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# NON-EQUILIBRIUM ISOTHERMAL TRANSFORMATIONS IN A TEMPERATURE GRADIENT FROM A MICROSCOPIC DYNAMICS

#### VIVIANA LETIZIA AND STEFANO OLLA

ABSTRACT. We consider a chain of anharmonic oscillators immersed in a heat bath with a temperature gradient and a time-varying tension applied to one end of the chain while the other side is fixed to a point. We prove that under diffusive space-time rescaling the volume strain distribution of the chain evolves following a non-linear diffusive equation. The stationary states of the dynamics are of non-equilibrium and have a positive entropy production, so the classical relative entropy methods cannot be used. We develop new estimates based on entropic hypocoercivity, that allow to control the distribution of the position configurations of the chain. The macroscopic limit can be used to model isothermal thermodynamic transformations between non-equilibrium stationary states.

#### 1. Introduction

Macroscopic isothermal thermodynamic transformations can be modeled microscopically by putting a system in contact with Langevin heat bath at a given temperature  $\beta^{-1}$ . In [9] a chain of n anharmonic oscillators is immersed in a heat bath of Langevin thermostats acting independently on each particle. Macroscopically equivalent isothermal dynamics is obtained by elastic collisions with an external gas of independent particles with maxwellian random velocities with variance  $\beta^{-1}$ . The effect is to quickly renew the velocities distribution of the particles, so that at any given time it is very close to a maxwellian at given temperature. The chain is pinned only on one side, while at the opposite site a force (tension)  $\tau$  is acting. The equilibrium distribution is characterized by the two control parameters  $\beta^{-1}$ ,  $\tau$  (temperature and tension). The total length and the energy of the system in equilibrium are in general non-linear functions of these parameters given by the standard thermodynamic relations.

By changing the tension  $\tau$  applied to the system, a new equilibrium state, with the same temperature  $\beta^{-1}$ , will be eventually reached. For large n, while the heat bath equilibrates the velocities at the corresponding temperature at time of order 1, the system converges to this global equilibrium length at a time scale of order  $n^2t$ . In [9] it is proven that the length stretch of the system evolves in a diffusive space-time scale, i.e. after a scaling limit the empirical distribution of the interparticle distances converges to the solution of a non-linear diffusive equation governed by the local tension. Consequently

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this diffusive equation describes the non-reversible isothermal thermodynamic transformation from one equilibrium to another with a different tension. By a further rescaling of the time dependence of the changing tension, a so called *quasi-static* or *reversible* isothermal transformation is obtained. Corresponding Clausius equalities/inequalities relating work done and change in free energy can be proven.

The results of [9] summarized above concern isothermal transformations from an equilibrium state to another, by changing the applied tension. In this article we are interested in transformations between non-equilibrium stationary states. We now consider the chain of oscillators immersed in a heat bath with a macroscopic gradient of temperature: each particle is in contact with thermostats at a different temperature. These temperatures slowly change from a particle to the neighboring one. A tension  $\tau$  is again applied to the chain. In the stationary state, that is now characterized by the tension  $\tau$  and the profile of temperatures  $\beta_1^{-1}, \ldots, \beta_n^{-1}$ , there is a continuous flow of energy through the chain from the hot thermostats to the cold ones. Unlike the equilibrium case, the probability distribution of the configurations of the chain in the stationary state cannot be computed explicitly.

By changing the applied tension we can obtain transitions from a non-equilibrium stationary state to another, that will happen in a diffusive space-time scale as in the equilibrium case. The main result in the present article is that these transformations are again governed by a diffusive equation that takes into account the local temperature profile. The free energy can be computed according to the local equilibrium rule and its changes during the transformation satisfy the Clausius inequality with respect to the work done. This provides a mathematically precise example for understanding non-equilibrium thermodynamics from microscopic dynamics.

The results in [9] where obtained by using the relative entropy method, first developed by H.T.Yau in [17] for the Ginzburg-Landau dynamics, which is just the overdamped version of the bulk dynamics of the oscillators chain. The relative entropy method is very powerful and flexible, and was already applied to interacting Ornstein-Uhlenbeck particles in the PhD thesis of Tremoulet [14] as well as many other cases, in particular in the hyperbolic scaling limit for Euler equation in the smooth regime [13, 4]. This method consists in looking at the time evolution of the relative entropy of the distribution of the particle with respect to the local Gibbs measure parametrized by the non-constant tension profile corresponding to the solution of the macroscopic diffusion equation. The point of the method is in proving that the time derivative of such relative entropy is small, so that the relative entropy itself remains small with respect to the size of the system and local equilibrium, in a weak but sufficient form, propagates in time. In the particular applications to interacting Ornstein-Uhlenbeck particles [14, 9], the local Gibbs measure needs to be corrected by a small recentering of the damped velocities due to the local gradient of the tension.

The relative entropy method seems to fail when the stationary measures are not the equilibrium Gibbs measure, like in the present case. The reason is that when taking the time derivative of the relative entropy mentioned above, a large term, proportional to the gradient of the temperature, appears. This term is related to the *entropy production* of the stationary measure. Consequently we could not apply the relative entropy method to the present problem.

A previous method was developed by Guo, Papanicolaou and Varadhan in [6] for overdamped dynamics. In this approach the main step in closing the macroscopic equation is the direct comparison of the coarse grained empirical density in the microscopic and macroscopic space scale. They obtain first a bound of the Dirichlet form (more precisely called Fisher information) from the time derivative of the relative entropy with respect to the equilibrium stationary measures. This bound implies that the system is close to equilibrium on a local microscopic scale, and that the density on a large microscopic interval is close to the density in a small macroscopic interval (the so called *one* and *two block estimates*, see [7] chapter 5).

In the over-damped dynamics considered in [6], the Dirichlet form appearing in the time derivative of the relative entropy controls the gradients of the probability distributions with respects to the position of the particles. In the damped models, the Dirichlet form appearing in the time derivative of the relative entropy controls only the gradients on the velocities of the probability distribution of the particles. In order to deal with damped models a different approach for comparing densities on the different scales was developed in [12], after the over-damped case in [15], based on Young measures. Unfortunately this approach requires a control of higher moments of the density that are difficult to prove for lattice models. Consequently we could not apply this method either in the present situation.

The main mathematical novelty in the present article is the use of entropic hypocoercivity, inspired by [16]. We introduce a Fisher information form  $I_n$  associated to the vector fields  $\{\partial_{p_i} + \partial_{q_i}\}_{i=1,\dots,n}$ , defined by (2.27). By computing the time derivative of this Fisher information form on the distribution at time t of the configurations, we obtain a uniform bound  $I_n \leq Cn^{-1}$ . This implies that, at the macroscopic diffusive time scale, velocity gradients of the distribution are very close to positions gradients. This allows to obtain a bound on the Fisher information on the positions from the bound on the Fisher information on the velocities. At this point we are essentially with the same information as in the over-damped model, and we proceed as in [6]. Observe that the Fisher information  $I_n$  we introduce in (2.27) is more specific and a bit different than the distorted Fisher information used by Villani in [16], in particular  $I_n$  is more degenerate. On the other hand the calculations, that are contained in appendix D are less miraculous than in [16], and they are stable enough to control the effect of the boundary tension and of the gradient of temperature. This also suggests that entropic hypocoercivity seems to be the right tool in order to obtain explicit estimates uniform in the dimension of the system.

Adiabatic thermodynamic transformations are certainly more difficult to be obtained from microscopic dynamics, for some preliminary results see [13, 4, 1, 10]. Equilibrium fluctuations for the dynamics with constant temperature can be treated as in [11]. The fluctuations in the case with a gradient of temperature are non-equilibrium fluctuation, and we believe that can be treated with the techniques of the present article together with those developed in the over-damped case in [5].

Large deviations for the stationary measure also require some further mathematical investigations, but we conjecture that the corresponding quasi-potential functional ([2]) is given by the free energy associated to the local Gibbs measure, without any non-local terms, unlike the case of the simple exclusion process.

The article is structured in the following way. In section 2 we define the dynamics and we state the main result (Theorem 2.1). In section 3 we discuss the consequences for the thermodynamic transformations from a stationary state to another, the Clausius inequality and the quasi-static limit. In section 4 are obtained the bounds on the

entropy and the various Fisher informations needed in the proof of the hydrodynamic limit. In section 5 we show that any limit point of the distribution of the empirical density on strain of the volume is concentrated in the weak solutions of the macroscopic diffusion equation. The compactness, regularity and uniqueness of the corresponding weak solution, necessary to conclude the proof, are proven in the first three appendices. Appendix D contains the calculations and estimates for the time derivative of the Fisher information  $I_n$ .

# 2. The dynamics and the results

We consider a chain of n coupled oscillators in one dimension. Each particle has the same mass, equal to one. The configuration in the phase space is described by  $\{q_i, p_i, i = 1, \ldots, n\} \in \mathbb{R}^{2n}$ . 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. The chain is attached on the left to a fixed point, so we set  $q_0 = 0, p_0 = 0$ . We call  $\{r_i = q_i - q_{i-1}, i = 1, \ldots, n\}$  the interparticle distance.

We assume V to be a positive smooth function, that satisfy the following assumptions:

i)

$$\lim_{|r| \to \infty} \frac{V(r)}{|r|} = \infty, \tag{2.1}$$

ii) there exists a constant  $C_2 > 0$  such that:

$$\sup_{r} |V''(r)| \le C_2,\tag{2.2}$$

iii) there exists a constant  $C_1 > 0$  such that:

$$V'(r)^{2} \le C_{1} (1 + V(r)). \tag{2.3}$$

In particular these conditions imply  $|V'(r)| \leq C_0 + C_2 |r|$  for some constant  $C_0$ . Notice that this conditions allows potentials that may grow like  $V(r) \sim |r|^{\alpha}$  for large r, with  $1 < \alpha \leq 2$ .

Energy is defined by the following Hamiltonian function:

$$\mathcal{H} := \sum_{i=1}^{n} \left( \frac{p_i^2}{2} + V(r_i) \right) \tag{2.4}$$

The particle dynamics is subject to an interaction with an environment given by Langevin heat bath at different temperatures  $\beta_i^{-1}$ . We choose  $\beta_i$  as slowly varying on a macroscopic scale, i.e.  $\beta_i = \beta(i/n)$  for a given smooth strictly positive function  $\beta(x)$ ,  $x \in [0,1]$  such that  $\inf_{y \in [0,1]} \beta(y) \ge \beta_- > 0$ .

