1 = S(\mathcal{L}_1, u_1) = S_0 + \int_0^\infty dt \int_0^1 \left[\mathcal{D} \left(\frac{\partial_x \beta}{\beta} \right)^2 + \frac{1}{2\gamma} \beta (\partial_x \boldsymbol{\tau})^2 \right] dx. \quad (4.4)$$

This is in agreement with the second principle of thermodynamics, in the statement that an irreversible adiabatic transformation increases the thermodynamic entropy of the system.

In the harmonic case, the thermodynamic entropy is a function of the temperature only, and

$$S_1 - S_0 = \log \left(\frac{\beta_0}{\beta_1} \right). \quad (4.5)$$

In other words, any increase of entropy implies an increase of temperature. It means that any adiabatic irreversible transformation can only increase the temperature of the system. In the harmonic case, the reversible transformations obtained by the quasi-static limit cannot change the entropy and the temperature.

4.2. Quasistatic limit. Notice that (3.1) suggests to define

$$\beta^{-1}(t, x) = u(t, x) - \frac{1}{2} r^2(t, x).$$

Equation (3.2) can be written as

$$\begin{aligned} \partial_t r(t, x) &= \frac{1}{2\gamma} \partial_{xx} r(t, x) \\ \partial_t [\beta^{-1}](t, x) &= \frac{1}{4\gamma} \partial_{xx} [\beta^{-1}](t, x) + \frac{1}{2\gamma} (\partial_x r(t, x))^2 \end{aligned} \quad (4.6)$$

with the boundary conditions, for $(t, x) \in \mathbb{R}_+ \times [0, 1]$

$$\begin{cases} \partial_x r(t, 0) = 0 \\ r(t, 1) = \bar{\tau}(t) \\ r(0, x) = r_0(x) \end{cases} \quad \begin{cases} \partial_x [\beta^{-1}](t, 0) = 0 = \partial_x [\beta^{-1}](t, 1) \\ \beta^{-1}(0, x) = u_0(x) - \frac{r_0^2(x)}{2}. \end{cases} \quad (4.7)$$

Consider the case when the exterior tension $\bar{\tau}(t)$ is equal to a value $\bar{\tau}_1$ for any $t \geq t_1$. It is clear that we have the following convergence to equilibrium:

$$r(t, x) \xrightarrow[t \rightarrow \infty]{} \bar{\tau}_1,$$

$$\beta^{-1}(t, x) \xrightarrow[t \rightarrow \infty]{} \bar{\beta}_1^{-1} = \int_0^1 \left(u_0(x') - \frac{r_0(x')^2}{2} \right) dx' + \frac{1}{2\gamma} \int_0^\infty dt \int_0^1 (\partial_x r(t, x))^2 dx.$$

Suppose, as above, that we start at equilibrium with tension τ_0 and temperature β_0^{-1} . This means $r(0, x) = \tau_0$, $u(0, x) = \beta_0^{-1} - \tau_0^2/2$, and an initial exterior force $\bar{\tau}(0) = \tau_0$. Then, after the limit $t \rightarrow \infty$, we have reached a new equilibrium with tension $\bar{\tau}_1$ and a higher temperature

$$\beta_1^{-1} = \beta_0^{-1} + \frac{1}{2\gamma} \int_0^\infty dt \int_0^1 (\partial_x r(t, x))^2 dx.$$

In particular the temperature, and consequently the entropy, always increase in this irreversible transformation.

We now consider the quasi-static limit, where we slow down the changing of the exterior tension, i.e. we consider the same system (4.6), but one of the boundary conditions (precisely, the second one of (4.7)) is changed into $r(t, 1) = \bar{\tau}(\varepsilon t)$. The corresponding solution is denote by $(r^\varepsilon, u^\varepsilon)$. Then Proposition 3.1 of [10] can be applied and it follows that

$$\lim_{\varepsilon \rightarrow 0} \int_0^\infty dt \int_0^1 (\partial_x r^\varepsilon(\varepsilon^{-1}t, x))^2 dx = 0$$

and $r^\varepsilon(\varepsilon^{-1}t, x) \rightarrow \bar{\tau}(t)$, for all $(t, x) \in \mathbb{R}_+ \times [0, 1]$. Consequently

$$(\beta^\varepsilon(\varepsilon^{-1}t, x))^{-1} \xrightarrow[\varepsilon \rightarrow 0]{} \beta_0^{-1}, \quad u^\varepsilon(\varepsilon^{-1}t, x) \xrightarrow[\varepsilon \rightarrow 0]{} \beta_0^{-1} - \frac{\bar{\tau}^2(t)}{2}$$

for all $(t, x) \in \mathbb{R}_+ \times [0, 1]$. Similar considerations are valid in the non-linear case.

5. PROOF OF THE HYDRODYNAMIC LIMIT

We approach this problem by using the relative entropy method [13]. We adapt the proof of [12], where the same harmonic perturbed chain is investigated, assuming periodic boundary conditions. We recall here the main steps of the argument, and give details only for computations that change due to boundary conditions.

In the context of diffusive systems, the relative entropy method works if the following conditions are satisfied.

- (1) First, the dynamics has to be *ergodic*: the only time and space invariant measures for the infinite system, with finite local entropy, are given by mixtures of Gibbs measures in infinite volume $\mu_{\tau, \beta}$. From [5], we know that the velocity-flip model is ergodic in the sense above. For a precise statement, we refer to [12, Theorem 1.3].

- (2) Next, we need to establish the so-called *fluctuation-dissipation equations*. Such equations express the microscopic currents $j_i^\mathcal{E}$ and j_i^r (respectively of energy and deformation) as the sum of a discrete gradient and a fluctuating term. Here, the conservation laws write for $i \geq 1$,

$$\mathcal{L}_n^\tau(\mathcal{E}_i) = n^2(j_{i+1}^\mathcal{E} - j_i^\mathcal{E}) \quad \text{with } j_i^\mathcal{E} := \begin{cases} r_i p_{i-1}, & \text{if } i \in \{1, \dots, n\}, \\ \tau p_n, & \text{if } i = n+1, \end{cases}$$

$$\mathcal{L}_n^\tau(r_i) = n^2(j_{i+1}^r - j_i^r) \quad \text{with } j_i^r = p_{i-1} \text{ for any } i \in \{1, \dots, n+1\}.$$

