Non-equilibrium macroscopic dynamics of chains of anharmonic oscillators

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Introduction

> *The objective of statistical mechanics is to explain the macroscopic properties of matter on the basis of the behavior of the atom and molecules of which it is composed.*
>
> Oscar R. Lanford III [9]

If we want to make the above definition specific for the *non-equilibrium* statistical mechanics, we can refrase it as

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This definition requires to be more specific about what we intend for *macroscopic evolution*. In most non-equilibrium problems it should be specified non only the space scale, but also the time scale of the macroscopic evolution. In fact, as we will see in this book, the same system can behave very differently at different space-time scaling.

This is also related to the choice of which observables we should follow in a macroscopic non-equilibrium evolution of a system. Here we are interested in the evolution of *conserved* quantities of the systems, like energy. A major concern is to distinguish these *slow* observables from the others (*fast*). In fact a deterministic hamiltonian dynamics with n degrees of freedom, may have other integrals of motion than energy. One could be total momentum, but there could be many others, and some systems are completely integrable (like a chain of harmonic oscillators, or the Toda lattice).

We are interested here in systems such that the only integrals of the motion that *survive* to the themodynamic limit $n \to \infty$ are given by energy, eventually momentum (if the infinite system has translation invariant properties), and number of particles. This is actually a very vague statement, since the corresponding infinite system typically has an infinite amount of energy, momentum and mass. So the precise definition of this property is that the only stationary translation invariant measures, enough regular so that are locally absolutely continuous with respect to Lebesgue measure, are given by Gibbs measures associated to the Hamiltonian of the system (see chapter 2 for a precise definition of all these notions). We call this property *ergodicity*, or *ergodicity of the infinite system* to distinguish it from the more classical definition of ergodicity of finite systems.

A well known conterexample to this ergodicity is given by the harmonic chain of oscillators, where the energy of each mode of vibration is conserved. This is a linear system, and this example suggests that ergodicity should be connected with some level of *chaoticity* induced by non-linearities in the interactions. The Toda lattice conterexample (non–linear) shows that the situation is not so simple, and in fact it is not easy to state necessary or sufficient conditions on the interaction between particles, that will imply this ergodicity property. This is one of the major open problem of statistical mechanics, since it is this property that allows, in a macroscopic (space-time) description, to separate an autonomous evolution of energy, momentum and density from the other observables.

In chapter 2 we give a proof that, if a stationary measure has an excheangeable distribution of velocities, then is a Gibbs measure, i.e. ergodicity follows from this excheageability of the velocities.

Since at the moment we are not able to prove ergodicity of the infinite system for any hamiltonian system, we consider stochastic perturbations of these hamiltonian dynamics. These stochastic perturbation exchange momentum between particles. They are local and conserve kinetic energy and eventually total momentum. Consequently the stationary measures for these infinite stochastic dynamics have excheangeable distributions of velocities, i.e. they are ergodic. All this is proven in chapter 2 for a one-dimensional chain of oscillators. One can think that these stochastic perturbations model the effect of the non-linearities, or of some other faster chaotic degree of freedom not included in the hamiltonian dynamics.

For these ergodic systems it is useful to define the concept of *local equilibrium*. This is not a property of a single probability measure on the configuration space of the finite of infinite system, but an asymptotic property of a sequence of probability measures. We define a sequence of probability measure a local equilibrium if *locally* they converge to a Gibbs measure for the infinite system corresponding to a given energy, momentum and density (cf. section 1.4 for a precise definition).

Thermodynamic entropy $S(r, \mathcal{E})$ is defined by formula (A.5.11) from the microcanonical ensemble, as the limit of the logarithm of the volume of the configurations with fixed total energy and volume of the system of n particles. Notice that this is actually a density of entropy, and it should be thought as the thermodynamic entropy of the *macroscopic* system of (macroscopic) length r at equilibrium with given value of energy $\mathcal{E}$. This is obtained from a one dimensional chain of n oscillators, with total length fixed to be nr and total energy fixed at $n\mathcal{E}$, as $n \to \infty$. It comes out from its definition that $S(r, \mathcal{E})$ is a concave function, and that

$$2S\left(\frac{r_1 + r_2}{2}, \frac{\mathcal{E}_1 + \mathcal{E}_2}{2}\right) \geq S(r_1, \mathcal{E}_1) + S(r_2, \mathcal{E}_2) \tag{0.0.1}$$

The quantity on the left in (0.0.1) is the thermodynamic entropy of a system of $2n$ oscillators with total length fixed at $n(r_1 + r_2)$ and energy fixed at $n(\mathcal{E}_1 + \mathcal{E}_2)$. This property of thermodynamic entropy has a classic interpretation. Suppose we have two systems of n oscillators in microcanonical equilibrium, with corresponding parameter $r_1, \mathcal{E}_1$ and $r_2, \mathcal{E}_2$, and we put them in contact fixing the two extremities

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We have then an inhomogeneous system of $2n$ oscillators with total length fixed to be $n(r_1 + r_2)$ and energy $n(\mathcal{E}_1 + \mathcal{E}_2)$. This system now is in non-equilibrium, and energy and density will evolve on a certain time scale depending on n that we will study later on. *If* this new system will reach equilibrium, then the thermodynamic entropy associated will be larger than the sum of the two initial thermodynamic entropies. This is the classic argument explaining increase with time of thermodynamic entropy, repeated probably thousand times by many authors. In principle it is correct even if we where not taking the limit as $n \to \infty$, i.e. using as entropy just the logarithm of the corresponding volume in the phase space. The usual objection to this argument is that the dynamics of the (*finite*) system may not reach equilibrium (and in fact typically it does not [1]). Here we insist in the inequality (0.0.1) for the thermodynamic entropy S defined in the limit $n \to \infty$, i.e. associated to the macroscopic (*infinite*) system in equilibrium. More precisely the sense of the entropy increase contained in (0.0.1) as to be understood in a *macroscopic* space-time limit, as we will make clear later on.