The equations of motion are given by

$$\begin{cases}
dr_i(t) = n^2(p_i(t) - p_{i-1}(t))dt \\
dp_i(t) = n^2(V'(r_{i+1}(t)) - V'(r_i(t))) dt - n^2\gamma p_i(t)dt + n\sqrt{\frac{2\gamma}{\beta_i}}dw_i(t), & i = 1, ..., N - 1 \\
dp_n(t) = n^2(\bar{\tau}(t) - V'(r_n(t))) dt - n^2\gamma p_n(t) dt + n\sqrt{\frac{2\gamma}{\beta_n}}dw_n(t).
\end{cases}$$
(2.5)

Here  $\{w_i(t)\}_i$  are *n*-independent Wiener processes,  $\gamma > 0$  is the coupling parameter with the Langevin thermostats. The time is rescaled according to the diffusive spacetime scaling, i.e. t is the macroscopic time. The tension  $\tilde{\tau} = \tilde{\tau}(t)$  changes at the

macroscopic time scale (i.e. very slowly in the microscopic time scale). The generator of the diffusion is given by

$$\mathcal{L}_n^{\bar{\tau}(t)} := n^2 \mathcal{A}_n^{\bar{\tau}(t)} + n^2 \gamma \mathcal{S}_n, \tag{2.6}$$

where  $\mathcal{A}_n^{\bar{\tau}}$  is the Liouville generator

$$A_n^{\bar{\tau}} = \sum_{i=1}^n (p_i - p_{i-1})\partial_{r_i} + \sum_{i=1}^{n-1} (V'(r_{i+1}) - V'(r_i))\partial_{p_i} + (\bar{\tau} - V'(r_n))\partial_{p_n}$$
 (2.7)

while  $S_n$  is the operator

$$S_n = \sum_{i=1}^n \left( \beta_i^{-1} \partial_{p_i}^2 - p_i \partial_{p_i} \right) \tag{2.8}$$

2.1. Gibbs measures. For  $\bar{\tau}(t) = \tau$  constant, and  $\beta_i = \beta$  homogeneous, the system has a unique invariant probability measure given by a product of invariant Gibbs measures  $\mu_{\tau,\beta}^n$ :

$$d\mu_{\tau,\beta}^{n} = \prod_{i=1}^{n} e^{-\beta(\mathcal{E}_{i} - \tau r_{i}) - \mathcal{G}(\tau,\beta)} dr_{i} dp_{i}$$

$$(2.9)$$

where  $\mathcal{E}_i$  is the energy of the particle i:

$$\mathcal{E}_i = \frac{p_i^2}{2} + V(r_i). \tag{2.10}$$

The function  $\mathcal{G}(\tau,\beta)$  is the Gibbs potential defined as:

$$\mathcal{G}(\tau,\beta) = \log \left[ \sqrt{2\pi\beta^{-1}} \int e^{-\beta(V(r) - \tau r)} dr \right]. \tag{2.11}$$

Notice that, thanks to condition (2.1),  $\mathcal{G}(\tau, \beta)$  is finite for any  $\tau \in \mathbb{R}$  and any  $\beta > 0$ . Furthermore it is strictly convex in  $\tau$ .

The free energy of the equilibrium state  $(r, \beta)$  is given by the Legendre transform of  $\beta^{-1}\mathcal{G}(\tau, \beta)$ :

$$\mathcal{F}(r,\beta) = \sup_{\tau} \{ \tau r - \beta^{-1} \mathcal{G}(\tau,\beta) \}$$
 (2.12)

The corresponding convex conjugate variables are the equilibrium average length

$$\mathfrak{r}(\tau,\beta) = \beta^{-1}\partial_{\tau}\mathcal{G}(\tau,\beta) \tag{2.13}$$

and the tension

$$\tau(r,\beta) = \partial_r \mathcal{F}(r,\beta).$$
 (2.14)

Observe that

$$\mathbb{E}_{\mu_{\tau,\beta}^n[r_i]} = \mathfrak{r}(\tau,\beta), \qquad \mathbb{E}_{\mu_{\tau,\beta}^n[V'(r_i)]} = \tau. \tag{2.15}$$

2.2. The hydrodynamic limit. We assume that for a given initial profile  $r_0(x)$  the initial probability distribution satisfies:

$$\frac{1}{n} \sum_{i=1}^{n} G(i/n) r_i(0) \xrightarrow[n \to \infty]{} \int_0^1 G(x) r_0(x) dx \quad \text{in probability}$$
 (2.16)

for any continuous test function  $G \in \mathcal{C}_0([0,1])$ . We expect that this same convergence happens at the macroscopic time t:

$$\frac{1}{n}\sum_{i=1}^{n}G(i/n)r_{i}(t)\longrightarrow \int_{0}^{1}G(x)r(x,t)dx \tag{2.17}$$

where r(x,t) satisfies the following diffusive equation

$$\begin{cases} \partial_t r(x,t) = \frac{1}{\gamma} \partial_x^2 \boldsymbol{\tau}(r(x,t), \beta(x)) & \text{for } x \in [0,1] \\ \partial_x \boldsymbol{\tau}(r(t,x), \beta(x))|_{x=0} = 0, \quad \boldsymbol{\tau}(r(t,x), \beta(x))|_{x=1} = \bar{\tau}(t), \quad t > 0 \\ r(0,x) = r_0(x), \quad x \in [0,1] \end{cases}$$
 (2.18)

We say that r(x,t) is a weak solution of (2.18) if for any smooth function G(x) on [0,1] such that G(1)=0 and G'(0)=0 we have

$$\int_0^1 G(x) \left( r(x,t) - r_0(x) \right) dx = \gamma^{-1} \int_0^t ds \left[ \int_0^1 G''(x) \tau(r(x,s), \beta(x)) dx - G'(1) \bar{\tau}(s) \right]. \tag{2.19}$$

In appendix C we prove that the weak solution is unique in the class of functions such that:

$$\int_0^t ds \int_0^1 \left(\partial_x \tau(r(x,s),\beta(x))\right)^2 dx < +\infty.$$
 (2.20)

Let  $\nu_{\beta}^n$  the inhomogeneous Gibbs measure

$$d\nu_{\beta.}^{n} = \prod_{i=1}^{n} \frac{e^{-\beta_{i}\mathcal{E}_{i}}}{Z_{\beta_{i}}}$$
 (2.21)

Observe that this is **not** the stationary measure for the dynamics defined by (2.5) and (2.6) for  $\bar{\tau} = 0$ .

Let  $f_t^n$  the density, with respect to  $\nu_{\beta}^n$ , of the probability distribution of the system at time t, i.e. the solution of

$$\partial_t f_t^n = \mathcal{L}_n^{\bar{\tau}(t),*} f_t^n, \tag{2.22}$$

where  $\mathcal{L}_n^{\bar{\tau}(t),*}$  is the adjoint of  $\mathcal{L}_n^{\bar{\tau}(t)}$  with respect to  $\nu_{\beta}^n$ , i.e. explicitly

$$\mathcal{L}_{n}^{\bar{\tau}(t),*} = -n^{2} \mathcal{A}_{n}^{\tau(t)} - n \sum_{i=1}^{n-1} \nabla_{n} \beta(i/n) p_{i} V'(r_{i+1}) + n^{2} \beta(1) p_{n} \bar{\tau} + n^{2} \gamma \mathcal{S}_{n}, \qquad (2.23)$$

where

$$\nabla_n \beta(i/n) = n \left( \beta \left( \frac{i+1}{n} \right) - \beta \left( \frac{i}{n} \right) \right), \qquad i = 1, \dots, n-1.$$
 (2.24)

Define the relative entropy of  $f_t^n d\nu_{\beta}^n$  with respect to  $d\nu_{\beta}^n$  as:

$$H_n(t) = \int f_t^n \log f_t^n d\nu_{\beta}^n. \tag{2.25}$$

We assume that the initial density  $f_0^n$  satisfy the bound

$$H_n(0) \le Cn. \tag{2.26}$$

We also need some regularity of  $f_0^n$ : define the hypercoercive Fisher information functional:

$$I_n(t) = \sum_{i=1}^{n-1} \beta_i^{-1} \int \frac{((\partial_{p_i} + \partial_{q_i}) f_t^n)^2}{f_t^n} d\nu_{\beta}.$$
 (2.27)

where  $\partial_{q_i} = \partial_{r_i} - \partial_{r_{i+1}}, i = 1, \dots, n-1$ , and  $\nu_{\beta} := \nu_{\beta}^n$ . We assume that

$$I_n(0) \le K_n \tag{2.28}$$

with  $K_n$  growing less than exponentially in n. We will show in Appendix D that for any t > 0 we have  $I_n(t) \leq Cn^{-1}$ .

Furthermore we assume that

$$\lim_{n \to \infty} \int \left| \frac{1}{n} \sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i - \int_0^1 G(x) r_0(x) dx \right| f_0^n d\nu_{\beta}. = 0$$
 (2.29)

for any continuous test function  $G \in \mathcal{C}_0([0,1])$ .

**Theorem 2.1.** Assume that the starting initial distribution satisfy the above conditions. Then

$$\lim_{n \to \infty} \int \left| \frac{1}{n} \sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i - \int_0^1 G(x) r(x, t) dx \right| f_t^n d\nu_{\beta}. = 0, \tag{2.30}$$

where r(x,t) is the unique weak solution of (2.18) satisfying (2.20).

Furthermore a local equilibrium result is valid in the following sense: consider a local function  $\phi(\mathbf{r}, \mathbf{p})$  such that for some positive finite constants  $C_1, C_2$  we have the bound

$$|\phi(\mathbf{r}, \mathbf{p})| \le C_1 \sum_{i \in \Lambda_{\phi}} (p_i^2 + V(r_i))^{\alpha} + C_2, \qquad \alpha < 1$$
(2.31)

where  $\Lambda_{\phi}$  is the local support of  $\phi$ . Let  $k_{\phi}$  the length of  $\Lambda_{\phi}$ , and let  $\theta_{i}\phi$  be the shifted function, well defined for  $k_{\phi} < i < n - k_{\phi}$ , and define

$$\hat{\phi}(r,\beta) = \mathbb{E}_{\mu_{\tau(r,\beta),\beta}}(\phi). \tag{2.32}$$

# Corollary 2.2.

$$\lim_{n \to \infty} \int \left| \frac{1}{n} \sum_{i=k_{\phi}+1}^{n-k_{\phi}} G\left(\frac{i}{n}\right) \theta_{i} \phi(\mathbf{r}, \mathbf{p}) - \int_{0}^{1} G(x) \hat{\phi}(r(x, t), \beta(x)) dx \right| f_{t}^{n} d\nu_{\beta} = 0, \quad (2.33)$$

# 3. Non-equilibrium thermodynamics

We collect in this section some interesting consequences of the main theorem for the non-equilibrium thermodynamics of this system. All statements contained in this section can be proven rigorously, except for one that will require more investigation in the future. The aim is to build a non equilibrium thermodynamics in the spirit of [3, 2]. The equilibrium version of these results has been already proven in [9]. As we already mentioned, stationary states of our dynamics are not given by Gibbs measures if a gradient in the temperature profile is present, but they are still characterized by the tension  $\bar{\tau}$  applied. We denote these stationary distributions as non-equilibrium stationary states (NESS). Let us denote  $f_{ss,\tau}^n$  the density of the stationary distribution with respect to  $\nu_{\beta}$ .

It is easy to see that

$$\int V'(r_i) f_{ss,\tau}^n \nu_{\beta.} = \tau, \qquad i = 1, \dots, n.$$
(3.1)

In fact, since  $\int p_i f_{ss,\tau}^n \nu_{\beta} = 0$  and

$$n^{-2}\mathcal{L}_{n}^{\tau}p_{i} = V'(r_{i+1}) - V'(r_{i}) - \gamma p_{i}, \quad i = 1, \dots, n-1,$$
  
$$n^{-2}\mathcal{L}_{n}^{\tau}p_{n} = \tau - V'(r_{n}) - \gamma p_{n},$$

we have

$$0 = \int (V'(r_{i+1}) - V'(r_i)) f_{ss,\tau}^n \nu_{\beta} = \int (\tau - V'(r_n)) f_{ss,\tau}^n \nu_{\beta}.$$

By the main theorem 2.1, there exists a stationary profile of stretch  $r_{ss,\tau}(y) = \mathfrak{r}(\tau,\beta(y))$  (defined by (2.13)) such that for any continuous test function G:

$$\lim_{n \to \infty} \int \left| \frac{1}{n} \sum_{i=1}^{n} G\left(\frac{i}{n}\right) r_i - \int_0^1 G(x) r_{ss,\tau}(x) dx \right| f_{ss,\tau}^n d\nu_{\beta.} = 0, \tag{3.2}$$

In order to study the transition from one stationary state to another with different tension, we start the system at time 0 with a stationary state with tension  $\tau_0$ , and we change tension with time, setting  $\bar{\tau}(t) = \tau_1$  for  $t \geq t_1$ . The distribution of the system will eventually converge to a stationary state with tension  $\tau_1$ . Let r(x,t) be the solution of the macroscopic equation (2.19) starting with  $r_0(x) = r_{ss,\tau_0}(x)$ . Clearly  $r(x,t) \to r_1(x) = r_{ss,\tau_1}(x)$ , as  $t \to \infty$ .