Notice that $j_1^\mathcal{E} = 0$ and $j_1^r = 0$. If $\tau_i f(\mathbf{r}, \mathbf{p})$ is a local function on the configurations, we define its discrete gradient as

$$\nabla(\theta_i f) := \theta_{i+1} f - \theta_i f.$$

We denote by $(\mathcal{L}_n^\tau)^* := -n^2 A_n^\tau + \gamma n^2 S_n$ the adjoint of \mathcal{L}_n^τ in $\mathbf{L}^2(\mu_{\tau, \beta}^n)$. We write down the fluctuation-dissipation equations: for $i \in \{2, \dots, n\}$,

$$j_i^\mathcal{E} = \nabla(u_i) + (\mathcal{L}_n^\tau)^* \left[-\frac{r_i(p_{i-1} + p_i - \gamma r_i)}{4\gamma n^2} \right] \quad (5.1)$$

$$j_i^r = \nabla\left(-\frac{r_{i-1}}{2\gamma}\right) + (\mathcal{L}_n^\tau)^* \left[-\frac{p_{i-1}}{2\gamma n^2} \right] \quad (5.2)$$

where for $i \in \{2, \dots, n\}$,

$$u_i = -\frac{p_{i-1}^2 + r_{i-1} r_i}{4\gamma} \quad \text{and} \quad u_{n+1} = -\frac{p_n^2 + \tau r_n}{4\gamma}.$$

For $i = n+1$, the fluctuation-dissipation equations read as

$$j_{n+1}^\mathcal{E} = \tau \left(\frac{r_n - \tau}{2\gamma} + (\mathcal{L}_n^\tau)^* \left[-\frac{p_n}{2\gamma n^2} \right] \right)$$

$$j_{n+1}^r = \frac{r_n - \tau}{2\gamma} + (\mathcal{L}_n^\tau)^* \left[-\frac{p_n}{2\gamma n^2} \right]$$

- (3) Since we observe the system on a diffusive scale and the system is non-gradient, we need second order approximations. If we want to obtain the entropy estimate of order $o(n)$, we can not work directly with the local Gibbs measure $\mu_{\tau(t, \cdot), \beta(t, \cdot)}^n$: we have to correct it with a small term.
- (4) Finally, we need to control all the following moments,

$$\int \left\{ \frac{1}{n} \sum_{i=1}^n |\mathcal{E}_i|^k \right\} d\mu_t^n, \quad k \geq 2 \quad (5.3)$$

uniformly in time and with respect to n . The harmonicity of the chain is crucial to get this result: roughly speaking, it ensures that the set of mixtures of Gaussian probability measures is left invariant during the time evolution.

In the two next subsections, we explain the relative entropy method, and highlight the role of the fluctuation-dissipation equations. In Subsection 5.3, we prove bounds (5.3).

5.1. Relative entropy method. Recall the definition of the relative entropy (3.6). The objective is to prove a Gronwall estimate of the entropy production in the form

$$\frac{d}{dt} \mathcal{H}_n(t) \leq C \mathcal{H}_n(t) + o(n), \quad (5.4)$$

where $C > 0$ does not depend on n . We begin with the following lemma, proved in [7, Chap. 6, Lemma 1.4].

Lemma 5.1.

$$\frac{d}{dt} \mathcal{H}_n(t) \leq \int \frac{1}{\phi_t^n} \{(\mathcal{L}_n^{\bar{\tau}(t)})^* \phi_t^n - \partial_t \phi_t^n\} f_t^n \, d\mathbf{r} d\mathbf{p} = \int \frac{1}{\phi_t^n} \{(\mathcal{L}_n^{\bar{\tau}(t)})^* \phi_t^n - \partial_t \phi_t^n\} \, d\mu_t^n.$$

We now choose the correction term: for $i \neq n$ let us define

$$\begin{cases} F(t, i/n) := (\partial_x \beta(t, i/n), -\partial_x(\tau \beta)(t, i/n)), \\ \theta_i h(\mathbf{r}, \mathbf{p}) := \left(-\frac{r_{i+1}(p_i + p_{i+1} - \gamma r_{i+1})}{4\gamma}, -\frac{p_i}{2\gamma} \right). \end{cases} \quad (5.5)$$

For $i = n$, we assume

$$\begin{cases} F(t, 1) := (0, (\beta \partial_x \tau)(t, 1)), \\ \theta_n h(\mathbf{r}, \mathbf{p}) := \left(0, -\frac{p_n}{2\gamma} \right). \end{cases}$$

For the sake of simplicity, we introduce the following notations

$$\xi_i := (\mathcal{E}_i, r_i), \quad \chi := (\tau, \beta), \quad \eta(t, x) := (u(t, x), r(t, x)).$$

If f is a vectorial function, we denote its differential by Df . We are now able to state the main technical result of the relative entropy method.

Proposition 5.2. *The term $(\phi_t^n)^{-1} \{(\mathcal{L}_n^{\bar{\tau}(t)})^* \phi_t^n - \partial_t \phi_t^n\}$ is given by a finite sum of microscopic expansions up to the first order. In other words, it can be written as a finite sum, for which each term k is of the form*

$$\sum_{i=1}^n v_k\left(t, \frac{i}{n}\right) \left[J_i^k - H_k\left(\eta\left(t, \frac{i}{n}\right)\right) - (DH_k)\left(\eta\left(t, \frac{i}{n}\right)\right) \cdot \left(\xi_i - \eta\left(t, \frac{i}{n}\right)\right) \right] + o_t(n) \quad (5.6)$$

where

- $o_t(n)$ is an error term in the sense that

$$\int_0^t ds \int n^{-1} o_s(n) f_s^n \, d\mathbf{r} \, d\mathbf{p} \xrightarrow[n \rightarrow \infty]{} 0,$$

- J_i^k are local functions on the configurations given in Subsection 5.2,
- $v_k(t, x)$ are smooth functions that depends on τ, β , given in Subsection 5.2,

- the functions H_k satisfy

$$H_k \left(\eta \left(t, \frac{i}{n} \right) \right) = \mu_{\chi(t, i/n)}^n [J_0^k]. \quad (5.7)$$

Before explaining the main steps to prove Proposition 5.2, let us achieve the proof of Theorem 3.1. A priori the first term on the right-hand side of (5.6) is of order n , but we can take advantage of these microscopic Taylor expansions. First, we need to cut-off large energies in order to work with bounded variables only. Second, the strategy consists in performing a one-block estimate: we replace the empirical truncated current which is averaged over a microscopic box centered at i by its mean with respect to a Gibbs measure with the parameters corresponding to the microscopic averaged profiles. This is achieved thanks to the ergodicity of the dynamics. A one-block estimate is performed for each term of the form

$$\sum_{i=1}^n v_k \left(t, \frac{i}{n} \right) \left[J_i^k - H_k \left(\eta \left(t, \frac{i}{n} \right) \right) - (DH_k) \left(\eta \left(t, \frac{i}{n} \right) \right) \cdot \left(\xi_i - \eta \left(t, \frac{i}{n} \right) \right) \right].$$

We deal with error terms by taking advantage of (5.7) and by using the large deviation properties of the probability measure $\nu_{\chi(t, \cdot)}^n$, that locally is almost homogeneous. Along the proof, we will need to control, uniformly in n , the quantity

$$\int \sum_{i=1}^n \exp \left(\frac{\mathcal{E}_i}{n} \right) d\mu_t^n.$$

In fact, to get the convenient estimate, it is not difficult to see that it is sufficient to prove (5.3). The rest of the proof follows by the standard arguments of the relative entropy method (cf. [7, 8, 9, 12, 13]).