The above procedure can be generalized to k chains of n oscillators at different equilibrium parameters obtaining

$$S\left(\frac{1}{k}\sum_{i=1}^{k} r_i, \frac{1}{k}\sum_{i=1}^{k} \mathcal{E}_i\right) \geq \sum_{i=1}^{k} S(r_i, \mathcal{E}_i)\frac{1}{k}$$

where as before we identify the right hand side as the entropy of an inhomogeneous system where we have prepared each subsystem in equilibrium at different parameters. Going further we can rescale the (macroscopic) size of the k macroscopic

[1] Even in presence of non-linearities the finite system may have periodicities and other phenomena that prevent the system to converge to equilibrium, this was in fact the main point of the Fermi-Pasta-Ulam numerical experiment. These phenomenas should disappear in the limit as $n \to \infty$, see the clear discussion of this problem in [13]

systems as k^{-1} and obtain with the limit procedure, as $k \to \infty$, the thermodynamic entropy of a system in *local equilibrium*[2] with profiles of energy $\mathcal{E}(y)$ and inverse density $r(y)$ as

$$\int_0^1 S(r(y), \mathcal{E}(y))\, dy$$

that by concavity is bigger or equal than $S(\int r(y)dy, \int \mathcal{E}(y)dy)$. This definition of thermodynamic entropy has precise mathematical meaning for a *macroscopic* inhomogeneous system in *local equilibrium*. Homogeneous systems (systems in local equilibrium with flat profile of energy and density) maximize this entropy.

Assume now that we have prove that in a certain macroscopic scale energy and density evolve deterministically, following some profiles densities $r(y,t), \mathcal{E}(y,t)$, solution of certain conservative macroscopic equations (i.e. $\int r(y,t)dy, \int \mathcal{E}(y,t)dy$ are constant in t). It follows that the problem of the macroscopic increase of the entropy in time is related to the evolution of the profiles of density and energy in this macroscopic scale.

More precisely, if one looks at the hyperbolic macroscopic space-time scale, where space and time are rescaled in the same way (see chapter 3), the momentum $\pi(y,t)$ is also a macroscopic observable, and the internal energy is given by $\mathcal{U}(y,t) = \mathcal{E}(y,t) - \pi(y,t)^2/2$, and the total thermodynamic entropy at time t is given by $\int_0^1 S(r(y,t), \mathcal{U}(y,t))\, dy$. The profiles triplet $r(y,t), \pi(y,t), \mathcal{E}(y,t)$ evolves in time as solution of the Euler non-linear hyperbolic system (3.1.3). If these solutions are smooth, then we prove in chapter 3, under the assumption that the infinite dynamics is ergodic, that they describe the macroscopic evolution of the corresponding observables. It turns out that in this smooth regime

$$\partial_t S(r(y,t), \mathcal{U}(y,t)) = 0 \tag{0.0.2}$$

for any y. This means that if shock are not present, thermodynamic entropy remains constant. Correspondingly the sysstem is also macroscopically reversible in time (in the smooth regime Eler equations are time reversible).

[2]see the precise definition in section 1.4, where this notion is intended as a macroscopic asymptotic property.

Chapter 1

Statistical mechanics and thermodynamics of one dimensional chain of oscillators

1.1 The model: grand canonical formalism

We study a system of n anharmonic oscillators. The particles are denoted by $j = 1, \dots n$. We denote with $q_j, j = 1, \dots, n$ their positions, and with p_j the corresponding momentum (which is equal to its velocity since we assume that all particles have mass 1). We consider first the system attached to a *wall*, and we set $q_0 = 0, p_0 = 0$. Between each pair of consecutive particles $(i, i+1)$ there is an anharmonic spring described by its potential energy $V(q_{i+1} - q_i)$. We assume V is a positive smooth function such that $V(r) \to +\infty$ as $|r| \to \infty$ and such that

$$Z(\lambda, \beta) := \int e^{-\beta V(r) + \lambda r} dr < +\infty \tag{1.1.1}$$

for all $\beta > 0$ and all $\lambda \in \mathbb{R}$. Let a be the equilibrium interparticle spacing, where V attains its minimum that we assume is 0: $V(a) = 0$. It is convenient to work with interparticle distance as coordinates, rather than absolute particle position, so we define $\{r_j = q_j - q_{j-1} - a,\ j = 1, \dots, n\}$. Without loosing any generality, we will choose $a = 0$ for the sequence.