3.1. Excess Heat. The (normalized) total internal energy of the system is defined by

$$U_n := \frac{1}{n} \sum_{i=1}^n \left( \frac{p_i^2}{2} + V(r_i) \right)$$
 (3.3)

It evolves as:

$$U_n(t) - U_n(0) = \mathcal{W}_n(t) + Q_n(t)$$

where

$$W_n(t) = \int_0^t \bar{\tau}(s) n p_n(s) ds = \int_0^t \bar{\tau}(s) \frac{dq_n(s)}{n}$$

is the (normalized) work done by the force  $\bar{\tau}(s)$  up to time t, while

$$Q_n(t) = \gamma \, n \sum_{j=1}^n \int_0^t ds \left( p_j^2(s) - \beta_j^{-1} \right) + \sum_{j=1}^n \sqrt{2\gamma \beta_j^{-1}} \int_0^t p_j(s) dw_i(s). \tag{3.4}$$

is the total flux of energy between the system and the heat bath (divided by n). As a consequence of theorem 2.1 we have that

$$\lim_{n \to \infty} W_n(t) = \int_0^t \bar{\tau}(s) d\mathcal{L}(s)$$

where  $\mathcal{L}(t) = \int_0^1 r(x,t)dx$ , the total macroscopic length at time t. While for the energy difference we expect that

$$\lim_{n \to \infty} (U_n(t) - U_n(0)) = \int_0^1 \left[ u(\boldsymbol{\tau}(r(x,t), \beta(x)), \beta(x)) - u(\tau_0, \beta(x)) \right] dx \tag{3.5}$$

where  $u(\tau, \beta)$  is the average energy for  $\mu_{\beta,\tau}$ , i.e.

$$u(\tau,\beta) = \int \mathcal{E}_1 d\mu_{\tau,\beta}^1 = \frac{1}{2\beta} + \int V(r)e^{-\beta(V(r) - \tau r) - \tilde{\mathcal{G}}(\tau,\beta)} dr$$

with  $\tilde{\mathcal{G}}(\tau,\beta) = \log \int e^{-\beta(V(r)-\tau r)} dr$ . Unfortunately (3.5) does not follow from (2.33), since (2.31) is not satisfied. Consequently at the moment we do not have a rigorous proof of (3.5). In the constant temperature profile case, treated in [9], this limit can be computed rigorously thanks to the use on the relative entropy method [17] that gives a better control on the local distribution of the energy.

Since  $\tau(r(x,t),\beta(x)) \to \tau_1$  as  $t \to \infty$ , it follows that

$$u(\boldsymbol{\tau}(r(x,t),\beta(x)),\beta(x)) \to u(\tau_1,\beta(x))$$

and the energy change will become

$$\int_0^1 \left( u(\tau_1, \beta(x)) - u(\tau_0, \beta(x)) \right) dx = \int_0^{+\infty} \bar{\tau}(s) d\mathcal{L}(s) ds + Q = \mathcal{W} + Q \tag{3.6}$$

where Q is the limit of (3.4), which is called *excess heat*. So equation (3.6) is the expression of the first principle of thermodynamics in this *isothermal* transformation between non–equilibrium stationary states. Here *isothermal* means that the profile of temperature does not change in time during the transformation.

3.2. Free energy. Define the free energy associated to the macroscopic profile r(x,t):

$$\widetilde{\mathcal{F}}(t) = \int_0^1 \mathcal{F}(r(x,t), \beta(x)) dx. \tag{3.7}$$

Correspondingly the free energy associated to the macroscopic stationary state is:

$$\widetilde{\mathcal{F}}_{ss}(\tau) = \int_0^1 \mathcal{F}(r_{ss,\tau}(x), \beta(x)) dx \tag{3.8}$$

A straightforward calculation using (2.19) gives

$$\widetilde{\mathcal{F}}(t) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}(t) - \gamma^{-1} \int_0^t ds \int_0^1 \left(\partial_x \boldsymbol{\tau}(r(x,s), \beta(x))\right)^2 dx \tag{3.9}$$

and after the time limit  $t \to \infty$ 

$$\widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W} - \gamma^{-1} \int_0^{+\infty} dt \int_0^1 \left(\partial_x \boldsymbol{\tau}(r(x,t), \beta(x))\right)^2 dx$$

$$< \mathcal{W}$$
(3.10)

i.e. Clausius inequality for NESS. Notice that in the case  $\beta_j$  constant, this is just the usual Clausius inequality (see [9]).

3.3. Quasi-static limit and reversible transformations. The thermodynamic transformation obtained above from the stationary state at tension  $\tau_0$  to the one at tension  $\tau_1$  is an irreversible transformation, where the work done on the system by the external force is strictly bigger than the change in free energy.

In thermodynamics the *quasi-static* transformations are (vaguely) defined as those processes where changes are so slow such that the system is in *equilibrium* at each instant of time. In the spirit of [3] and [9], these quasi static transformations are precisely defined as a limiting process by rescaling the time dependence of the driving tension  $\bar{\tau}$  by a small parameter  $\varepsilon$ , i.e. by choosing  $\bar{\tau}(\epsilon t)$ . Of course the right time scale at which the evolution appears is  $\varepsilon^{-1}t$  and the rescaled solution  $\tilde{r}^{\varepsilon}(x,t) = r(x,\varepsilon^{-1}t)$  satisfy the equation

$$\begin{cases}
\partial_t \tilde{r}^{\varepsilon}(x,t) = \frac{1}{\epsilon \gamma} \partial_x^2 \boldsymbol{\tau}(\tilde{r}^{\varepsilon}(x,t), \beta(x)) & \text{for } x \in [0,1] \\
\partial_x \boldsymbol{\tau}(\tilde{r}^{\varepsilon}(t,x), \beta(x))|_{x=0} = 0, \quad \boldsymbol{\tau}(\tilde{r}^{\varepsilon}(t,x), \beta(x))|_{x=1} = \bar{\tau}(t), \quad t > 0 \\
\boldsymbol{\tau}(\tilde{r}^{\varepsilon}(0,x), \beta(x)) = \tau_0, \quad x \in [0,1]
\end{cases}$$
(3.11)

By repeating the argument above, equation (3.10) became:

$$\widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}^{\varepsilon} - \frac{1}{\epsilon \gamma} \int_0^{+\infty} dt \int_0^1 \left( \partial_x \boldsymbol{\tau}(\widetilde{r}^{\varepsilon}(x, t), \beta(x)) \right)^2 dx \tag{3.12}$$

By the same argument used in [9] for  $\beta$  constant, it can be proven that the last term on the right hand side of (3.12) converges to 0 as  $\varepsilon \to 0$ , and that  $\tau(\tilde{r}^{\varepsilon}(x,t),\beta(x)) \to \bar{\tau}(t)$  for almost any  $x \in [0,1]$  and  $t \geq 0$ . Consequently in the quasi-static limit we have the Clausius equality

$$\widetilde{\mathcal{F}}_{ss}(\tau_1) - \widetilde{\mathcal{F}}_{ss}(\tau_0) = \mathcal{W}$$

This implies the following equality for the heat in the quasi-static limit:

$$Q = \int_0^1 \beta^{-1}(x) \left( S(r_{ss}(x, \tau_1), u_{ss}(x, \tau_1)) - S(r_{ss}(x, \tau_0), u_{ss}(x, \tau_0)) \right) dx$$
 (3.13)

analogous of the equilibrium equality  $Q = T\Delta S$ .

In [8] a direct quasi-static limit is obtained form the microscopic dynamics without passing through the macroscopic equation (2.19), by choosing a driving tension  $\bar{\tau}$  that changes at a slower time scale.

# 4. Entropy and hypercoercive bounds

In this section we prove the bounds on the relative entropy and the different Fisher informations that we need in the proof of the hydrodynamic limit in section section 5. These bounds provide a quantitative information on the closeness of the local distributions of the particles to some equilibrium measure.

In order to shorten formulas, we introduce here some vectorial notation. Given two vectors  $u = (u_1, \ldots, u_n), v = (v_1, \ldots, v_n)$ , define

$$u \odot v = \sum_{i=1}^{n} \beta_i^{-1} u_i v_i, \qquad u \tilde{\odot} v = \sum_{i=1}^{n-1} \beta_i^{-1} u_i v_i, \qquad |u|_{\tilde{\odot}}^2 = u \odot u, \quad |u|_{\tilde{\tilde{\odot}}}^2 = u \tilde{\odot} u.$$

We also use the notations

$$\partial_p = (\partial_{p_1}, \dots, \partial_{p_n}) \qquad \partial_p^* = (\partial_{p_1}^*, \dots, \partial_{p_n}^*), \qquad \partial_{p_i}^* = \beta_i p_i - \partial_{p_i}$$

$$\partial_q = (\partial_{q_1}, \dots, \partial_{q_n}), \qquad \partial_{q_i} = \partial_{r_i} - \partial_{r_{i+1}}, \qquad \partial_{q_n} = \partial_{r_n}.$$

$$(4.1)$$

Observe that with this notations we can write

$$S_n = -\partial_p^* \odot \partial_p, \qquad A_n^{\tau} = p \cdot \partial_q - \partial_q \mathcal{V} \cdot \partial_p + \tau \partial_{p_n}$$
(4.2)

where  $\mathcal{V} = \sum_{i} V(r_i)$  and the · denotes the usual scalar product in  $\mathbb{R}^n$ . Then we define the following Fisher informations forms on a probability density distribution (with respect to  $\nu_{\beta}$ .):

$$\mathcal{D}_{n}^{p}(f) = \int \frac{|\partial_{p} f|_{\odot}^{2}}{f} d\nu_{\beta}, \qquad \tilde{\mathcal{D}}_{n}^{p}(f) = \int \frac{|\partial_{p} f|_{\tilde{\odot}}^{2}}{f} d\nu_{\beta}.$$

$$\mathcal{D}_{n}^{r}(f) = \int \frac{|\partial_{q} f|_{\tilde{\odot}}^{2}}{f} d\nu_{\beta}.$$

$$I_{n}(f) = \int \frac{|\partial_{p} f + \partial_{q} f|_{\tilde{\odot}}^{2}}{f} d\nu_{\beta}. = \tilde{\mathcal{D}}_{n}^{p}(f) + \mathcal{D}_{n}^{r}(f) + 2 \int \frac{\partial_{q} f \tilde{\odot} \partial_{p} f}{f} d\nu_{\beta}. \geq 0$$
(4.3)

**Proposition 4.1.** Let  $f_t^n$  the solution of the forward equation (2.22). Then there exist a constant C such that

$$H_n(t) \le Cn, \qquad \int_0^t \mathcal{D}_n^p(f_s^n) ds \le \frac{C}{n}, \qquad \int_0^t \mathcal{D}_n^r(f_s^n) ds \le \frac{C}{n}.$$
 (4.4)

*Proof.* Taking the time derivative of the entropy we obtain:

$$\frac{d}{dt}H_n(t) = \int (\mathcal{L}_n^{\bar{\tau}(t)})^* f_t^n \log f_t^n d\nu_{\beta}. \tag{4.5}$$

So that, using (2.23), we have

$$\frac{d}{dt}H_n(t) = \int f_t^n \mathcal{L}_n^{\bar{\tau}(t)} \log f_t^n d\nu_{\beta.} = \int n^2 \mathcal{A}_n^{\bar{\tau}(t)} f d\nu_{\beta.} - \gamma n^2 \mathcal{D}_n^p(f_t^n)$$

$$= -n \sum_{i=1}^{n-1} \nabla_n \beta(i/n) \int V'(r_{i+1}) p_i f_t^n d\nu_{\beta.} + n^2 \beta_n \bar{\tau}(t) \int p_n f_t^n d\nu_{\beta.} - \gamma n^2 \mathcal{D}_n^p(f_t^n) \tag{4.6}$$