5.2. Taylor expansion. First, let us give the explicit expressions for all the functions given in Proposition 5.2. For $i = 1, \dots, n-1$, we have:

k	J_i^k	$H_k(u, r)$	$v_k(t, x)$
1	$p_i^2 + r_i r_{i+1} + 2\gamma r_i p_{i-1}$	$u + \frac{r^2}{2}$	$-\frac{1}{4\gamma} \partial_{xx} \beta(t, x)$
2	$r_i + \gamma p_{i-1}$	r	$\frac{1}{2\gamma} \partial_{xx} (\tau \beta)(t, x)$
3	$p_i^2 (r_i + r_{i+1})^2$	$(2u - r^2) \left(u + \frac{3}{2} r^2 \right)$	$\frac{1}{8\gamma} [\partial_x \beta(t, x)]^2$
4	$p_i^2 (r_i + r_{i+1})$	$r (2u - r^2)$	$-\frac{1}{2\gamma} \partial_x \beta(t, x) \partial_x (\tau \beta)(t, x)$
5	p_i^2	$u - \frac{r^2}{2}$	$\frac{1}{2\gamma} [\partial_x (\tau \beta)(t, x)]^2$

For $i = n$, the local functions J_n^k read:

$$J_n^1 = p_n^2 + \tau r_n, \quad J_n^2 = r_n, \quad J_n^3 = J_n^4 = 0, \quad J_n^5 = p_n^2$$

associated to

$$v_1 = -\frac{1}{4\gamma}\partial_{xx}\beta, \quad v_2 = \frac{1}{2\gamma}\partial_{xx}(\tau\beta), \quad v_5 = \frac{1}{2\gamma}(\beta\partial_x\tau)^2.$$

The fluctuation-dissipation equations are crucial: the role of functions F, h is to compensate the fluctuating terms. For the sake of clarity, we write down three different lemmas. Let us introduce the notation, for $i \in \{1, \dots, n\}$,

$$\delta_i(\mathbf{r}, \mathbf{p}) = F(t, i/n) \cdot \theta_i h(\mathbf{r}, \mathbf{p}),$$

where we denote by $a \cdot b$ the usual scalar product in \mathbb{R}^2 .

Lemma 5.3 (Antisymmetric part).

$$\begin{aligned} n^2 A_n^{\bar{\tau}(t)} \phi_t^n &= \phi_t^n \sum_{i=0}^{n-1} \left\{ \partial_{xx}\beta\left(t, \frac{i}{n}\right) \left[\frac{r_{i+1}p_i}{2} - u_{i+2} \right] - \partial_{xx}(\beta\tau)\left(t, \frac{i}{n}\right) \left[\frac{p_i}{2} + \frac{r_{i+1}}{2\gamma} \right] \right\} \\ &+ \phi_t^n n \sum_{i=1}^{n-1} \left\{ (n^2 \mathcal{L}_n^{\bar{\tau}(t)})^*(\delta_i) + A_n^{\bar{\tau}(t)}(\delta_i) \right\} + n \frac{\phi_t^n}{2\gamma} (\tau\beta\partial_x\tau)(t, 1) + o(n). \end{aligned}$$

Proof. The first step consists in performing an integration by part coming from the conservation laws. One can easily check that

$$\begin{aligned} n^2 A_n^{\bar{\tau}(t)} \phi_t^n &= \phi_t^n \sum_{i=1}^{n-1} n \left[\partial_x\beta\left(t, \frac{i}{n}\right) j_{i+1}^{\mathcal{E}} - \partial_x(\beta\tau)\left(t, \frac{i}{n}\right) j_{i+1}^r \right] \\ &+ \phi_t^n \sum_{i=1}^{n-1} \frac{1}{2} \left[\partial_{xx}\beta\left(t, \frac{i}{n}\right) j_{i+1}^{\mathcal{E}} - \partial_{xx}(\beta\tau)\left(t, \frac{i}{n}\right) j_{i+1}^r \right] + o(n) \\ &+ \phi_t^n n \sum_{i=1}^n A_n^{\bar{\tau}(t)}(\delta_i) + n^2 \left((\beta\tau)(t, 1)p_n - \beta(t, 1)\bar{\tau}(t)p_n \right). \end{aligned}$$

Note that the boundary conditions $\partial_x\beta(t, 0) = 0$ and $\partial_x(\tau\beta)(t, 0) = 0$ permit to introduce the boundary gradients. Moreover, the condition $\tau(t, 1) = \bar{\tau}(t)$ makes the last two terms compensate.

The next step makes use of the fluctuation-dissipation equations. The fluctuating terms in the range of $(\mathcal{L}_n^{\bar{\tau}(t)})^*$ give the contribution $\sum (\mathcal{L}_n^{\bar{\tau}(t)})^*(\delta_i)$ (for $i = 1, \dots, n-1$) whereas the gradient terms are turned into a second integration by parts. The term $A_n^{\bar{\tau}(t)}(\delta_n)$ is going to be treated separately. Then, one can check that

$$\begin{aligned} n^2 A_n^{\bar{\tau}(t)} \phi_t^n &= \phi_t^n \sum_{i=0}^{n-1} \left\{ \partial_{xx}\beta\left(t, \frac{i}{n}\right) \left[\frac{r_{i+1}p_i}{2} - u_{i+2} \right] - \partial_{xx}(\beta\tau)\left(t, \frac{i}{n}\right) \left[\frac{p_i}{2} + \frac{r_{i+1}}{2\gamma} \right] \right\} \\ &+ n \phi_t^n \sum_{i=1}^{n-1} \left\{ (n^{-2} \mathcal{L}_n^{\bar{\tau}(t)})^*(\delta_i) + A_n^{\bar{\tau}(t)}(\delta_i) \right\} + o(n) \\ &+ n \phi_t^n \left[-\partial_x\beta(t, 1) \frac{p_n^2 + \bar{\tau}(t)r_n}{4\gamma} + \partial_x(\tau\beta)(t, 1) \frac{r_n}{2\gamma} + A_n^{\bar{\tau}(t)}(\delta_n) \right]. \end{aligned}$$