The configuration of the system is given by $\{p_j, r_j, j = 1, \dots, n\} \in \mathbb{R}^{2n}$, and energy function (Hamiltonian) defined on each configuration is given by

$$\mathcal{H} = \sum_{j=1}^{n} \mathcal{E}_j$$

where

$$\mathcal{E}_j = \frac{1}{2}p_j^2 + V(r_j), \quad j = 1, \dots, n$$

is the energy of each oscillator. This choice is a bit arbitrary, because we associate the potential energy of the bond $V(r_j)$ to the particle j. Different choices can be made, but this one is notationally convenient.

At the other end of the chain we apply a constant force $\tau \in \mathbb{R}$ on the particle n (tension). The position of the particle n is given by $q_n = \sum_{j=1}^n r_j$. We consider the Hamiltonian dynamics:

$$\begin{aligned} \dot{r}_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 1, \dots, n, \\ \dot{p}_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)), \qquad j = 1, \dots, n-1, \\ \dot{p}_n(t) &= \tau - V'(r_n(t)), \end{aligned} \tag{1.1.2}$$

It is easy to see that, for any $\beta > 0$, the grand canonical measure $\mu^{gc}_{\tau,\beta}$ defined by

$$d\mu^{n,gc}_{\tau,\beta} = \prod_{j=1}^n \frac{e^{-\beta(\mathcal{E}_j - \tau r_j)}}{\sqrt{2\pi\beta^{-1}}Z(\beta\tau, \beta)} dr_j dp_j \tag{1.1.3}$$

is stationary for this dynamics. The distribution $\mu^{n,gc}_{\tau,\beta}$ is called grand canonical Gibbs measure at temperature $T = \beta^{-1}$ and tension (or pressure) τ. Notice that $\{r_1, \dots, r_n, p_1, \dots, p_n\}$ are independently distributed under this probability measure.

Let us now fix a reference measure $\mu^{gc}_{\tau_0,\beta_0}$, corresponding to a given temperature $T_0 = \beta_0^{-1}$ and with external force τ_0. We define $\lambda_0 = \tau_0\beta_0$. If we consider the random vector $\mathbf{X}_j = (r_j, \mathcal{E}_j) \in \mathbb{R}\times\mathbb{R}\times\mathbb{R}_+$, then applying the result of appendix A, we obtain that the sum $\frac{1}{n}\sum_1^n \mathbf{X}_j$ has a large deviation function given by

$$I(r, \mathcal{E}) = \sup_{\lambda, \eta < \beta_0} \{\lambda r + \eta\mathcal{E} - \Lambda(\lambda, \eta; \lambda_0, \beta_0)\}$$

with

$$\Lambda(\lambda, \eta; \lambda_0, \beta_0) = \log\left(\frac{Z(\lambda + \lambda_0, \beta_0 - \eta)}{Z(\lambda_0, \beta_0)}\sqrt{\frac{\beta_0}{\beta_0 - \eta}}\right)$$

and $\Lambda(\lambda, \eta; \lambda_0, \beta_0) = +\infty$ if $\eta > \beta_0$.

Then we obtain

$$\begin{aligned} I(r, \mathcal{E}) = \sup_{\lambda, \beta > 0} &\left\{\lambda r - \beta\mathcal{E} - \log\left(\sqrt{2\pi\beta^{-1}}Z(\lambda, \beta)\right)\right\} \\ &- \lambda_0 r + \beta_0\mathcal{E} + \log\left(\sqrt{2\pi\beta_0^{-1}}Z(\lambda_0, \beta_0)\right) \end{aligned}$$

The function

$$S(r,u) = \inf_{\lambda,\beta>0}\left\{-\lambda r + \beta u + \log Z(\lambda,\beta) + \frac{1}{2}\log\frac{2\pi}{\beta}\right\} \tag{1.1.4}$$

is called *thermodynamic entropy.*

So we have obtained that

$$I(r,\mathcal{E}) = -S(r,\mathcal{E}) - \lambda_0 r + \beta_0\mathcal{E} + \log Z(0,\beta_0) + \frac{1}{2}\log\frac{2\pi}{\beta_0}$$

The density of the distribution of $\frac{1}{n}\sum_{j=1}^n \mathbf{X}_j$ under $\mu^{n,gc}_{\tau_0,\beta_0}$ is given by

$$\begin{aligned} f_n(r,\mathcal{E}) & \\ &= \int_{\mathbb{R}^{2n}} \frac{e^{-\beta_0\sum_j \mathcal{E}_j + \lambda_0 \sum_j r_j}}{(2\pi\beta_0^{-1})^{n/2} Z(\lambda_0,\beta_0)^n}\delta\left(\frac{1}{n}\sum_{j=1}^n \mathcal{E}_j - \mathcal{E}; \frac{1}{n}\sum_{j=1}^n r_j - r\right)\prod_j dr_j dp_j \\ &= \frac{e^{-n(\beta_0\mathcal{E}-\lambda_0 r)}}{(2\pi\beta_0^{-1})^{n/2} Z(\lambda_0,\beta_0)^n}\int_{\mathbb{R}^{2n}} \delta\left(\frac{1}{n}\sum_{j=1}^n \mathcal{E}_j - \mathcal{E}; \frac{1}{n}\sum_{j=1}^n r_j - r\right)\prod_j dr_j dp_j \\ &= \frac{e^{-n(\beta_0\mathcal{E}-\lambda_0 r)}}{(2\pi\beta_0^{-1})^{n/2} Z(\lambda_0,\beta_0)^n}\Gamma_n(r,\mathcal{E}). \end{aligned} \tag{1.1.5}$$