Recall that  $q_n = \sum_{i=1}^n r_i$ , then the time integral of the second term on the RHS of (4.6) gives

$$n^{2}\beta_{n} \int_{0}^{t} ds \,\bar{\tau}(s) \int p_{n} f_{s}^{n} d\nu_{\beta} = \beta_{n} \int_{0}^{t} ds \,\bar{\tau}(s) \int \mathcal{L}_{n}^{\bar{\tau}(s)} q_{n} f_{s}^{n} d\nu_{\beta}$$

$$= \beta_{n} \bar{\tau}(t) \int q_{n} f_{t}^{n} d\nu_{\beta} - \beta_{n} \bar{\tau}(0) \int q_{n} f_{0}^{n} d\nu_{\beta} - \beta_{n} \int_{0}^{t} ds \,\bar{\tau}'(s) \int q_{n} f_{s}^{n} d\nu_{\beta}.$$

$$(4.7)$$

By the entropy inequality, for any  $a_1 > 0$ , using the first of the conditions (2.1),

$$\int |q_{n}| f_{s}^{n} d\nu_{\beta} \leq \frac{1}{a_{1}} \log \int e^{a_{1}|q_{n}|} d\nu_{\beta} + \frac{1}{a_{1}} H_{n}(s) \leq \frac{1}{a_{1}} \log \int \prod_{i=1}^{n} e^{a_{1}|r_{i}|} d\nu_{\beta} + \frac{1}{a_{1}} H_{n}(s)$$

$$\leq \frac{1}{a_{1}} \sum_{i=1}^{n} \log \int \left( e^{a_{1}r_{i}} + e^{-a_{1}r_{i}} \right) d\nu_{\beta} + \frac{1}{a_{1}} H_{n}(s)$$

$$= \frac{1}{a_{1}} \sum_{i=1}^{n} \left( \mathcal{G}(a_{1}, \beta_{i}) + \mathcal{G}(-a_{1}, \beta_{i}) - 2\mathcal{G}(0, \beta_{i}) \right) + \frac{1}{a_{1}} H_{n}(s) \leq nC(a_{1}, \beta) + \frac{1}{a_{1}} H_{n}(s)$$

$$(4.8)$$

We apply (4.8) to the three terms of the RHS of (4.7). So after this time integration we can estimate, for any  $a_1 > 0$ ,

$$n^{2}\beta(1)\left|\int_{0}^{t}ds\ \bar{\tau}(t)\int p_{n}f_{t}^{n}d\nu_{\beta.}\right| \leq \frac{\beta(1)K_{\bar{\tau}}}{a_{1}}\left(H_{n}(t) + H_{n}(0) + \int_{0}^{t}H_{n}(s)ds\right) + n(2+t)\beta(1)K_{\bar{\tau}}C(a_{1},\beta.)$$
(4.9)

where  $K_{\bar{\tau}} = \sup_{s>0} (|\bar{\tau}(s)| + |\bar{\tau}'(s)|).$ 

By integration by part and Schwarz inequality, for any  $a_2 > 0$  we have

$$\left| n \sum_{i=1}^{n-1} \nabla_n \beta(i/n) \int V'(r_{i+1}) p_i f_t^n d\nu_{\beta.} \right| = \left| n \sum_{i=1}^{n-1} \frac{\nabla_n \beta(i/n)}{\beta(i/n)} \int V'(r_{i+1}) \partial_{p_i} f_t^n d\nu_{\beta.} \right|$$

$$\leq \frac{1}{2a_2} \sum_{i=1}^{n-1} \frac{(\nabla_n \beta(i/n))^2}{\beta_i} \int V'(r_{i+1})^2 f_t^n d\nu_{\beta.} + \frac{a_2 n^2}{2} \tilde{\mathcal{D}}_n^p (f_t^n)$$

By our assumptions on  $\beta(\cdot)$  and assumption (2.3) on V, we have that for some constant  $C_{\beta} > 0$  depending on  $\beta(\cdot)$  and V,

$$\sum_{i=1}^{n-1} \frac{(\nabla_n \beta(i/n))^2}{\beta_i} V'(r_{i+1})^2 \le C_{\beta} \cdot \sum_{i=1}^{n-1} V'(r_{i+1})^2 \le C_{\beta} \cdot C_1 \sum_{i=1}^n (V(r_i) + 1)$$
 (4.10)

By the entropy inequality, for any  $\delta$  such that  $0 < \delta < \inf_y \beta(y)$ , there exists a finite constant  $C_{\delta,\beta}$  depending on  $V,\delta$  and  $\beta(\cdot)$  such that:

$$\sum_{i=1}^{n} \int V(r_{i}) f_{t}^{n} d\nu_{\beta} \leq \frac{1}{\delta} \log \int e^{\delta \sum_{i=1}^{n} \int V(r_{i})} d\nu_{\beta} + \frac{1}{\delta} H_{n}(t)$$

$$= \frac{1}{\delta} \sum_{i=1}^{n} \left( \mathcal{G}(0, \beta_{i} - \delta) - \mathcal{G}(0, \beta_{i}) \right) + \frac{1}{\delta} H_{n}(t) \leq C_{\delta,\beta} \cdot n + \frac{1}{\delta} H_{n}(t) \tag{4.11}$$

At this point we have obtained the following inequality, for some constant C not depending on n,

$$H_{n}(t) - H_{n}(0) \leq -n^{2} \left(\gamma - \frac{a_{2}}{2}\right) \int_{0}^{t} \mathcal{D}_{n}^{p}(f_{s}^{n}) ds + \left(\frac{C_{\beta}}{2a_{2}\delta} + \frac{\beta(1)K_{\bar{\tau}}}{a_{1}}\right) \int_{0}^{t} H_{n}(s) ds + \frac{\beta(1)K_{\bar{\tau}}}{a_{1}} \left(H_{n}(t) + H_{n}(0)\right) + nc(a_{1}, a_{2}, \delta, \bar{\tau}, \beta.)$$

$$(4.12)$$

consequently, choosing  $a_2 = \gamma$  and  $a_1 = 2\beta(1)K_{\bar{\tau}}$ , we have

$$H_n(t) \le 3H_n(0) + C' \int_0^t H_n(s)ds + cn - n^2 \gamma \int_0^t \mathcal{D}_n^p(f_s^n)ds$$
 (4.13)

where C' and c are constants independent of n. Given the initial bound on  $H_n(0) \leq cn$ , by Gronwall inequality we have for some c'' independent on n:

$$H_n(t) \le c'' e^{C't} n. \tag{4.14}$$

Inserting this in (4.13) we obtain, for some  $\tilde{C}$  independent of n,

$$\gamma \int_0^t \mathcal{D}_n^p(f_s^n) ds \le \frac{\tilde{C}}{n} \tag{4.15}$$

The bound (4.15) gives only informations about the distribution of the velocities, but we actually need a corresponding bound of the distribution of the positions.

In appendix D we prove that, as a consequence of (4.15), we have

$$I_n(t) \le \frac{C}{n} \qquad \forall t > 0.$$
 (4.16)

Consequently

$$\mathcal{D}_{n}^{r}(f_{t}^{n}) = I_{n}(f_{t}^{n}) - \tilde{\mathcal{D}}_{n}^{p}(f_{t}^{n}) - 2\int \frac{\partial_{q}f_{t}^{n}\tilde{\odot}\partial_{p}f_{t}^{n}}{f_{t}^{n}}d\nu_{\beta}.$$

$$\leq \frac{C}{n} - \tilde{\mathcal{D}}_{n}^{p}(f_{t}^{n}) - 2\int \frac{\partial_{q}f_{t}^{n}\tilde{\odot}\partial_{p}f_{t}^{n}}{f_{t}^{n}}d\nu_{\beta}.$$

$$\leq \frac{C}{n} - \tilde{\mathcal{D}}_{n}^{p}(f_{t}^{n}) + 2\tilde{\mathcal{D}}_{n}^{p}(f_{t}^{n}) + \frac{1}{2}\mathcal{D}_{n}^{r}(f_{t}^{n})$$

that gives

$$\mathcal{D}_n^r(f_t^n) \le 2\tilde{\mathcal{D}}_n^p(f_t^n) + \frac{2C}{n}$$

Since we have already the bound (4.15), (4.4) follows.

## 5. Characterization of the limit points

Define the empirical measure

$$\pi_t^n(dx) := \frac{1}{n} \sum_{i=1}^n r_i(t) \delta_{i/n}(dx).$$

and we use the notation, for a given smooth function  $G:[0,1]\to\mathbb{R}$ ,

$$\langle \pi_t^n, G \rangle := \frac{1}{n} \sum_{i=1}^n G\left(\frac{i}{n}\right) r_i(t)$$

Computing the time derivative we have:

$$\langle \pi_t^n, G \rangle - \langle \pi_0^n, G \rangle = \int_0^t \frac{1}{n} \sum_{i=1}^n G\left(\frac{i}{n}\right) \mathcal{L}_n^{\tilde{\tau}(t)} r_i(t)$$
 (5.1)

Since

$$\mathcal{L}_n^{\tilde{\tau}(t)} r_i = n^2 (p_i - p_{i-1}), \qquad i = 1, \dots, n, \quad p_0 = 0,$$

after performing a summation by parts, we obtain

$$\mathcal{L}_n^{\bar{\tau}(t)}\langle \pi_t^n, G \rangle = -\sum_{i=1}^{n-1} \nabla_n G\left(\frac{i}{n}\right) p_i(t) + n p_n(t) G(1). \tag{5.2}$$

where  $\nabla_n G$  is defined by (2.24). We define also

$$\nabla_n^* G\left(\frac{i}{n}\right) = n \left[ G\left(\frac{i-1}{n}\right) - G\left(\frac{i}{n}\right) \right] \qquad i = 2, \dots, n.$$

Now observe that

$$\mathcal{L}_{n}^{\bar{\tau}(t)} \left[ \frac{1}{n^{2}} \sum_{i=1}^{n-1} \nabla_{n} G\left(\frac{i}{n}\right) p_{i} - \frac{1}{n} p_{n} G(1) \right] = -\gamma \sum_{i=1}^{n-1} \nabla_{n} G\left(\frac{i}{n}\right) p_{i} + \gamma n p_{n} G(1) 
+ \sum_{i=1}^{n-1} \nabla_{n} G\left(\frac{i}{n}\right) \left(V'(r_{i+1}) - V'(r_{i})\right) - n G(1) \left(\bar{\tau}(t) - V'(r_{n})\right) 
= -\gamma \sum_{i=1}^{n-1} \nabla_{n} G\left(\frac{i}{n}\right) p_{i} + \gamma n p_{n} G(1) 
+ \frac{1}{n} \sum_{i=2}^{n-1} \nabla_{n}^{*} \nabla_{n} G\left(\frac{i}{n}\right) V'(r_{i+1}) + \nabla_{n} G\left(\frac{n-1}{n}\right) V'(r_{n}) - \nabla_{n} G\left(\frac{1}{n}\right) V'(r_{1}) 
- n G(1) \left(\bar{\tau}(t) - V'(r_{n})\right)$$
(5.3)

Recall that, by the weak formulation of the macroscopic equation, cf. (2.19), it is enough to consider test functions G such that G(1) = 0 and G'(0) = 0. This takes care of the last term on the RHS of the above expression and in (5.2), and putting these two expression together and dividing by  $\gamma$ , we obtain

$$\mathcal{L}_{n}^{\bar{\tau}(t)}\langle \pi^{n}, G \rangle = \frac{1}{\gamma n} \sum_{i=2}^{n-1} (-\nabla_{n}^{*} \nabla_{n}) G\left(\frac{i}{n}\right) V'(r_{i+1}) - \gamma^{-1} \nabla_{n} G\left(\frac{n-1}{n}\right) V'(r_{n}) 
+ \gamma^{-1} \nabla_{n} G\left(\frac{1}{n}\right) V'(r_{1}) + \mathcal{L}_{n}^{\bar{\tau}(t)} \frac{1}{\gamma n^{2}} \sum_{i=1}^{n-1} \nabla_{n} G\left(\frac{i}{n}\right) p_{i}$$
(5.4)

It is easy to show, by using the entropy inequality, that the last two terms are negligible. In fact, since G'(0) = 0 we have that  $|\nabla_n G\left(\frac{1}{n}\right)| \leq C_G n^{-1}$ . Furthermore

$$\int e^{\alpha|V'(r)|-\beta_1 V(r)} dr < +\infty \qquad \forall \alpha > 0.$$

Then, using the entropy inequality we have for any  $\alpha > 0$ :

$$\int \left| \gamma^{-1} \nabla_n G\left(\frac{1}{n}\right) V'(r_1) \right| f_s^n d\nu_{\beta} \leq \frac{C_G}{n\gamma} \int |V'(r_1)| f_s^n d\nu_{\beta} 
\leq \frac{C_G}{n\gamma\alpha} \int e^{\alpha |V'(r_1)|} d\nu_{\beta}^n + \frac{C_G}{n\gamma\alpha} H_n(s) \leq \frac{C(\alpha)}{n} + \frac{C'}{\alpha}$$
(5.5)

that goes to 0 after taking the limit as  $n \to \infty$  then  $\alpha \to \infty$ . About the last term of the RHS in (5.4), after time integration we have to estimate

$$\int \frac{1}{\gamma n^2} \sum_{i=1}^{n-1} \left| \nabla_n G\left(\frac{i}{n}\right) \right| |p_i| f_s^n d\nu_{\beta}$$

for s=0,t. By similar use of the entropy inequality it follows that also this term disappear when  $n\to\infty$ .