Remind that $\partial_x \beta(t, 1) = 0$. After simplifications in the last line above, we get

$$\begin{aligned} n^2 A_n^{\bar{r}(t)} \phi_t^n &= \phi_t^n \sum_{i=0}^{n-1} \left\{ \partial_{xx} \beta \left(t, \frac{i}{n} \right) \left[\frac{r_{i+1} p_i}{2} - u_{i+2} \right] - \partial_{xx} (\beta \tau) \left(t, \frac{i}{n} \right) \left[\frac{p_i}{2} + \frac{r_{i+1}}{2\gamma} \right] \right\} \\ &\quad + n \phi_t^n \sum_{i=1}^{n-1} \left\{ (n^{-2} \mathcal{L}_n^{\bar{r}(t)})^* (\delta_i) + A_n^{\bar{r}(t)} (\delta_i) \right\} + n \frac{\phi_t^n}{2\gamma} (\tau \beta \partial_x \tau)(t, 1) + o(n). \end{aligned}$$

□

The following lemma is widely inspired from [12]. As previously, we keep the term $S_n(\delta_n) = -2\gamma \delta_n$ isolated.

Lemma 5.4 (Symmetric part).

$$\frac{n^2 S_n(\phi_t^n)}{\phi_t^n} = n \sum_{i=1}^{n-1} S_n(\delta_i) + n(\beta \partial_x \tau)(t, 1) p_n + \frac{1}{4} \sum_{y=1}^n \left(\sum_{i=1}^n \delta_i(\mathbf{p}^y) - \delta_i(\mathbf{p}) \right)^2 + \varepsilon(n),$$

where $\mu_t^n[\varepsilon(n)] = o(n)$.

The proof of Lemma 5.4 is the same as in [12, Lemma A.2], provided that moment bounds have been proved (see Section 5.3). The last result below can also be proved by following straightforwardly [12].

Lemma 5.5 (Logarithmic derivative).

$$\partial_t \{\log(\phi_t^n)\} = \sum_{i=1}^n - \left[\mathcal{E}_i - u \left(t, \frac{i}{n} \right) \right] \partial_t \beta \left(t, \frac{i}{n} \right) + \left[r_i - r \left(t, \frac{i}{n} \right) \right] \partial_t (\tau \beta) \left(t, \frac{i}{n} \right) + O(1).$$

We are now able to prove the Taylor expansion. According to the three previous results and to the notations introduced at the beginning of Subsection 5.2 we have

$$\begin{aligned} \frac{1}{\phi_t^n} (\mathcal{L}_n^{\bar{r}(t)})^* \phi_t^n - \partial_t \{\log(\phi_t^n)\} &= \sum_{k=1}^5 \sum_{i=1}^n v_k \left(t, \frac{i}{n} \right) J_i^k \\ &\quad + \sum_{i=1}^n \left\{ \left[\mathcal{E}_i - u \left(t, \frac{i}{n} \right) \right] \partial_t \beta \left(t, \frac{i}{n} \right) - \left[r_i - r \left(t, \frac{i}{n} \right) \right] \partial_t (\tau \beta) \left(t, \frac{i}{n} \right) \right\} \\ &\quad + n(\beta \partial_x \tau)(t, 1) \left(\frac{\tau(t, 1)}{2\gamma} + p_n \right) + o(n). \end{aligned} \tag{5.8}$$

In (5.8), the two boundary terms are treated in the following way: the first term

$$n(\beta \partial_x \tau)(t, 1) \frac{\tau(t, 1)}{2\gamma}$$

cancels out with the Taylor expansion (see below), and we are going to prove in Lemma 5.6 that the term $n p_n$ is of order $o(n)$ when integrated with respect to μ_t^n . Recall that H_k is the function defined as follows:

$$H_k \left(\eta \left(t, \frac{i}{n} \right) \right) = \mu_{\chi(t, i/n)}^n [J_0^k].$$

The next step consists in introducing in (5.8) the sum

$$\begin{aligned} \Sigma_n := & \sum_{i=1}^n \left\{ -\frac{1}{4\gamma} \partial_{xx}\beta\left(t, \frac{i}{n}\right) H_1\left(\eta\left(t, \frac{i}{n}\right)\right) + \frac{1}{2\gamma} \partial_{xx}(\tau\beta)\left(t, \frac{i}{n}\right) H_2\left(\eta\left(t, \frac{i}{n}\right)\right) \right. \\ & + \frac{1}{8\gamma} \left[\partial_{xx}\beta\left(t, \frac{i}{n}\right) \right]^2 H_3\left(\eta\left(t, \frac{i}{n}\right)\right) - \frac{1}{2\gamma} \partial_x\beta\partial_x(\tau\beta)\left(t, \frac{i}{n}\right) H_4\left(\eta\left(t, \frac{i}{n}\right)\right) \\ & \left. + \frac{1}{2\gamma} \left[\partial_x(\tau\beta)\left(t, \frac{i}{n}\right) \right]^2 H_5\left(\eta\left(t, \frac{i}{n}\right)\right) \right\}. \end{aligned}$$

Here, Σ_n is not of order $o(n)$ because of the boundary conditions. We let the reader write the two suitable integrations by part implying the Riemann convergence

$$\frac{1}{n} \left(\Sigma_n - n \frac{(\beta\tau\partial_x\tau)(t, 1)}{2\gamma} \right) \xrightarrow{n \rightarrow \infty} 0. \quad (5.9)$$

There is one remaining lemma to prove:

Lemma 5.6. *Let $\varphi(t)$ a smooth function on \mathbb{R}_+ . The following bound holds:*

$$\int_0^t ds \int \varphi(s) p_n f_s^n d\mathbf{r}d\mathbf{p} \leq \frac{C}{n} \left(\frac{1}{n} + \int_0^t \mathcal{H}_n(s) ds + \mathcal{H}_n(t) + \mathcal{H}_n(0) \right)$$

for some positive constant C independent of n .