Observe that $\Gamma_n(r,\mathcal{E})$ defined by the equation above, does not depend on τ_0 and β_0. It is clearly sub–multiplicative

$$\Gamma_{n+m}(r,\mathcal{E}) \geq \Gamma_n(r,\mathcal{E})\Gamma_m(r,\mathcal{E})$$

that implies the existence of the limit

$$\lim_{n\to\infty}\frac{1}{n}\log\Gamma_n(r,\mathcal{E}) = S(r,\mathcal{E}) \ . \tag{1.1.6}$$

and applying (A.5.8) we identify as the thermodynamic entropy defined by (1.1.4). This is the fundamental relation that connects the microscopic system to its thermodynamic macroscopic description.

We can now define the other thermodynamic quantities from the entropy definition (1.1.4). From equation (1.1.4) we have

$$\lambda(r,u) = -\frac{\partial S(r,u)}{\partial r}, \qquad \beta(r,u) = \frac{\partial S(r,u)}{\partial u} \tag{1.1.7}$$

and we will always define the tension as $\tau(r,u) = \lambda(r,u)/\beta(r,u)$.

$$
\begin{aligned}
r(\lambda,\beta) &= \frac{\partial \log Z(\lambda,\beta)}{\partial\lambda} = \int r \,\frac{e^{\lambda r-\beta V(r)}}{Z(\lambda,\beta)}\, dr = \int r_j \; d\mu^{gc}_{\tau,\beta} \\
u(\lambda,\beta) &= -\frac{\partial \log\left(Z(\lambda,\beta)\sqrt{2\pi/\beta}\right)}{\partial\beta} = \int V(r)\frac{e^{\lambda r-\beta V(r)}}{Z(\lambda,\beta)}\, dr + \frac{1}{2\beta} = \int \mathcal{E}_j \; d\mu^{gc}_{\tau,\beta}
\end{aligned}
\tag{1.1.8}
$$

In thermodynamics is used the following terminology

- r is the *length*,
- u is the *internal energy*,
- $T = \beta^{-1}$ is the *temperature*,
- $\tau = \beta^{-1}\lambda$ is the pressure or the *tension* [16].

The above are the basic thermodynamics coordinates. Usually one choose two of these as independent variables, and express the others as functions of these.

Computing the total differential of $S(r,u)$ we have

$$
dS = -\beta\tau dr + \beta du = \frac{dQ}{T} \tag{1.1.9}
$$

where dQ is the (non-exact) differential

$$
dQ = -\tau dr + du \tag{1.1.10}
$$

and represents the energy gained (or lost) by the system under the infinitesimal change dr, du. In fact τdr is the infinitesimal *work* done on the system by the force τ to perform the infinitesimal displacement dr, while du is the infinitesimal change of *internal energy*, so that we can identify dQ as the energy exchanced from the system to the *exterior* during the *thermodynamic* infinitesimal change dr, du.

Equation (1.1.10) is the differential form of the *first law of thermodynamics*, while (1.1.9) is the one corresponding to the *second law of thermodynamics*.

1.2 Microcanonical measure

Instead of applying a force (tension) to one side of the chain, one can fix the particle n to another wall at distance nr ($q_n = \sum_{j=1}^n r_j = nr$ and $p_n = \dot{p}_n = 0$). The corresponding constrained dynamics is

$$\begin{aligned}
\dot{r}_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 1, \dots, n-1, \\
\dot{p}_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)), \qquad j = 1, \dots, n-1, \\
r_n(t) &= nr - \sum_{j=1}^{n-1} r_j(t)\ .
\end{aligned} \tag{1.2.1}$$

The dynamics now is conserving the total energy $\mathcal{H} = \sum_j \mathcal{E}_j = nu$ and the total length $\sum_{j=1}^n r_j = nr$. The microcanonical measures $\mu_{r,u}^{n,mc}$ are now stationary for this dynamics. These are defined in the following way:

Consider the vector valued i.i.d. random variables

$$\{\mathbf{X}_j = (r_j, \mathcal{E}_j), j = 1, \dots, n\},$$

distributed by $d\mu_{\tau_0,\beta_0}^{n,gc}$. Fix $\mathbf{x} = (r, u)$, and define $\mu_{\mathbf{x}}^{n,mc}$ the conditional distribution of $(r_1, p_1, \dots, r_n, p_n)$ on the manifold $\sum_{j=1}^n \mathbf{X}_j = n\mathbf{x}$. This is defined, for any bounded continuous function $G : \mathbb{R} \times \mathbb{R}_+ \to \mathbb{R}$ and $H : \mathbb{R}^{2n} \to \mathbb{R}$, by

$$\begin{aligned}
&\int G(\hat{\mathbf{S}}_n) H(r_1, p_1, \dots, r_n, p_n)\ d\mu_{\tau_0,\beta_0}^{n,gc}(r_1, p_1, \dots, r_n, p_n) \\
&= \int_{\mathbb{R}\times\mathbb{R}_+} d\mathbf{x}\ G(\mathbf{x}) f_n(\mathbf{x}) \int H(r_1, p_1, \dots, r_n, p_n)\ d\mu_{\mathbf{x}}^{n,mc}
\end{aligned}$$

where $\hat{\mathbf{S}}_n = \frac{1}{n} \sum_{i=1}^n \mathbf{X}_i$. It is easy to see that $\mu_{\mathbf{x}}^{n,mc}$ does not depend on τ_0, β_0. We call $\mu_{\mathbf{x}}^{n,mc}$ the *microcanonical measure*.