To deal with the second term of the RHS of (5.4), we need the following lemma:

#### Lemma 5.1.

$$\lim_{n \to \infty} \mathbb{E}\left(\left| \int_0^t \int \left( V'(r_n(s)) - \bar{\tau}(s) \right) ds \right| \right) = 0$$
 (5.6)

*Proof.* Observe that

$$V'(r_n) - \bar{\tau}(s) = -\frac{1}{n^2} \mathcal{L}^{\bar{\tau}(s)} p_n - \gamma p_n = -\frac{1}{n^2} \mathcal{L}^{\bar{\tau}(s)} (p_n + \gamma q_n).$$
 (5.7)

Then after time integration:

$$\int_0^t \left( V'(r_n(s)) - \bar{\tau}(s) \right) ds = \frac{1}{n^2} \left( p_n(0) - p_n(t) \right) - \frac{\gamma}{n^2} (q_n(t) - q_n(0)) + \frac{\sqrt{2\gamma\beta_n}}{n} w_n(t).$$

It is easy to show that, using similar estimate as (4.7) and (4.8), the expectation of the absolute value of the right hand side of the above expression converges to 0 as  $n \to \infty$ .

It follows that

$$\lim_{n \to \infty} \mathbb{E}\left( \left| \int_0^t \left( \nabla_n G\left( \frac{n-1}{n} \right) V'(r_n(s)) - G'(1)\bar{\tau}(s) \right) ds \right| \right) = 0. \tag{5.8}$$

We are finally left to deal with the first term of the RHS of (5.4). We will proceed as in [6]. For any  $\varepsilon > 0$  define

$$\bar{r}_{i,\varepsilon} = \frac{1}{2n\varepsilon + 1} \sum_{|j-i| \le n\varepsilon} r_j, \qquad n\varepsilon < i < n(1-\varepsilon).$$
 (5.9)

We first prove that the boundary terms are negligible:

#### Lemma 5.2.

$$\lim_{\varepsilon \to 0} \lim_{n \to \infty} \int_0^t \int \left| \frac{1}{\gamma n} \left( \sum_{i=2}^{[n\varepsilon]} + \sum_{i=[n(1-\varepsilon)]+1}^{[n-1]} \right) (-\nabla_n^* \nabla_n) G\left(\frac{i}{n}\right) V'(r_{i+1}) \right| f_s^n d\nu_{\beta} ds = 0$$

$$(5.10)$$

*Proof.* For simplicity of notation let us estimate just one side. Since our conditions on V imply that  $|V'(r)| \leq C_2|r| + C_0$ , we only need to prove that for any  $t \geq 0$ :

$$\lim_{\varepsilon \to 0} \lim_{n \to \infty} \int \frac{1}{n} \sum_{i=2}^{[n\varepsilon]} |r_i| f_t^n d\nu_{\beta} = 0$$
 (5.11)

By the entropy inequality we have:

$$\int \frac{1}{n} \sum_{i=2}^{[n\varepsilon]} |r_i| f_t^n d\nu_{\beta} \leq \frac{1}{n\alpha} \log \int \prod_{i=2}^{[n\varepsilon]} e^{\alpha |r_i|} d\nu_{\beta} + \frac{H_n(t)}{\alpha n}$$
$$\leq \frac{1}{n\alpha} \sum_{i=2}^{[n\varepsilon]} (\mathcal{G}(\alpha, \beta_i) + \mathcal{G}(-\alpha, \beta_i) - 2\mathcal{G}(0, \beta_i)) + \frac{C}{\alpha}$$

Since  $\mathcal{G}(\alpha, \beta_i) + \mathcal{G}(-\alpha, \beta_i) - 2\mathcal{G}(0, \beta_i) \leq C'\alpha^2$ , for a constant C' independent on i, we have

$$\int \frac{1}{n} \sum_{i=2}^{[n\varepsilon]} |r_i| f_t^n d\nu_{\beta} \leq C' \varepsilon \alpha + \frac{C}{\alpha},$$

and by choosing  $\alpha = \varepsilon^{-1/2}$  (5.11) follows.

We are only left to show that

$$\lim_{\varepsilon \to 0} \lim_{n \to \infty} \int_0^t \int \left| \frac{1}{\gamma n} \sum_{i=[n\varepsilon]+1}^{[n(1-\varepsilon)]} (-\nabla_n^* \nabla_n) G\left(\frac{i}{n}\right) \left(V'(r_{i+1}) - \boldsymbol{\tau}(\bar{r}_{i,\varepsilon}, \beta_i)\right) \right| f_s^n d\nu. ds = 0$$

$$(5.12)$$

Thanks to the bound (4.4), we are now in the same position as in the proof of the over-damped dynamics, as considered in [6], and by using similar argument as used there (the so called one-block/two blocks) (5.12) follows. A slight difference is due to the dependence of  $\tau$  on  $\beta_i$ , but since this changes very slowly and smoothly in space it is easy to consider microscopic blocks of size k with constant temperature inside.

At this point the proof of theorem 2.1 follows by standard arguments. Let  $Q_n$  the probability distribution of  $\pi_n^n$  on  $\mathcal{C}([0,T],\mathcal{M}([0,1]))$ , where  $\mathcal{M}([0,1])$  are the signed measures on [0,1]. In appendix B we prove that the sequence  $Q_n$  is compact. Then, by the above results any limit point Q of  $Q_n$  is concentrated on absolutely continuous measures with densities  $\bar{r}(y,t)$  such that for any  $0 \le t \le T$ ,

$$\mathbb{E}^{Q} \Big| \int_{0}^{1} G(y) \left( \bar{r}(y,t) - \bar{r}(y,0) \right) dy - \gamma^{-1} \int_{0}^{t} ds \left[ \int_{0}^{1} G''(y) \boldsymbol{\tau}(\bar{r}(y,s),\beta(y)) dy - G'(1)\bar{\tau}(s) \right] \Big| = 0$$
(5.13)

Furthermore in appendix A we prove that Q is concentrated on densities that satisfy the regularity condition to have uniqueness of the solution of the equation.

#### 6. Appendix A: Proof of the regularity bound 2.20

**Proposition 6.1.** There exists a finite constant C such that for any limit point distribution Q we have the bound:

$$\mathbb{E}^{Q}\left(\int_{0}^{t} ds \int_{0}^{1} dx \left(\partial_{x} \boldsymbol{\tau}(\bar{r}(s, x), \beta(x))\right)^{2}\right) < C. \tag{6.1}$$

*Proof.* It is enough to prove that for any function  $F \in C^1([0,1])$  such that F(0) = 0 the following inequality holds:

$$\mathbb{E}^{Q}\left(\int_{0}^{t} ds \left[\int_{0}^{1} dx F'(x) \boldsymbol{\tau}(\bar{r}(s, x), \beta(x)) - F(1)\bar{\tau}(s)\right]\right) \le C\left(\int_{0}^{1} F(x)^{2} dx\right)^{1/2}.$$
(6.2)

In fact by a duality argument, since  $\tau(\bar{r}(s,1),\beta(1)) = \bar{\tau}(s)$ , we have:

$$\int_0^1 dx \, (\partial_x \boldsymbol{\tau}(\bar{r}(s,x),\beta(x)))^2 = \sup_{F \in \mathcal{C}^1([0,1])} \frac{\int_0^1 dx F'(x) \boldsymbol{\tau}(\bar{r}(s,x),\beta(x)) - F(1)\bar{\tau}(s)}{\int_0^1 F(x)^2 dx}.$$

Observe that (6.2) corresponds to a choice of test functions G(x) in (2.19) such that G' = F. In order to obtain (6.2), compute

$$\frac{1}{n^2} \mathcal{L}_n^{\bar{\tau}} \sum_{i=1}^n F(i/n)(p_i + \gamma q_i) = \sum_{i=1}^n F(i/n) A_n^{\bar{\tau}} p_i$$

$$= \sum_{i=1}^{n-1} F(i/n) \left( V'(r_{i+1}) - V'(r_i) \right) + F(1) \left( \bar{\tau} - V'(r_n) \right)$$

$$= \frac{1}{n} \sum_{i=2}^n \nabla_n^* F(i/n) V'(r_i) + F(1) \bar{\tau} - F(1/n) V'(r_1)$$

and after time integration and averaging over trajectories we have

$$\frac{1}{n^2} \int \sum_{i=1}^n F(i/n)(p_i + \gamma q_i)(f_t^n - f_0^n) d\nu_{\beta}.$$

$$= \int_0^t ds \int \frac{1}{n} \sum_{i=2}^n \nabla_n^* F(i/n) V'(r_i) f_s^n d\nu_{\beta}. + F(1) \int_0^t \bar{\tau}(s) ds$$

$$-F(1/n) \int_0^t ds \int V'(r_1) f_s^n d\nu_{\beta}.$$
(6.3)

It is easy to see that, since F(0) = 0 and differentiable, the last term of the right hand side is negligible as  $n \to \infty$ , by the same argument used in (5.5).

About the first term on the RHS of (6.3), by the results of section 5, it converges, through subsequences, to

$$-\mathbb{E}^{Q}\left(\int_{0}^{t}ds\int_{0}^{1}dxF'(x)\boldsymbol{\tau}(\bar{r}(s,x),\beta(x))\right).$$

About the left hand side of (6.3), one can see easily that

$$\frac{1}{n^2} \int \sum_{i=1}^n F(i/n) p_i (f_t^n - f_0^n) d\nu_{\beta} \underset{n \to \infty}{\longrightarrow} 0.$$

Using the inequality  $\sum_i q_i^2 \le n^2 \sum_i r_i^2$ , we can bound the other term of the LHS of (6.3) by observing that, for s = 0, t,

$$\left| \frac{\gamma}{n} \int \sum_{i=1}^{n} F(i/n) \frac{q_i}{n} f_s^n d\nu_{\beta} \right| \le \gamma \left( \frac{1}{n} \sum_{i=1}^{n} F(i/n)^2 \right)^{1/2} \left( \int \frac{1}{n} \sum_{i=1}^{n} \frac{q_i^2}{n^2} f_s^n d\nu_{\beta} \right)^{1/2}$$

$$\le \gamma \left( \frac{1}{n} \sum_{i=1}^{n} F(i/n)^2 \right)^{1/2} \left( \int \frac{1}{n} \sum_{i=1}^{n} r_i^2 f_s^n d\nu_{\beta} \right)^{1/2} \le C\gamma \left( \frac{1}{n} \sum_{i=1}^{n} F(i/n)^2 \right)^{1/2} .$$

Since F is a continuous function on [0,1] the rhs of the above expression is bounded in n and converges to the  $L^2$  norm of F as  $n \to \infty$ . Thus (6.2) follows.