Proof. Since $\frac{d}{dt} \sum_{i=1}^n r_i(t) = n^2 p_n(t)$, we have:

$$\int_0^t \varphi(s) p_n(s) ds = -\frac{1}{n^2} \int_0^t \varphi'(s) \sum_{i=1}^n r_i(s) ds + \frac{1}{n^2} \varphi(t) \sum_{i=1}^n r_i(t) - \frac{1}{n^2} \varphi(0) \sum_{i=1}^n r_i(0).$$

Recall the entropy inequality: for any $\alpha > 0$ and any positive measurable function F we have

$$\int F d\mu \leq \frac{1}{\alpha} \left\{ \log \left(\int e^{\alpha F} d\nu \right) + \mathcal{H}(\mu|\nu) \right\}, \quad (5.10)$$

where $\mathcal{H}(\mu|\nu)$ is the relative entropy of μ with respect to ν . Therefore,

$$\int \frac{1}{n^2} \sum_{i=1}^n r_i f_s^n d\mathbf{r}d\mathbf{p} \leq \frac{1}{\alpha n} \log \int \exp \left(\frac{\alpha}{n} \sum_{i=1}^n r_i \right) \phi_s^n d\mathbf{r}d\mathbf{p} + \frac{1}{\alpha n} \mathcal{H}_n(s)$$

and it is easy to see that the first term of the right-hand side of the above bound is bounded by Cn^{-2} for some constant $C > 0$. \square

Eventually, further computations give

$$\begin{aligned} -\frac{\partial_{xx}\beta}{4\gamma} \partial_u H_1 + \frac{\partial_{xx}(\tau\beta)}{2\gamma} \partial_u H_2 + \frac{[\partial_x\beta]^2}{8\gamma} \partial_u H_3 - \frac{\partial_x\beta\partial_x(\tau\beta)}{2\gamma} \partial_u H_4 \\ + \frac{[\partial_x(\tau\beta)]^2}{2\gamma} \partial_u H_5 = -\partial_t\beta, \quad (5.11) \end{aligned}$$

and

$$\begin{aligned}
-\frac{\partial_{xx}\beta}{4\gamma} \partial_r H_1 + \frac{\partial_{xx}(\tau\beta)}{2\gamma} \partial_r H_2 + \frac{[\partial_x\beta]^2}{8\gamma} \partial_r H_3 + \frac{\partial_x\beta\partial_x(\tau\beta)}{2\gamma} \partial_r H_4 \\
+ \frac{[\partial_x\tau\beta]^2}{2\gamma} \partial_r H_5 = -\partial_t(\tau\beta). \quad (5.12)
\end{aligned}$$

It remains to rewrite (5.8) after introducing Σ_n , and making a suitable use of (5.11), (5.12) and (5.9). Eventually, Proposition 5.2 is proven.

5.3. Moment bounds. In this last part we are going to control all the energy moments. The precise statement is the following:

Theorem 5.7. *For every positive integer $k \geq 1$, there exists a positive constant C which does not depend on n (but depends on k), such that*

$$\mu_t^n \left[\sum_{i=1}^n \mathcal{E}_i^k \right] \leq C \times n. \quad (5.13)$$

The dependence on k could be precised: we refer the interested reader to [12]. The first two bounds ($k = 1, 2$) would be sufficient to justify the cut-off of currents, but here we need more bounds because of the Taylor expansion (Proposition 5.2). Since the chain is harmonic, Gibbs states are Gaussian. Remarkably, all Gaussian moments can be expressed in terms of variances and covariances. We start with a graphical representation of the dynamics of the process given by the generator $\mathcal{L}_n^{\tau(t)}/n^2$. Notice that time is not accelerated in the diffusive scale. To avoid any confusion, the law of this new process is denoted by ν_t^n . Then, we recover the diffusive time accelerated process by:

$$\mu_t^n = \nu_{tn^2}^n.$$

In the following, we always respect the decomposition of the space $\mathbb{R}^n \times \mathbb{R}^n$, where the first n components stand for \mathbf{r} and the last n components stand for \mathbf{p} . All vectors and matrices are written according to this decomposition.

Let ν be a measure on $\mathbb{R}^n \times \mathbb{R}^n$. We denote by $\mathbf{m} \in \mathbb{R}^{2n}$ its mean vector and by $\mathbf{C} \in \mathfrak{M}_{2n}(\mathbb{R})$ its covariance matrix. There exist $\rho := \nu[\mathbf{r}] \in \mathbb{R}^n$, $\pi := \nu[\mathbf{p}] \in \mathbb{R}^n$ and $U, V, Z \in \mathfrak{M}_n(\mathbb{R})$ such that

$$\mathbf{m} = (\rho, \pi) \in \mathbb{R}^{2n} \quad \text{and} \quad \mathbf{C} = \begin{pmatrix} U & {}^t Z \\ Z & V \end{pmatrix} \in \mathfrak{S}_{2n}(\mathbb{R}). \quad (5.14)$$

Hereafter, we denote by ${}^t Z$ the real transpose of the matrix Z . Thanks to a trivial convexity inequality, instead of proving (5.13) we are going to show

$$\nu_t^n \left[\sum_{i=1}^n p_i^{2k} \right] \leq C \times n \quad \text{and} \quad \nu_t^n \left[\sum_{i=1}^n r_i^{2k} \right] \leq C \times n, \quad (5.15)$$

where C is a constant that does not depend on t nor on n .

Proof. (i) Poisson Process and Gaussian Measures – We start by giving a graphical representation of the process, based on the Harris description. Let us define the antisymmetric $(2n, 2n)$ -matrix, written by blocks as

$$A := \begin{pmatrix} 0_n & \mathfrak{A}_n \\ -{}^t\mathfrak{A}_n & 0_n \end{pmatrix} \quad \text{where} \quad \mathfrak{A}_n := \begin{pmatrix} 1 & & & (0) \\ -1 & \ddots & & \\ & \ddots & \ddots & \\ (0) & & -1 & 1 \end{pmatrix} \in \mathfrak{M}_n(\mathbb{R}).$$

Above 0_n is the null (n, n) -matrix. We also define the n -vector

$$b(t) := \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \bar{\tau}(t) \end{pmatrix}.$$