The multidimensional application of theorem A.5.4 gives the following *equivalence between microcanonical and grandcanonical measure*:

Theorem 1.2.1 *Given* $\mathbf{x} = (r, u)$, *let*

$$\beta = \beta(r, u), \qquad \tau = \lambda(r, u)\beta^{-1}.$$

Then for any bounded continuous function $F : \mathbb{R}^{2k} \to \mathbb{R}$ *we have*

$$\begin{aligned}
&\lim_{n\to\infty} \int F(r_1, p_1, \dots, r_k, p_k)\ d\mu_{\mathbf{x}}^{n,mc}(r_1, p_1, \dots, r_n, p_n) \\
&\qquad = \int F(r_1, p_1, \dots, r_k, p_k)\ d\mu_{\tau,\beta}^{gc}(\dots, r_1, p_1, \dots, r_n, p_n, \dots)
\end{aligned}$$

It will be useful later the equivalence of ensembles in the following form:

Theorem 1.2.2 *Under the same conditions of Theorem 1.2.1, assume that*

$$\int F(r_1, p_1, \dots, r_k, p_k)\, d\mu^{k,gc}_{\tau,\beta}(r_1, p_1, \dots, r_k, p_k) = 0.$$

Then

$$\lim_{n\to\infty} \int \left| \frac{1}{n-k} \sum_{i=1}^{n-k} F(r_i, p_i, \dots, r_{i+k}, p_{k+i}) \right| d\mu^{n,mc}_{\mathbf{x}} = 0$$

The proof of these two theorems follows the argument used for Theorems A.5.4 and A.5.5.

1.3 Canonical measure

Applying a Langevin's thermostat at temperature $T = \beta^{-1}$ to the particle n (or to any other particle), we obtain a dynamics that has the canonical measure $\mu^{n,c}_{r,\beta}$ as stationary measure:

$$\begin{aligned}
\dot r_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 1, \dots, n-1, \\
dp_j(t) &= \left(V'(r_{j+1}(t)) - V'(r_j(t))\right) dt \\
&\qquad + \delta_{j,n-1}\left(-p_j(t)dt + \sqrt{\beta} dw(t)\right), \qquad j = 1, \dots, n-1, \qquad (1.3.1)\\
r_n(t) &= nr - \sum_{j=1}^{n-1} r_j(t)\ .
\end{aligned}$$

This is defined as follows:

If we condition the grand canonical measure $\mu^{n,gc}_{0,0,\beta}$ on the total length of the chain equal to $L = nr = \sum_j r_j = q_n - q_0$, we obtain the canonical measure that we denote by $\mu^{n,c}_{r,\beta}$. We can formally write

$$d\mu^{n,c}_{r,\beta} = \prod_j \frac{e^{-\beta p_j^2/2}}{\sqrt{2\pi\beta^{-1}}} dp_j \otimes \frac{e^{-\beta \sum_j V(r_j)}}{Z_{n,c}(r,\beta)} \delta\left(\sum_j r_j = nr\right) \prod_j dr_j$$

where $Z_{n,c}(r, \beta)$ is the normalization constant (canonical partition function).

Similar statements as theorems 1.2.1 and 1.2.2 holds, $\mu^{n,c}_{r,\beta}$ converging to the grand-canonical measure $\mu^{n,gc}_{\tau,\beta}$, with τ given by the thermodynamic relations (1.1.7).

Other boundary conditions can be made, like applying a tension τ and a Langevin thermostat at temperature β^{-1} to the n particle, obtaining a system with $\mu^{gc}_{\tau,\beta}$ as stationary measure.

1.4 Local equilibrium, local Gibbs measures

The Gibbs distributions defined in the above sections are also called equilibrium distributions for the dynamics. Studying the non-equilibrium behaviour we need the concept of local equilibrium distributions. These are probability distributions that have some asymptotic properties when the system became large ($n \to \infty$), vaguely speaking *locally* they look like Gibbs measure. We need a precise mathematical definition, that will be useful later for proving macroscopic behaviour of the system.

Definition 1.4.1 *Given two functions $\beta(y) > 0, \tau(y), y \in [0,1]$, we say that the sequence of probability measures μ_n on $\mathbb{R}^{2n}$ has the local equilibrium property (with respect to the profiles $\beta(\cdot), \tau(\cdot)$) if for any $k > 0$ and $y \in (0,1)$,*

$$\lim_{n\to\infty} \mu_n\big|_{([ny],[ny]+k)} = \mu^{k,gc}_{\tau(y),\beta(y)} \tag{1.4.1}$$

Sometimes we will need some weaker definition of local equilibrium (for example relaxing the pointwise convergence in y). It is important here to understand that *local equilibrium* is a property of a *sequence* of probability measures.