## 7. Appendix B: Compactness

We prove in this section that the sequence of probability distributions  $Q_n$  on  $\mathcal{C}([0,t],\mathcal{M})$  induced by  $\pi_n$  is tight. Here  $\mathcal{M}$  is the space of the signed measures on [0,1] endowed

by the weak convergence topology. This tightness is consequence of the following statement.

**Proposition 7.1.** For any function  $G \in C^1([0,1])$  such that G(1) = 0, G'(0) = 0 and any  $\varepsilon > 0$  we have

$$\lim_{\delta \to 0} \limsup_{n \to \infty} \mathbb{P}^{\mu_0} \left[ \sup_{0 \le s < t \le T, |s-t| < \delta} |<\pi_n(t), G > - < \pi_n(s), G > | \ge \varepsilon \right] = 0$$
 (7.1)

*Proof.* By doing similar calculations as done in section 5 (see (5.2) and following ones)

$$<\pi_{n}(t), G> - <\pi_{n}(s), G> = -\int_{s}^{t} du \sum_{i=1}^{n-1} \nabla_{n} G\left(\frac{i}{n}\right) p_{i}(u)$$

$$= \int_{s}^{t} du \frac{1}{\gamma n} \sum_{i=2}^{n-1} (-\nabla_{n}^{*} \nabla_{n}) G\left(\frac{1}{n}\right) V'(r_{i+1}(u)) - \int_{s}^{t} du \frac{1}{\gamma} \nabla_{n} G\left(\frac{n-1}{n}\right) V'(r_{n}(u))$$

$$+ \int_{s}^{t} du \frac{1}{\gamma} \nabla_{n} G\left(\frac{1}{n}\right) V'(r_{1}(u)) + \frac{1}{\gamma n^{2}} \sum_{i=2}^{n-1} \nabla_{n} G\left(\frac{i}{n}\right) (p_{i}(t) - p_{i}(s))$$

$$+ \frac{1}{n} \sum_{i}^{n} \sqrt{2\gamma \beta_{j}^{-1}} \nabla_{n} G\left(\frac{i}{n}\right) (w_{i}(t) - w_{i}(s))$$

$$:= I_{1}(s, t) + I_{2}(s, t) + I_{3}(s, t) + I_{4}(s, t) + I_{5}(s, t)$$

We treat the corresponding 5 terms separately. The term  $I_3 = \int_s^t du \frac{1}{\gamma} \nabla_n G\left(\frac{1}{n}\right) V'(r_1(u))$  is the easiest to estimate, since G'(0) = 0, and using Schwarz inequality we have

$$\sup_{0 \le s < t \le T, |s-t| < \delta} |I_3(s,t)| \le \sup_{0 \le s < t \le T, |s-t| < \delta} \frac{C}{n\gamma} \int_s^t |V'(r_1(u))| du$$

$$\le \sup_{0 \le s < t \le T, |s-t| < \delta} \frac{C}{n\gamma} |t-s|^{1/2} \left( \int_s^t |V'(r_1(u))|^2 du \right)^{1/2}$$

$$\le \frac{C\delta^{1/2}}{n\gamma} \left( \int_0^T |V'(r_1(u))|^2 du \right)^{1/2}.$$

Since, by entropy inequality,

$$\mathbb{E}\left[\left(\int_{0}^{T} |V'(r_{1}(u))|^{2} du\right)^{1/2}\right] \leq \left[\int_{0}^{T} \mathbb{E}\left(|V'(r_{1}(u))|^{2}\right) du\right]^{1/2}$$
$$\leq C\left[\int_{0}^{T} \mathbb{E}\left(\sum_{i=1}^{n} (V(r_{i}(u)) + 1)\right) du\right]^{1/2} \leq CT^{1/2}n^{1/2}$$

so that

$$\mathbb{E}\left[\sup_{0\leq s< t\leq T, |s-t|<\delta} |I_3(s,t)|\right] \leq \frac{C\delta^{1/2}T^{1/2}}{\gamma n^{1/2}} \underset{n\to\infty}{\longrightarrow} 0.$$

About  $I_2$ , this is equal to

$$-\frac{1}{\gamma}\nabla_n G\left(\frac{n-1}{n}\right) \int_s^t du \left(V'(r_n(u)) - \bar{\tau}(u)\right) - \frac{1}{\gamma}\nabla_n G\left(\frac{n-1}{n}\right) \int_s^t du \bar{\tau}(u) \tag{7.2}$$

The second term of the above expression is trivially bounded by  $C\delta$  since  $|t - s| \le \delta$ . For the first term on the right hand side of (7.2), by (5.7), we have

$$\int_{s}^{t} du \left( V'(r_n(u)) - \bar{\tau}(u) \right) = \frac{p_n(s) - p_n(t)}{n^2} - \gamma \int_{s}^{t} p_n(u) du + \frac{\sqrt{2\gamma \beta_n^{-1}}}{n} \left( w_n(t) - w_n(s) \right)$$

The last term of the right hand side of the above is estimated by the standard modulus of continuity of the Wiener process  $w_n$ . For the second term of the right hand side, this is bounded by

$$\mathbb{E}\left[\sup_{0 \le s < t \le T, |s-t| < \delta} \gamma \left| \int_{s}^{t} p_{n}(u) du \right| \right] \le \gamma \delta^{1/2} \mathbb{E}\left[\left(\int_{0}^{T} p_{n}^{2}(u) du\right)^{1/2}\right] \\
\le \gamma \delta^{1/2} \left[\int_{0}^{T} \mathbb{E}(p_{n}^{2}(u)) du \right]^{1/2} = \gamma \delta^{1/2} \left[\int_{0}^{T} \mathbb{E}(p_{n}^{2}(u) - \beta_{n}^{-1}) du + T \beta_{n}^{-1}\right]^{1/2} \\
\le C \gamma \delta^{1/2} \left[\int_{0}^{T} \int p_{n} \partial_{p_{n}} f_{u}^{n} d\nu_{\beta} du + T \beta_{n}^{-1}\right]^{1/2} \\
\le C \gamma \delta^{1/2} \left[\left(\int_{0}^{T} \int p_{n}^{2} f_{u}^{n} d\nu_{\beta} du\right)^{1/2} \left(\int_{0}^{T} \int \frac{(\partial_{p_{n}} f_{u}^{n})^{2}}{f_{u}^{n}} d\nu_{\beta} du\right)^{1/2} + T \beta_{n}^{-1}\right]^{1/2} \\
\le C \gamma \delta^{1/2} \left[\left(\int_{0}^{T} \int p_{n}^{2} f_{u}^{n} d\nu_{\beta} du\right)^{1/2} \left(\int_{0}^{T} \int \frac{(\partial_{p_{n}} f_{u}^{n})^{2}}{f_{u}^{n}} d\nu_{\beta} du\right)^{1/2} + T \beta_{n}^{-1}\right]^{1/2} \\
\le C \gamma \delta^{1/2} \left[\left(\int_{0}^{T} \int p_{n}^{2} f_{u}^{n} d\nu_{\beta} du\right)^{1/2} \left(\int_{0}^{T} \int \frac{(\partial_{p_{n}} f_{u}^{n})^{2}}{f_{u}^{n}} d\nu_{\beta} du\right)^{1/2} + T \beta_{n}^{-1}\right]^{1/2} \\
\le C \gamma \delta^{1/2} \left[\left(\int_{0}^{T} \int p_{n}^{2} f_{u}^{n} d\nu_{\beta} du\right)^{1/2} \left(\int_{0}^{T} \int \frac{(\partial_{p_{n}} f_{u}^{n})^{2}}{f_{u}^{n}} d\nu_{\beta} du\right)^{1/2} + T \beta_{n}^{-1}\right]^{1/2} \\
\le C \gamma \delta^{1/2} \left[\left(\int_{0}^{T} \int p_{n}^{2} f_{u}^{n} d\nu_{\beta} du\right)^{1/2} \left(\int_{0}^{T} \int \frac{(\partial_{p_{n}} f_{u}^{n})^{2}}{f_{u}^{n}} d\nu_{\beta} du\right)^{1/2} + T \beta_{n}^{-1}\right]^{1/2}$$

where the last inequality is justified by the inequalities:

$$\int p_n^2 f_u^n d\nu \le Cn$$

$$\int_0^T \int \frac{(\partial_{p_n} f_u^n)^2}{f_u^n} d\nu du \le \frac{C}{n}$$

To deal with the first term we have to prove that

$$\lim_{n \to \infty} \mathbb{E}\left(\sup_{0 \le t \le T} \frac{1}{n^2} |p_n(t)|\right) = 0 \tag{7.3}$$

Since

$$\frac{p_n(t)}{n^2} = \frac{1}{n^2} p_n(0) e^{-\gamma n^2 t} + \int_0^t e^{-\gamma n^2 (t-u)} \left[ \bar{\tau}(u) - V'(r_n(u)) \right] du + \sqrt{2\gamma \beta_n^{-1}} \frac{1}{n} \int_0^t e^{-\gamma n^2 (t-u)} dw_n(u) \tag{7.4}$$

The stochastic integral is easy to estimate by Doob's inequality:

$$\mathbb{E}\left(\sup_{0 \le t \le T} \left| \sqrt{2\gamma\beta_n^{-1}} \frac{1}{n} \int_0^t e^{-\gamma n^2(t-u)} dw_n(u) \right|^2 \right) \le \frac{CT}{n^2}$$

About the second term, by Schwarz inequality we have that

$$\mathbb{E} \sup_{0 \le t \le T} \left| \int_0^t e^{-\gamma n^2 (t-u)} \left[ \bar{\tau}(u) - V'(r_n(u)) \right] du \right|$$

$$\le \frac{1}{n\sqrt{2\gamma}} \left( \int_0^T \mathbb{E} \left( \left[ \bar{\tau}(u) - V'(r_n(u)) \right]^2 \right) du \right)^{1/2}$$

and by the entropy bound we have

$$\mathbb{E}\left(\left[\bar{\tau}(u) - V'(r_n(u))\right]^2\right) \le Cn$$

so that this term goes to zero like  $n^{-1/2}$ . The first term in (7.4) is trivial to estimate. This conclude the estimate of  $I_2$ .

The estimation of  $I_4$  is similar to the proof of (7.3), but require a little extra work. We need to prove that

$$\lim_{n \to \infty} \mathbb{E} \sup_{0 \le t \le T} \left| \frac{1}{n^2} \sum_{i=2}^{n-1} \nabla_n G\left(\frac{i}{n}\right) p_i(t) \right| = 0.$$
 (7.5)

By the evolution equations we have

$$\frac{1}{n^2} \sum_{i=2}^{n-1} \nabla_n G\left(\frac{i}{n}\right) p_i(t) = \frac{1}{n^2} \sum_{i=2}^{n-1} \nabla_n G\left(\frac{i}{n}\right) p_i(0) e^{-\gamma n^2 t}$$

$$+ \int_0^t ds \ e^{-\gamma n^2 (t-s)} \frac{1}{n} \sum_{i=3}^{n-1} \nabla_n^* \nabla_n G\left(\frac{i}{n}\right) V'(r_i(s))$$

$$+ \int_0^t ds \ e^{-\gamma n^2 (t-s)} \left(\nabla_n G(1) V'(r_n(s)) - \nabla_n G\left(\frac{2}{n}\right) V'(r_2(s))\right)$$

and all these terms can be estimated as in the proof of (7.3), so that (7.5) follows.

Also  $I_5$  can be easily estimated by Doob inequality and using the independence of  $w_i(t)$ .