Let $(N_i)_{i=1\dots n}$ be a sequence of independent standard Poisson processes of intensity γ . At time 0 the process has an initial state $(\mathbf{r}, \mathbf{p})(0)$. Let

$$T_1 = \inf_{t \geq 0} \left\{ \text{there exists } i \in \{1, \dots, n\} \text{ such that } N_i(t) = 1 \right\}$$

and i_1 the site where the infimum is achieved. During the interval $[0, T_1)$, the process (not accelerated in time) follows the deterministic evolution given by the generator $A_n^{\bar{\tau}(t)}$. More precisely, during the time interval $[0, T_1)$, $(\mathbf{r}, \mathbf{p})(t)$ follows the evolution given by the system:

$$\frac{dy}{dt} = A \cdot y(t) + b(t). \quad (5.16)$$

At time T_1 , the momentum p_{i_1} is flipped, and gives a new configuration. Then, the system starts again with the deterministic evolution up to the time of the next flip, and so on. Let $\xi := (i_1, T_1), \dots, (i_q, T_q), \dots$ be the sequence of sites and ordered times for which we have a flip, and let us denote its law by \mathbb{P} . Conditionally to ξ , the evolution is deterministic, and the state of the process $(\mathbf{r}, \mathbf{p})^\xi(t)$ is given for all $t \in [T_q, T_{q+1})$ by

$$(\mathbf{r}, \mathbf{p})^\xi(t) = e^{(t-T_q)A} \circ F_{i_q} \circ e^{(T_q-T_{q-1})A} \circ F_{i_{q-1}} \circ \dots \circ e^{T_1 A}(\mathbf{r}, \mathbf{p})(0) + \Omega^\xi(t) \quad (5.17)$$

where

- F_i is the map $(\mathbf{r}, \mathbf{p}) \mapsto (\mathbf{r}, \mathbf{p}^i)$.
- $\Omega^\xi(t)$ is a vector that depends only on A , $b(t)$ and ξ , and can be written as

$$\begin{aligned} \Omega^\xi(t) = \sum_{\ell=0}^{q-1} e^{(t-T_q)A} \circ F_{i_q} \circ e^{(T_q-T_{q-1})A} \circ \dots \circ F_{i_{\ell+1}} \circ e^{(T_{\ell+1}-T_\ell)A} \int_{T_\ell}^{T_{\ell+1}} e^{-uA} b(u) du \\ + e^{(t-T_q)A} \int_{T_q}^t e^{-uA} b(u) du. \end{aligned}$$

If initially the process starts from $(\mathbf{r}, \mathbf{p})(0)$ which is distributed according to a Gaussian measure ν_0^n , then $(\mathbf{r}, \mathbf{p})^\xi(\mathbf{t})$ is distributed according to a Gaussian measure ν_t^ξ . Finally, the density ν_t^n is given by the convex combination

$$\nu_t^n(\cdot) = \int \nu_t^\xi(\cdot) d\mathbb{P}(\xi). \quad (5.18)$$

Moreover, we are able to write the evolution of the mean vector \mathbf{m}_t^ξ and the covariance matrix \mathbf{C}_t^ξ of ν_t^ξ . During the interval $[0, T_1)$, \mathbf{m}_t follows the evolution given by system (5.16). At time T_1 , the component $m_{i_1+n} = \pi_{i_1}$ (which corresponds to the mean of p_{i_1}) is flipped, and gives a new mean vector. Then, the deterministic evolution goes on up to the time of the next flip, and so on.

In the same way, during the interval $[0, T_1)$, \mathbf{C}_t follows the evolution given by the (matrix) system:

$$\frac{dM}{dt} = AM(t) - M(t)A. \quad (5.19)$$

At time T_1 , all the components $C_{i_1+n, j}$ and C_{i, i_1+n} when $i, j \neq i_1 + n$ are flipped and the matrix \mathbf{C}_{T_1} becomes $\Sigma_{i_1} \cdot \mathbf{C}_{T_1} \cdot {}^t\Sigma_{i_1}$, where Σ_{i_1} is defined as

$$\Sigma_{i_1} := \begin{pmatrix} I_n & 0_n \\ 0_n & I_n - 2E_{i_1, i_1} \end{pmatrix},$$

and so on up to the next flip. Above, I_n is the (n, n) -identity matrix, and $E_{i, i}$ is the (n, n) -matrix composed by the elements $(\delta_{i, k} \delta_{i, \ell})_{1 \leq k, \ell \leq n}$ where $\delta_{i, k}$ is the Kronecker delta function. More precisely,

$$\mathbf{C}_t^\xi = e^{(t-T_q)A} \cdot \Sigma_{i_q} \cdots \Sigma_{i_1} \cdot e^{T_1 A} \cdot \mathbf{C}_0 \cdot e^{-T_1 A} \cdot {}^t\Sigma_{i_1} \cdots {}^t\Sigma_{i_q} e^{-(t-T_q)A}. \quad (5.20)$$

Finally, the density ν_t^n is equal to

$$\nu_t^n(\cdot) = \int \nu_t^\xi(\cdot) d\mathbb{P}(\xi) = \int G_{\mathbf{m}, \mathbf{C}}(\cdot) d\theta_{\mathbf{m}_0, \mathbf{C}_0}^t(\mathbf{m}, \mathbf{C}), \quad (5.21)$$

where $G_{\mathbf{m}, \mathbf{C}}(\cdot)$ denotes the Gaussian measure on $(\mathbb{R} \times \mathbb{R})^n$ with mean \mathbf{m} and covariance matrix \mathbf{C} , and $\theta_{\mathbf{m}_0, \mathbf{C}_0}^t(\cdot, \cdot)$ is the law of the random variable $(\mathbf{m}_t, \mathbf{C}_t)$, knowing that the Markov process $(\mathbf{m}_t, \mathbf{C}_t)_{t \geq 0}$ described by the graphical representation above starts from $(\mathbf{m}_0, \mathbf{C}_0)$. We denote by $\mathbb{P}_{\mathbf{m}_0, \mathbf{C}_0}$ the law of the Markov process $(\mathbf{m}_t, \mathbf{C}_t)_{t \geq 0}$, and by $\mathbb{E}_{\mathbf{m}_0, \mathbf{C}_0}$ the corresponding expectation. Observe that we have, from (5.21),

$$\nu_t^n[p_i] = \int G_{\mathbf{m}, \mathbf{C}}(p_i) d\theta_{\mathbf{m}_0, \mathbf{C}_0}^t(\mathbf{m}, \mathbf{C}) = \int \pi_i d\theta_{\mathbf{m}_0, \mathbf{C}_0}^t(\mathbf{m}, \mathbf{C}),$$

$$\nu_t^n[r_i] = \int G_{\mathbf{m}, \mathbf{C}}(r_i) d\theta_{\mathbf{m}_0, \mathbf{C}_0}^t(\mathbf{m}, \mathbf{C}) = \int \rho_i d\theta_{\mathbf{m}_0, \mathbf{C}_0}^t(\mathbf{m}, \mathbf{C}).$$