The most simple example of local equilibrium sequence is given by the local Gibbs measures:

$$\prod_{j=1}^{n} \frac{e^{-\beta(j/n)(\mathcal{E}_j - \tau(j/n) r_j)}}{\sqrt{2\pi\beta(j/n)^{-1}} Z(\beta(j/n)\tau(j/n), \beta(j/n))} dr_j dp_j = g^n_{\tau(\cdot),\beta(\cdot)} \prod_{j=1}^{n} dr_j dp_j \tag{1.4.2}$$

Of course are local equilibrium sequence also *small order* perturbation of this sequence like

$$e^{\sum_j F_j(r_{j-h},p_{j-h},\dots,r_{j+h},p_{j+h})/n} g^n_{\tau(\cdot),\beta(\cdot)} \prod_{j=1}^{n} dr_j dp_j \tag{1.4.3}$$

where F_j are local functions.

To a local equilibrium sequence we can associate a thermodynamic entropy, defined as

$$S(r(\cdot), u(\cdot)) = \int_0^1 S(r(y), u(y))\, dy \tag{1.4.4}$$

where $r(y), u(y)$ are computed from $\tau(y), \beta(y)$ using (1.1.8).

Chapter 2

Dynamics

In this chapter we study the dynamics of the infinite chain and we set the problem of its ergodicity. We need first to give a proper definition of ergodicity for an infinite dynamics. We need some stochastic perturbation in order to prove something about this ergodicity. We introduce then some stochastic perturbation acting only on the velocities such that will conserve the total energy and momentum of the chain.

2.1 Dynamics of the infinite system

In order to avoid technical difficulties we assume the potential V satisfies

$$V'(r)^2 \le CV(r), \qquad V''(r) \le C \tag{2.1.1}$$

Basically we require that V grows to infinity quadratically.

We consider now the system in the infinite lattice $\mathbb{Z}$. As before, $r_j = q_j - q_{j-1}$ is the interparticle distance. Let us denote $\Omega = (\mathbb{R}^2)^{\mathbb{Z}}$ the configuration space and $\omega = (p_i, r_i)_{i\in\mathbb{Z}} \in \Omega$ the generic configuration. We introduce the space $C_0^k(\Omega)$ composed of local functions which are k differentiable with continuous bounded derivatives and $\mathcal{D}(\Omega) = \cap_{k\ge 0} C_0^k(\Omega)$.

The hamiltonian dynamics is given by the solution of the infinite system of differential equations

$$\begin{aligned} \dot r_j(t) &= p_j(t) - p_{j-1}(t) \\ \dot p_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)), \qquad j \in \mathbb{Z}. \end{aligned} \tag{2.1.2}$$

and the formal *generator* of the dynamics is the Liouville operator

$$\mathcal{A} = \sum_{j\in\mathbb{Z}} \left\{ (p_j - p_{j-1})\, \partial_{r_j} + (V'(r_{j+1}) - V'(r_j))\, \partial_{p_j} \right\} \tag{2.1.3}$$

with domain $\mathcal{D}(\Omega)$.

The existence of the solution for (2.1.2) can be proven for a wide class of initial conditions, in particular for a set of configurations that has measure one for any Gibbs grand-canonical distribution

$$d\mu^{gc}_{\tau,\bar{p},\beta} = \prod_{j\in\mathbb{Z}} \frac{e^{-\beta(\mathcal{E}_j - \bar{p}p_j - \tau r_j)}}{\mathcal{Z}(\beta\tau, \beta\bar{p}, \beta)} dr_j dp_j \ . \tag{2.1.4}$$

for all parameters $\tau, \bar{p}, \beta > 0$. We will prove this existence by an iteration scheme. Notice that the momentum is formally conserved, which follows from the translation invariance of the dynamics. This is why we have the third parameter $\bar{p}$ in the stationary measures.

A set of initial conditions can be defined in the following way. For $a > 0$, we denote

$$\Omega_a = \left\{ \omega = (r_j, p_j)_{j\in\mathbb{Z}} \in (\mathbb{R}^2)^{\mathbb{Z}} \ : \ \|\omega\|_a^2 = \sum_{j\in\mathbb{Z}} (p_j^2 + r_j^2) e^{-a|j|} < \infty \right\}$$

the Hilbert space equipped with the norm $\|\cdot\|_a$. It is easy to check that any probability measure ν such that $\int (r_j^2 + p_j^2) d\nu \leq C e^{bj}$ with $b < a$ gives measure one to Ω_a. In particular any Gibbs measure $\mu^{gc}_{\tau,\bar{p},\beta}$ satisfies this condition since

$$\int r^2 e^{-\beta(V(r) - \tau r)} dr \leq C\left[Z(\tau\beta + 1, \beta) + Z(\tau\beta - 1, \beta)\right]$$

We also introduce the Banach space $\mathcal{H}_a$ composed of all continuous Ω_a-valued functions ω on the time interval $[0, T]$ with norm

$$N(\omega) = \sup_{t\in[0,T]} \|\omega(t)\|_a$$

The two next lemmas are proved in a more general context in section 2.3.