Finally estimating  $I_1$ , notice that since G is a smooth function, it can be bounded by

$$\sup_{0 \le s < t \le T, |s-t| < \delta} |I_1(s,t)| \le \frac{C}{\gamma n} \sup_{0 \le s < t \le T, |s-t| < \delta} \int_s^t du \sum_{i=2}^{n-1} |V'(r_{i+1}(u))|$$

$$\le \frac{C\delta^{1/2}}{\gamma} \left( \int_0^T \frac{1}{n} \sum_{i=2}^{n-1} |V'(r_{i+1}(u))|^2 du \right)^{1/2}$$
(7.6)

and, by entropy inequality

$$\mathbb{E}\left[\left(\int_0^T \frac{1}{n} \sum_{i=2}^{n-1} |V'(r_{i+1}(u))|^2 du\right)^{1/2}\right] \le \left[\int_0^T \frac{1}{n} \sum_{i=2}^{n-1} \mathbb{E}\left(|V'(r_{i+1}(u))|^2\right) du\right]^{1/2} \le C,$$

so that the expression in (7.6) is negligible after  $\delta \to 0$ .

# 8. Appendix C: Uniqueness of Weak solutions

**Proposition 8.1.** The weak solution of (2.19) is unique in the class of function such that

$$\int_0^t ds \int_0^1 \left(\partial_x \tau(r(x,s),\beta(x))\right)^2 dx < +\infty \tag{8.1}$$

*Proof.* Let  $g(x) \ge 0$  a smooth function with compact support contained in [-1/4, 1/4] such that  $\int_{\mathbb{R}} g(y)dy = 1$ . Then for  $\lambda > 0$  large enough, define the function

$$G_{\lambda}(y,x) = 1 - \int_{-\infty}^{y} \lambda g(\lambda(z-x))dz$$

Then for  $1/(4\lambda) < x < 1 - 1/(4\lambda)$ , we have  $G_{\lambda}(0,x) = 0$  and  $\partial_y G_{\lambda}(1,x) = 0$ , and it can be used as test function in (2.19). So if r(x,t) is a solution in the given class, we have

$$\int_0^1 G_{\lambda}(y,x) \left( r(y,t) - r_0(y) \right) dx = \gamma^{-1} \int_0^t ds \left[ \int_0^1 \lambda g(\lambda(y-x)) \partial_y \tau(r(y,s),\beta(y)) dy \right].$$

Letting  $\lambda \to +\infty$  we obtain:

$$\int_{0}^{x} (r(y,t) - r_{0}(y)) dx = \gamma^{-1} \int_{0}^{t} ds \partial_{y} \tau(r(x,s), \beta(x)), \quad \forall x \in (0,1).$$

Let  $r_1(x,t), r_2(x,t)$  two solutions in the class considered, and define

$$R_j(x,t) = \int_0^x r_j(y,t)dy, \qquad j = 1, 2.$$

By the approximation argument done at the beginning of the proof, we have that

$$\partial_t R_i(x,t) = \gamma^{-1} \partial_x \tau(r_i(x,s), \beta(x))$$

for every  $x \in (0,1)$  and t > 0.

Since  $\tau(r_i(1,t),\beta(1)) = \bar{\tau}(t)$ , and since  $\tau(r,\beta)$  is a strictly increasing function of r,

$$\begin{split} &\frac{d}{dt} \int_0^1 \left( R_1(x,t) - R_2(x,t) \right)^2 dx \\ &= 2 \gamma^{-1} \int_0^1 \left( R_1(x,t) - R_2(x,t) \right) \partial_x \left( \tau(r_1(x,t),\beta(x)) - \tau(r_2(x,t),\beta(x)) \right) dx \\ &= -2 \gamma^{-1} \int_0^1 \left( r_1(x,t) - r_2(x,t) \right) \left( \tau(r_1(x,t),\beta(x)) - \tau(r_2(x,t),\beta(x)) \right) dx \le 0. \end{split}$$

## 9. Appendix D: proof of the entropic hypocoercive bound (4.16)

We will prove in this appendix that there exists constants  $\lambda>0$  and C>0 independent of n such that

$$\frac{d}{dt}I_n(f) \le -\lambda n^2 I_n(f) + Cn. \tag{9.1}$$

We will use the following commutation relations:

$$[\partial_{p_i}, \beta_j^{-1} \partial_{p_i}^*] = \delta_{i,j}, \qquad [\partial_{p_i}, \mathcal{A}_n^{\tau}] = \partial_{q_i}, \qquad [\partial_{q_i}, \mathcal{A}_n^{\tau}] = -(\partial_q^2 \mathcal{V} \partial_p)_i$$
(9.2)

where  $\partial_q^2 \mathcal{V}$  is the corresponding hessian matrix of  $\mathcal{V} = \sum_{i=1}^n V(r_n)$ .

Denote  $g_t = \sqrt{f_t^n}$  and observe that

$$I_n(g_t^2) = 4 \int \left( |\partial_p g_t|_{\tilde{\odot}}^2 + |\partial_q g_t|_{\tilde{\odot}}^2 + 2 |\partial_q g_t \tilde{\odot} \partial_p g_t \right) d\nu_{\beta}. \tag{9.3}$$

Recall that

$$n^2 \mathcal{A}_n^{\tau,*} = -n^2 \mathcal{A}_n^{\tau} + B_n^{\tau} \tag{9.4}$$

where

$$B_n^{\tau} = -n \sum_{i=1}^{n-1} \nabla_n \beta(i/n) p_i V'(r_{i+1}) + n^2 \beta(1) p_n \tau$$

Consequently  $g_t$  solves the equation:

$$\partial_t g = -n^2 \mathcal{A}_n^{\bar{\tau}(t)} g_t + n^2 \gamma \mathcal{S}_n g_t + n^2 \gamma \frac{|\partial_p g_t|_{\odot}^2}{g_t} + \frac{1}{2} B_n^{\bar{\tau}(t)} g_t$$

We then compute the time derivative of  $I_n(g_t^2)$  by considering the three terms separately. The first one gives:

$$\frac{d}{dt} \int |\partial_{p}g_{t}|_{\tilde{\odot}}^{2} d\nu_{\beta} = -2n^{2} \int \partial_{p}g_{t}\tilde{\odot}\partial_{p}(\mathcal{A}^{\bar{\tau}(t)}g_{t}) d\nu_{\beta}.$$

$$-2n^{2}\gamma \int \partial_{p}g_{t}\tilde{\odot}\partial_{p}(\partial_{p}^{*}\odot\partial_{p}g_{t}) d\nu_{\beta}.$$

$$+2n^{2}\gamma \int \partial_{p}g_{t}\tilde{\odot}\partial_{p}\left(\frac{|\partial_{p}g_{t}|_{\tilde{\odot}}^{2}}{g_{t}}\right) d\nu_{\beta}.$$

$$+\int \partial_{p}g_{t}\tilde{\odot}\partial_{p}(B_{n}^{\bar{\tau}(t)}g_{t}) d\nu_{\beta}.$$
(9.5)

By the commutation relations (9.2), and using (9.4), the first term on the RHS of (9.5) is equal to

$$-2n^{2} \int \partial_{p} g_{t} \tilde{\odot} \partial_{q} g_{t} \ d\nu_{\beta} - 2n^{2} \int \partial_{p} g_{t} \tilde{\odot} \mathcal{A}^{\bar{\tau}(t)} \partial_{p} g_{t} \ d\nu_{\beta}$$

$$= -2n^{2} \int \partial_{p} g_{t} \tilde{\odot} \partial_{q} g_{t} \ d\nu_{\beta} - \int \partial_{p} g_{t} \tilde{\odot} B_{n}^{\bar{\tau}(t)} \partial_{p} g_{t} \ d\nu_{\beta}$$

Then the RHS of (9.5) is equal to

$$-2n^{2} \int \partial_{p}g_{t} \tilde{\odot} \partial_{q}g_{t} \ d\nu_{\beta}. -2n^{2} \gamma \int \partial_{p}g_{t} \tilde{\odot} \partial_{p}(\partial_{p}^{*} \odot \partial_{p}g_{t}) \ d\nu_{\beta}.$$

$$+2n^{2} \gamma \int \partial_{p}g_{t} \tilde{\odot} \partial_{p} \left(\frac{|\partial_{p}g_{t}|_{\odot}^{2}}{g_{t}}\right) \ d\nu_{\beta}. + \int g_{t} \partial_{p}g_{t} \tilde{\odot} \partial_{p}B_{n}^{\bar{\tau}(t)} \ d\nu_{\beta}.$$

The last term of the above equation is equal to

$$\int g_t \partial_p g_t \tilde{\odot} \partial_p B_n \ d\nu_{\beta} = -n \int g_t \sum_{i=1}^{n-1} \beta_i^{-1} \nabla_n \beta(\frac{i}{n}) V'(r_{i+1}) \partial_{p_i} g_t \ d\nu_{\beta}. \tag{9.6}$$

Notice that the term involving  $n^2\tau p_n$  does not appear in the above expression, because the particular definition of  $\tilde{\odot}$ . For any  $\alpha_1 > 0$ , using Schwarz inequality, (4.10) and (4.11), (9.6) is bounded by

$$\frac{1}{2\alpha_1} \int g_t^2 \sum_{i=1}^{n-1} \frac{(\nabla_n \beta(\frac{i}{n}))^2}{\beta_i} V'(r_{i+1})^2 d\nu_{\beta} + \frac{\alpha_1 n^2}{2} \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta}.$$

$$\leq \frac{Cn}{\alpha_1} + \frac{\alpha_1 n^2}{2} \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta}.$$

for a constant C depending on  $\beta$ , and the initial entropy, but independent of n.

Computing the second term of the RHS of (9.5) we have:

$$\int \partial_p g_t \tilde{\odot} \partial_p (\partial_p^* \odot \partial_p g_t) \ d\nu_{\beta.} = \int \sum_{j=1}^{n-1} \beta_j^{-1} |\partial_p \partial_{p_j} g|_{\tilde{\odot}}^2 \ d\nu_{\beta.} + \int |\partial_p g|_{\tilde{\odot}}^2 \ d\nu_{\beta.}$$

$$= \int \sum_{j=1}^n \sum_{j=1}^{n-1} \beta_j^{-1} \beta_i^{-1} (\partial_{p_i} \partial_{p_j} g)^2 \ d\nu_{\beta.} + \int |\partial_p g|_{\tilde{\odot}}^2 \ d\nu_{\beta.}$$

About the third term on the RHS:

$$\partial_p g_t \tilde{\odot} \partial_p \left( \frac{|\partial_p g_t|_{\odot}^2}{g_t} \right) = \frac{2 \sum_{j=1}^{n-1} \sum_{i=1}^n \beta_j^{-1} \beta_i^{-1} \ \partial_{p_j} g_t \ \partial_{p_i} g_t \ \partial_{p_i} g_t}{g_t} - \frac{|\partial_p g|_{\odot}^2 |\partial_p g|_{\tilde{\odot}}^2}{g_t^2}$$

Summing all together we have obtained

$$\frac{d}{dt} \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta} = -2n^2 \int \partial_p g_t \tilde{\odot} \partial_q g_t d\nu_{\beta} - n^2 \left(2\gamma - \frac{\alpha_1}{2}\right) \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta} 
-2n^2 \gamma \int \sum_{j=1}^{n-1} \sum_{i=1}^n \beta_j^{-1} \beta_j^{-1} \left(\partial_{p_i} \partial_{p_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{p_j} g_t\right)^2 d\nu_{\beta} + \frac{Cn}{\alpha_1}.$$
(9.7)