Notice that we conveniently denote by $G_{\mathbf{m}, \mathbf{C}}(f)$ the mean of the function f with respect to the Gaussian measure $G_{\mathbf{m}, \mathbf{C}}$. Therefore, we rewrite (5.15) as

$$\nu_t^n \left[\sum_{i=1}^n p_i^{2k} \right] = \int \sum_{i=1}^n G_{\mathbf{m}, \mathbf{C}}(p_i^{2k} + r_i^{2k}) d\theta_{\mathbf{m}_0, \mathbf{C}_0}^t(\mathbf{m}, \mathbf{C}).$$

(ii) *Control in the covariance matrix* – First, let us focus on $G_{\mathbf{m},\mathbf{C}}(p_i^{2k} + r_i^{2k})$. Notice that

$$G_{\mathbf{m},\mathbf{C}}(p_i^{2k}) = G_{\mathbf{m},\mathbf{C}}([p_i - \pi_i + \pi_i]^{2k}) \leq 2^{2k-1} \{G_{\mathbf{m},\mathbf{C}}([p_i - \pi_i]^{2k}) + \pi_i^{2k}\}.$$

Remarkably, we can express all the centered moments of a Gaussian random variable as functions of the variance only. In other words, there exists a constant K_k that depends on k but not on n such that

$$G_{\mathbf{m},\mathbf{C}}([p_i - \pi_i]^{2k}) \leq K_k G_{\mathbf{m},\mathbf{C}}([p_i - \pi_i]^2)^k = K_k (C_{i+n,i+n})^k(t).$$

Therefore, after repeating the same argument for $G_{\mathbf{m},\mathbf{C}}(r_i^{2k})$ we are reduced to control, for any ξ ,

$$\sum_{i=1}^{2n} (C_{i,i}^\xi)^k(t) \tag{5.22}$$

and besides

$$\sum_{i=1}^n \pi_i^{2k}(t), \quad \sum_{i=1}^n \rho_i^{2k}(t). \tag{5.23}$$

In the following we treat separately (5.22) and (5.23).

(iii) *Control of (5.22) using the trace* – Let us fix once for all a sequence ξ a sequence of sites and ordered times for which we have a flip. The matrix C_t^ξ is symmetric, hence diagonalizable, and after denoting its eigenvalues by $\lambda_1, \dots, \lambda_{2n}$, we can write

$$\text{Tr}([C_t^\xi]^k) = \sum_{i=1}^{2n} \lambda_i^k.$$

We have now to compare $\sum_i \lambda_i^k$ with $\sum_i [C_{i,i}^\xi]^k(t)$. If we denote by P_t^ξ the orthogonal matrix of the eigenvectors of C_t^ξ , then we get $C_t^\xi = (P_t^\xi)^* \cdot D \cdot P_t^\xi$, where D is the diagonal matrix with entries $\lambda_1, \dots, \lambda_{2n}$. For the sake of simplicity, we denote by $(P_{i,j})$ the components of P_t^ξ . Then,

$$[C_{i,i}^\xi]^k(t) = \left(\sum_{j,\ell} P_{i,j}^* D_{j,\ell} P_{\ell,i} \right)^k = \left(\sum_j P_{i,j}^* \lambda_j P_{j,i} \right)^k = \left(\sum_j P_{i,j}^* P_{j,i} \cdot \lambda_j \right)^k.$$

Since P is an orthogonal matrix, $\sum_j P_{i,j}^* P_{j,i} = 1$. Consequently, we can use the convexity inequality, and we obtain

$$\sum_i [C_{i,i}^\xi]^k(t) \leq \sum_i \sum_j P_{i,j}^* P_{j,i} \lambda_j^k \leq \sum_j \lambda_j^k = \text{Tr}([C_t^\xi]^k).$$

Since C_0 and C_t^ξ are similar, we have:

$$\text{Tr}([C_t^\xi]^k) = \text{Tr}(C_0^k) = \sum_{i=1}^n \frac{1}{\beta_0^k(i/n)} + \left(\frac{1}{\beta_0(i/n)} + \tau_0^2(i/n) \right)^k \leq K'_1 n,$$

for some constant $K'_1 > 0$. Therefore, the same inequality holds for $\sum_i [C_{i,i}^\xi]^k(t)$.

(iv) *Control of (5.23)* – For this last paragraph we go back to the diffusive time scale, namely we are going to bound the two quantities

$$\sum_{i=1}^n \pi_i^{2k}(tn^2) \quad \text{and} \quad \sum_{i=1}^n \rho_i^{2k}(tn^2).$$

Notice that the sequences $\{\pi_i(t)\}_i$ and $\{\rho_i(t)\}_i$ satisfy the following system of differential equations: for $i = 1, \dots, n$ and $t \geq 0$,

$$\begin{cases} \pi'_i = \rho_{i+1} - \rho_i - 2\gamma \pi_i, \\ \rho'_i = \pi_i - \pi_{i-1}, \end{cases} \quad \text{with} \quad \begin{cases} \rho_{n+1}(t) = \bar{\tau}(t/n^2), \\ \pi_0(t) = 0. \end{cases}$$

Let us recenter $\tilde{\rho}_i(t) = \rho_i(t) - \bar{\tau}(t/n^2)$, then the equations become

$$\begin{cases} \pi'_i = \tilde{\rho}_{i+1} - \tilde{\rho}_i - 2\gamma \pi_i, \\ \tilde{\rho}'_i = \pi_i - \pi_{i-1} - \bar{\tau}'(t/n^2)n^{-2}, \end{cases} \quad \text{with} \quad \begin{cases} \tilde{\rho}_{n+1}(t) = 0, \\ \pi_0(t) = 0. \end{cases}$$

Denote by Π the column vector ${}^t(\pi_1, \dots, \pi_n, \pi'_1, \dots, \pi'_n)$. It is not difficult to see that $\Pi(t)$ follows a first order ordinary differential equation written as

$$\frac{dy}{dt} = M^\pi \cdot y(t) + T^\pi(t), \quad (5.24)$$

where M^π is the following constant block matrix:

$$M^\pi := \begin{pmatrix} 0_n & I_n \\ D^\pi & -2\gamma I_n \end{pmatrix} \quad \text{where} \quad D^\pi := \begin{pmatrix} -2 & 1 & & (0) \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & 1 & -2 & 1 \\ (0) & & & 1 & -1 \end{pmatrix}.$$