Lemma 2.1.1 *For any $\sigma \in \Omega_a$, there exists a unique stochastic process $\omega(\cdot, \sigma) = (r_i(\cdot), p_i(\cdot))_{i\in\mathbb{Z}}$ belonging to $\mathcal{H}_a$ and satisfying (2.3.5) with initial condition $\omega(0, \sigma) = \sigma$. The application $\sigma \in \Omega_a \to \omega(\cdot, \sigma) \in \mathcal{H}_a$ is continuously differentiable.*

For any $\omega \in \Omega_a$, the quantity $\left[\sum_j e^{-a|j|}\mathcal{E}_j(\omega)\right]$ is finite (thanks to (2.1.1)). Starting from ω, (2.1.1) gives

$$\frac{d}{dt}\left(\sum_{j\in\mathbb{Z}} e^{-a|j|}\mathcal{E}_j(\omega(t))\right) \leq C \sum_{j\in\mathbb{Z}} e^{-a|j|}\mathcal{E}_j(\omega(t)) \tag{2.1.5}$$

and then the following a priori bound

$$\left[\sum_{j\in\mathbb{Z}} e^{-a|j|}\mathcal{E}_j(\omega(t))\right] \le C_0 e^{c_1 t}\left[\sum_{j\in\mathbb{Z}} e^{-a|j|}\mathcal{E}_j(\omega)\right] \tag{2.1.6}$$

We define a semigroup $(P_t)_{t\geq 0}$ on the space $B(\Omega_a)$ of bounded measurable functions on Ω_a by:

$$\forall f \in B(\Omega_a), \quad \forall \sigma \in \Omega_a, \quad (P_t f)(\sigma) = f(\omega(t,\sigma))$$

where $\omega(t,\sigma) = \{r_j(t), p_j(t);\ j \in \mathbb{Z}\}$ is the solution of (2.1.2) starting from σ.

We have the following lemma

Lemma 2.1.2 *Stationary states μ satisfying the moment condition*

$$\sup_{j\in\mathbb{Z}} \int \mathcal{E}_j d\mu < +\infty \tag{2.1.7}$$

are characterized by the stationary Kolmogorov equation:

$$\int \mathcal{A}\phi(\omega)d\mu(\omega) = 0 \textit{ for } \ \phi \in \mathcal{D}(\Omega)$$

The moment condition (2.3.3) is here to ensure that the support of μ is included in $\cap_{a>0}\Omega_a$.

2.2 Ergodicity

Ergodicity is one of the main open problem for Hamiltonian systems, in fact we think there is not a general agreement on what it means for an infinite system.

For us *ergodicity* will mean a characterization of the stationary translation invariant probability measure, in a class of *locally regular* measure, as convex combination of Gibbs measures.

Definition 2.2.1 *We say that the dynamics defined by (2.1.2) is ergodic if any probability measure ν on the configuration space that*

1. *has finite density entropy :* $\exists C > 0, \forall \Lambda \Subset \mathbb{Z}, \quad H_\Lambda(\nu|\mu^{gc}_{0,0,1}) \le C|\Lambda|$

2. is translation invariant,

3. is stationary, i.e. for any function $F(r,p) \in \mathcal{D}(\Omega)$

$$\int \mathcal{A}F \; d\nu = 0 \tag{2.2.1}$$

is a convex combination of Gibbs measures $\mu^{gc}_{\tau,\bar{p},\beta}$.

Remark 2.2.2 *In the first assumption $\mu^{gc}_{0,0,1}$ does not play any role and can be replaced by any Gibbs measure $\mu^{gc}_{\tau,\bar{p},\beta}$.*

It is clear that this property is not always true. The easier example is the harmonic case, i.e. V quadratic. We are tempted to conjecture that for generic non-linear dynamics the system is ergodic. But for Toda lattice interaction $V(r) = ae^r - r - b$, the dynamics is completely integrable in its finite dimensional version (like the harmonic case) and constitute another conterexample. So it is not clear on which class of anharmonic V the ergodic property can be conjectured.

The idea is that the nonlinearity should mess up sufficiently the distribution of the velocity.

Theorem 2.2.3 *Let ν satisfy the three conditions of definition 2.2.1, and furthermore the distribution of the velocities conditioned to the position $\nu(dp|r)$ is excheangeable. Then ν is a convex combination of Gibbs measures $\mu^{gc}_{\tau,\bar{p},\beta}$.*

Let $\mathcal{F}_{inv}$ be the σ-field of the sets of Ω invariant for translations.