Now we deal with the derivative of the second term:

$$\frac{d}{dt} \int |\partial_{q}g_{t}|_{\tilde{\odot}}^{2} d\nu_{\beta} = -2n^{2} \int \partial_{q}g_{t}\tilde{\odot}\partial_{q}(\mathcal{A}^{\bar{\tau}(t)}g_{t}) d\nu_{\beta} - 2n^{2}\gamma \int \partial_{q}g_{t}\tilde{\odot}\partial_{q}(\partial_{p}^{*}\odot\partial_{p}g_{t}) d\nu_{\beta} 
+2n^{2}\gamma \int \partial_{q}g_{t}\tilde{\odot}\partial_{q}\left(\frac{|\partial_{p}g_{t}|_{\tilde{\odot}}^{2}}{g_{t}}\right) d\nu_{\beta} + \int \partial_{q}g_{t}\tilde{\odot}\partial_{q}(B_{n}g_{t}) d\nu_{\beta} 
= -2n^{2} \int \partial_{q}g_{t}\tilde{\odot}\partial_{q}(\mathcal{A}^{\bar{\tau}(t)}g_{t}) d\nu_{\beta} - 2n^{2}\gamma \int \sum_{j=1}^{n-1} \sum_{i=1}^{n} \beta_{i}^{-1}\beta_{j}^{-1} \left(\partial_{p_{i}}\partial_{q_{j}}g - g_{t}^{-1}\partial_{p_{i}}g\partial_{q_{j}}g\right)^{2} d\nu_{\beta} 
+ \int \partial_{q}g_{t}\tilde{\odot}\partial_{q}(B_{n}g_{t}) d\nu_{\beta} . \tag{9.8}$$

The first and the last term give:

$$-2n^{2} \int \partial_{q} g_{t} \tilde{\odot} \partial_{q} (\mathcal{A}^{\bar{\tau}(t)} g_{t}) d\nu_{\beta} + \int \partial_{q} g_{t} \tilde{\odot} \partial_{q} (B_{n} g_{t}) d\nu_{\beta}$$

$$= 2n^{2} \int \partial_{q} g_{t} \tilde{\odot} (\partial_{q}^{2} \mathcal{V} \partial_{p}) g_{t} d\nu_{\beta} + \int g_{t} \partial_{q} g_{t} \tilde{\odot} \partial_{q} B_{n} d\nu_{\beta}$$

The last term on the RHS of the above expression is equal to

$$\int g_t \partial_q g_t \tilde{\odot} \partial_q B_n \, d\nu_{\beta}.$$

$$= n \sum_{i=2}^{n-1} \int \beta_i^{-1} g_t(\partial_{q_i} g_t) \left[ \nabla_n \beta \left( \frac{i}{n} \right) V''(r_{i+1}) p_i - \nabla_n \beta \left( \frac{i-1}{n} \right) V''(r_i) p_{i-1} \right] \, d\nu_{\beta}.$$

$$+ n \int \beta_1^{-1} g_t(\partial_{q_1} g_t) \nabla_n \beta \left( \frac{1}{n} \right) V''(r_2) p_1.$$

Since V'' and  $\nabla_n \beta$  are bounded and  $\beta(\cdot)$  is positive bounded away from 0, this last quantity is bounded for any  $\alpha_2 > 0$  by

$$n^{2}\alpha_{2} \int |\partial_{q}g_{t}|_{\tilde{\odot}}^{2} d\nu_{\beta} + C\alpha_{2}^{-1} \int \sum_{i=1}^{n-1} p_{i}^{2} g_{t}^{2} d\nu_{\beta} \leq n^{2}\alpha_{2} \int |\partial_{q}g_{t}|_{\tilde{\odot}}^{2} d\nu_{\beta} + C'\alpha_{2}^{-1} n.$$

Since V'' is bounded, for any  $\alpha_3 > 0$  we have

$$2n^2 \int \partial_q g_t \tilde{\odot}(\partial_q^2 \mathcal{V} \partial_p) g_t \ d\nu_{\beta} \leq \alpha_3 n^2 \int |\partial_q g_t|_{\tilde{\odot}}^2 \ d\nu_{\beta} + \frac{|V''|_{\infty}^2 n^2}{\alpha_3} \int |\partial_p g_t|_{\tilde{\odot}}^2 \ d\nu_{\beta}.$$

Putting all the terms together, the time derivative of the second term is bounded by

$$\frac{d}{dt} \int |\partial_q g_t|_{\tilde{\odot}}^2 d\nu_{\beta} \leq (\alpha_2 + \alpha_3) n^2 \int |\partial_q g_t|_{\tilde{\odot}}^2 d\nu_{\beta} + \frac{Cn^2}{\alpha_3} \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta} 
- 2n^2 \gamma \int \sum_{i=1}^{n-1} \sum_{i=1}^n \beta_i^{-1} \beta_j^{-1} \left( \partial_{p_i} \partial_{q_j} g - g_t^{-1} \partial_{p_i} g \partial_{q_j} g \right)^2 d\nu_{\beta} + C' \alpha_2^{-1} n$$
(9.9)

About the derivative of the third term, using the third of the commutation relations (9.2), gives

$$\frac{d}{dt}2\int \partial_{q}g_{t}\tilde{\odot}\partial_{p}g_{t}d\nu_{\beta}. = -2n^{2}\int \left[\partial_{q}(\mathcal{A}^{\tau(t)}g_{t})\tilde{\odot}\partial_{p}g_{t} + \partial_{q}g_{t}\tilde{\odot}\partial_{p}(\mathcal{A}^{\tau(t)}g_{t})\right]d\nu_{\beta}.$$

$$+\int \left[\partial_{q}(B_{n}g_{t})\tilde{\odot}\partial_{p}g_{t} + \partial_{q}g_{t}\tilde{\odot}\partial_{p}(B_{n}g_{t})\right]d\nu_{\beta}.$$

$$-2n^{2}\gamma\int \left[\partial_{q}g_{t}\tilde{\odot}\partial_{p}(\partial_{p}^{*}\odot\partial_{p}g_{t}) + \partial_{q}(\partial_{p}^{*}\odot\partial_{p}g_{t})\tilde{\odot}\partial_{p}g_{t}\right]d\nu_{\beta}.$$

$$+2n^{2}\gamma\int \left[\partial_{q}g_{t}\tilde{\odot}\partial_{p}\left(\frac{|\partial_{p}g_{t}|_{\odot}^{2}}{g_{t}}\right) + \partial_{q}\left(\frac{|\partial_{p}g_{t}|_{\odot}^{2}}{g_{t}}\right)\tilde{\odot}\partial_{p}g_{t}\right]d\nu_{\beta}.$$

$$=2n^{2}\int (\partial_{q}^{2}\mathcal{V}\partial_{p})g_{t}\tilde{\odot}\partial_{p}g_{t}d\nu_{\beta}. - 2n^{2}\int |\partial_{q}g_{t}|_{\odot}^{2}d\nu_{\beta}.$$

$$+\frac{1}{2}\int g_{t}\left[\partial_{q}B_{n}\tilde{\odot}\partial_{p}g_{t} + \partial_{q}g_{t}\tilde{\odot}\partial_{p}B_{n}\right]d\nu_{\beta}.$$

$$-4n^{2}\gamma\int\sum_{j=1}^{n-1}\sum_{i=1}^{n}\beta_{i}^{-1}\beta_{j}^{-1}\left[\left(\partial_{p_{i}}\partial_{q_{j}}g\right)\left(\partial_{p_{i}}g_{t}\right)\left(\partial_{p_{j}}g_{t}\right)\right]d\nu_{\beta}.$$

$$+2n^{2}\gamma\int\sum_{j=1}^{n-1}\sum_{i=1}^{n}2\beta_{i}^{-1}\beta_{j}^{-1}g_{t}^{-1}\left[\left(\partial_{p_{i}}\partial_{p_{j}}g\right)\left(\partial_{p_{i}}g_{t}\right)\left(\partial_{q_{j}}g_{t}\right) + \left(\partial_{q_{j}}\partial_{p_{i}}g\right)\left(\partial_{p_{j}}g_{t}\right)\left(\partial_{p_{j}}g_{t}\right)d\nu_{\beta}.$$

$$-4n^{2}\gamma\int\sum_{j=1}^{n-1}\sum_{i=1}^{n}\beta_{i}^{-1}\beta_{j}^{-1}g^{-2}(\partial_{p_{i}}g_{t})^{2}(\partial_{q_{j}}g_{t})\left(\partial_{p_{j}}g_{t}\right)d\nu_{\beta}.$$

$$(9.10)$$

The last three terms of the RHS of the (9.10) can be written as

$$-4n^2\gamma \int \sum_{i=1}^{n-1} \sum_{i=1}^{n} \beta_i^{-1} \beta_j^{-1} \left[ \left( \partial_{p_i} \partial_{q_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{q_j} g_t \right) \left( \partial_{p_i} \partial_{p_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{p_j} g_t \right) \right] d\nu_{\beta}.$$

so they combine with the corresponding terms coming from the time derivative of the first two terms of  $I_n$  giving an exact square.

The second term of (9.10), by the same arguments used before, can be bounded by

$$n^2\alpha_4 \int |\partial_q g_t|_{\tilde{\odot}}^2 d\nu_{\beta}. + n^2\alpha_5 \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta}. + Cn(\alpha_4^{-1} + \alpha_5^{-1})$$

About the first term of (9.10), since V'' is bounded, it is bounded by  $V''_{\infty}n^2 \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta}$ . Putting all these bounds together we obtain that

$$\frac{d}{dt}I_n(f_t) \le -n^2 \kappa_p \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta} - n^2 \kappa_q \int |\partial_q g_t|_{\tilde{\odot}}^2 d\nu_{\beta} - 2n^2 \int \partial_p g_t \tilde{\odot} \partial_q g_t d\nu_{\beta} + Cn$$

$$-2N^2\gamma \int \sum_{i=1}^{n-1} \sum_{i=1}^n \beta_i^{-1} \beta_j^{-1} \left[ \left( \partial_{p_i} \partial_{q_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{q_j} g_t \right) + \left( \partial_{p_i} \partial_{p_j} g_t - g_t^{-1} \partial_{p_i} g_t \partial_{p_j} g_t \right) \right]^2 d\nu_{\beta}.$$

with

$$\kappa_p = 2\gamma - \frac{\alpha_1}{2} - \frac{C}{\alpha_3} - \alpha_5 - V_{\infty}''$$

$$\kappa_q = 2 - \alpha_2 - \alpha_3 - \alpha_4$$

By choosing  $\alpha_2 + \alpha_3 + \alpha_4 \leq 1$  we have obtained that for some constants  $C_1, C_2 > 0$  independent of n

$$\frac{d}{dt}I_n(f_t) \le -n^2I_n(f_t) + C_1n + C_2 \int |\partial_p g_t|_{\tilde{\odot}}^2 d\nu_{\beta}..$$

By recalling that

$$\int_0^t ds \int |\partial_p g_s|_{\tilde{\odot}}^2 d\nu_{\beta} \leq \frac{C'}{n}$$

after time integration we have for some constant  $C_3$ :

$$I_n(f_t) \le e^{-n^2 t} I_n(f_0) + \frac{C_3}{n} (1 - e^{-n^2 t})$$

that implies

$$I_n(f_t) \le \frac{C_4}{n} \tag{9.11}$$

for any reasonable initial conditions such that  $I_n(f_0)$  is finite and not growing too fast with n.

**Remark 9.1.** An important example for understanding the meaning of a density with small  $I_n$  functional, consider the inhomogeneous Gibbs density:

$$f = \exp\left(\sum_{i=1}^{n} \beta_i \tau_i r_i + \sum_{i=1}^{n-1} \frac{1}{n} \nabla_n(\beta_i \tau_i) p_i\right) / \mathcal{N}$$
(9.12)

where  $\mathcal{N}$  is a normalization constant. In the case of constant temperature these densities play an important role in the relative entropy method (cf [14, 9]), as to a non-constant profile of tension corresponds a profile of small damped velocities averages. Computing  $I_n$  on f we have

$$I_n(f) = \sum_{i=1}^{n-1} \left[ \beta_i \tau_i - \beta_{i+1} \tau_{i+1} + \frac{1}{n} \nabla_n(\beta_i \tau_i) \right] = 0.$$

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