Above I_n is the (n, n) -identity matrix, and the vector $T^\pi(t)$ is the $(2n)$ -vector

$$T^\pi(t) := {}^t\left(\underbrace{0, \dots, 0}_{2n-1}, \bar{\tau}'(t/n^2)n^{-2}\right).$$

In the same way, denote by R the column vector ${}^t(\tilde{\rho}_1, \dots, \tilde{\rho}_n, \tilde{\rho}'_1, \dots, \tilde{\rho}'_n)$. It is not difficult to see that $R(t)$ follows a first order ordinary differential equation written as

$$\frac{dy}{dt} = M^\rho \cdot y(t) + T^\rho(t), \quad (5.25)$$

where M^ρ is the following constant block matrix:

$$M^\rho := \begin{pmatrix} 0_n & I_n \\ D^\rho & -2\gamma I_n \end{pmatrix} \quad \text{where} \quad D^\rho := \begin{pmatrix} -1 & 1 & & (0) \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & 1 & -2 & 1 \\ (0) & & & 1 & -2 \end{pmatrix}$$

and $T^\rho(t)$ is the $(2n)$ -vector

$$T^\rho(t) := \mathbf{t} \left(\underbrace{0, \dots, 0}_{2n-1}, \bar{\tau}(t/n^2) \right) - \left[\bar{\tau}''(t/n^2)n^{-4} + 2\gamma\bar{\tau}'(t/n^2)n^{-2} \right] \times \mathbf{t} \left(\underbrace{0, \dots, 0}_n, \underbrace{1, \dots, 1}_n \right).$$

Both matrices D^π and D^ρ represents the discrete Laplacian operator with mixed Dirichlet-Neumann boundary conditions. Let us focus on $\Pi(t)$. We are going to compute the characteristic polynomial of M^π , that is $\chi^\pi(X) := \det(XI_{2n} - M^\pi)$. One can easily check that

$$\chi^\pi(X) = \det(D^\pi - X(X + 2\gamma)I_n).$$

In other words, the eigenvalues of M^π are exactly equal to the solutions of

$$x(x + 2\gamma) = -\lambda,$$

where $-\lambda$ takes any eigenvalue of D^π . It is well-known that the eigenvalues of D^π are all negatives. Therefore, we need to solve $x(x + 2\gamma) + \lambda = 0$, where λ is positive. Precisely,

(i) if $\gamma^2 > \lambda$, then the two solutions are real negative numbers written as

$$x_\pm = -\gamma \pm \sqrt{\gamma^2 - \lambda} < 0,$$

(ii) if $\gamma^2 < \lambda$, then the two solutions are complex numbers written as

$$x_\pm = -\gamma \pm i\sqrt{-\gamma^2 + \lambda},$$

(iii) if $\gamma^2 = \lambda$, then $-\gamma$ is the unique solution.

As a consequence, every eigenvalue of M^π has a negative real part, and the system (5.24) is hyperbolic (and the same holds for M^ρ). Let us write the solution of system (5.24) at time tn^2 :

$$\Pi(tn^2) = \exp(tn^2 M^\pi) \Pi(0) + \int_0^{tn^2} \exp((tn^2 - s) M^\pi) T^\pi(s) ds.$$

We are interested in the quantity $\sum_i |\pi_i(tn^2)|^m$, which is less or equal than the following norm

$$\left(\|\Pi(tn^2)\|_m \right)^m := \sum_{i=1}^n \left\{ |\pi_i(tn^2)|^m + |\pi'_i(tn^2)|^m \right\}.$$

Since the system is hyperbolic, there exists a constant $C > 0$ such that, for every $s \in [0, t]$,

$$\left\| \exp((tn^2 - s) M^\pi) \Pi(0) \right\|_m \leq C \|\Pi(0)\|_m.$$

Observe that the initial condition writes

$$\|\Pi(0)\|_m^m = \sum_{j=1}^{n-1} \left| \tau_0 \left(\frac{j+1}{n} \right) - \tau_0 \left(\frac{j}{n} \right) \right|^m + |\bar{\tau}(0) - \tau_0(1)|^m.$$

The last term above vanishes due to the assumptions on the boundary (3.3). Since the profile τ_0 is smooth, it is clear that $\|\Pi(0)\|_m^m$ is of order n^{1-m} . On the other hand,

$$\begin{aligned} \left\| \int_0^{tn^2} \exp((tn^2 - s) M^\pi) T^\pi(s) ds \right\|_m^m &\leq C^m \left(\int_0^{tn^2} \|T^\pi(s)\|_m ds \right)^m \\ &= \left(\int_0^{tn^2} n^{-2} \left| \bar{\tau}'\left(\frac{s}{n^2}\right) \right| ds \right)^m \\ &= \left(\int_0^t |\bar{\tau}'(u)| du \right)^m \end{aligned}$$

so that the bound does not depend on n . Therefore, we proved that there exists a constant K'_2 that does not depend on n nor on t such that

$$\sum_{i=1}^n |\pi_i(tn^2)|^m \leq \|\Pi(tn^2)\|_m^m \leq K'_2 n.$$

The same argument is valid for $R(t)$, except two different estimates: the first one appears in the initial condition, which now reads

$$\|R(0)\|_m^m = \sum_{j=1}^n \left| \tau_0\left(\frac{j}{n}\right) - \bar{\tau}(0) \right|^m + \sum_{j=1}^n |\bar{\tau}'(0) n^{-2}|^m.$$

Hence, $\|R(0)\|_m^m$ is of order n (instead of n^{1-m}), but this is enough. The second difference comes from the vector $T^\rho(t)$. Now we have to control

$$\left(\int_0^{tn^2} \left[\left| \bar{\tau}\left(\frac{s}{n^2}\right) \right|^m + n^m \left| \bar{\tau}''\left(\frac{s}{n^2}\right) n^{-4} + \bar{\tau}'\left(\frac{s}{n^2}\right) n^{-2} \right|^m \right]^{1/m} ds \right)^m,$$

which is also bounded uniformly in n . Therefore, we conclude that there exists a constant K'_3 that does not depend on n such that

$$\sum_{i=1}^n |\rho_i(tn^2) - \bar{\tau}(t)|^m \leq \|R(tn^2)\|_m^m \leq K'_3 n,$$

which implies

$$\sum_{i=1}^n |\rho_i(tn^2)|^m \lesssim K'_3 n + \sum_{i=1}^n |\bar{\tau}(t)|^m \leq K'_4 n.$$

□

ACKNOWLEDGMENTS

The authors warmly thank Cedric Bernardin for his useful suggestions on this work.

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