Lemma 2.2.4 *If ν is a translation invariant probability measure on Ω such that $\nu(dp|r)$ is exchangeable then conditionally to $\mathcal{F}_{inv}$ the p's and the r's.*

Proof:

Let $\mathcal{F}_k$ be the σ-field generated by $\{\omega_x, x \in \{-k, \dots, k\}\}$. A measurable transformation $T : \Omega \to \Omega$ is called local if $T(\omega)$ is $\mathcal{F}_k$-measurable for some $k \geq 1$. For example the map $T_{x,y} : (p,r) \to (p^{x,y}, r)$, where $p^{x,y}$ is the configuration of velocities obtained by the exchange of p_x and p_y, is a local transformation. Any bounded function θ is the limit of $\theta_k = \nu(\theta|\mathcal{F}_k)$ as $k \to \infty$ a.s. and in mean square. Let θ be a bounded $\mathcal{F}_{inv}$-measurable function. Then $\theta = \nu(\theta|\mathcal{F}_{inv}) = \lim_{k\to\infty} \nu(\theta_k|\mathcal{F}_{inv})$ a.s. and in mean square and using the ergodic theorem we have

$$\theta = \lim_{k\to\infty} \lim_{N\to\infty} \frac{1}{2N+1} \sum_{j=-N}^{N} \tau_j \theta_k \tag{2.2.2}$$

Since θ_k is a local function for any k this shows that any $\mathcal{F}_{inv}$-measurable function is in fact invariant w.r.t. any local transformation T.

Let $\phi(r)$ and $\psi(p)$ be two bounded local functions depending respectively only on the velocities and on the positions. Let θ be a bounded $\mathcal{F}_{inv}$-measurable function. Consider two integers k and j. Since ψ is local there exists a local transformation T_k obtained as the composition of exchange transformations $T_{x,y}$ such that $T_k p = \tau_k p$. Let $\chi_k(r) = \nu(\psi(\tau_k p)\theta(p,r)|r)$ and observe that $\chi_0(r) = \nu\left(\psi(T_k p)\theta(T_k p, r)|r\right) = \nu\left(\psi(\tau_k p)\theta(p,r)|r\right) = \chi_k(r)$ because $\nu(dp|r)$ is T_k-invariant and θ is T_k-invariant.

We have

$$\begin{aligned}
\int \phi(r)\psi(p)\, \theta(p,r)\, d\nu &= \int \nu(\phi\psi|\mathcal{F}_{inv})\, \theta\, d\nu \\
&= \int \phi(r)\chi_0(r)\, d\nu = \int \phi(r)\chi_k(r)\, d\nu \\
&= \int \phi(\tau_j r)\chi_k(\tau_j r)\, d\nu = \int \phi(\tau_j r)\psi(\tau_k p)\theta(p,r)\, d\nu
\end{aligned}$$

We now sum over $j, k = -N \dots N$ and divide by $(2N+1)^2$. Taking the limit $N \to \infty$ ergodic theorem implies

$$\int \nu(\phi\psi|\mathcal{F}_{inv})\theta\, d\nu = \int \nu(\phi|\mathcal{F}_{inv})\mu(\psi|\mathcal{F}_{inv})\theta\, d\nu \tag{2.2.3}$$

and the claim is proved.

□

Because ν has finite entropy density the entropy inequality (proposition B.1.1) gives the following bound on the energy density

$$\exists C > 0, \forall j \in \mathbb{Z}, \qquad \int \mathcal{E}_j d\nu \le C \tag{2.2.4}$$

Then the ergodic theorem allows us to define ν a.s. the following quantities

$$
\begin{aligned}
z_0 &= \lim_{\ell\to\infty} z_0^\ell = \lim_{\ell\to\infty} \frac{1}{\ell}\sum_{j=1}^{\ell} r_j = \nu(r_j|\mathcal{F}_{inv})\\
z_1 &= \lim_{\ell\to\infty} z_1^\ell = \lim_{\ell\to\infty} \frac{1}{\ell}\sum_{j=1}^{\ell} p_j = \nu(p_j|\mathcal{F}_{inv})\\
z_2 &= \lim_{\ell\to\infty} z_2^\ell = \lim_{\ell\to\infty} \frac{1}{\ell}\sum_{j=1}^{\ell} p_j^2 = \nu(p_j^2|\mathcal{F}_{inv})
\end{aligned}
$$

and we denote by $\mathbf{z}(r,p) = (z_0, z_1, z_2)$ the corresponding random vector (with values on $\mathbb{R}\times\mathbb{R}\times\mathbb{R}_+$). Denote $\hat\beta$ the $\mathcal{F}_{inv}$-measurable function defined by

$$
\hat\beta^{-1} = \nu(p_j(p_j - z_1)|\mathcal{F}_{inv}) = z_2 - z_1^2 \tag{2.2.5}
$$

and observe that

$$
\hat\beta^{-1}\delta_{i,j} = \nu(p_i(p_j - z_1)|\mathcal{F}_{inv}) \tag{2.2.6}
$$

Let us first show that the degenerate situation of null temperature: $\hat\beta^{-1} = 0$ is impossible. We have

Lemma 2.2.5 *Let ν a translation invariant measure with finite entropy density. Then ν a.s. we have $z^2 - z_1^2 > 0$.*

Proof :

Let $A_{\ell,\varepsilon}$ be the event

$$
A_{\ell,\varepsilon} = \left\{ \left| \frac{1}{\ell}\sum_{j=1}^{\ell} p_j^2 - \left(\frac{1}{\ell}\sum_{j=1}^{\ell} p_j\right)^2 \right| \le \varepsilon \right\} \in \mathcal{F}_{\Lambda_\ell}
$$

By the entropy inequality we have

$$
\nu(A_{\ell,\varepsilon}) \le \frac{\log 2 + H_{\Lambda_\ell}(\nu|\mu)}{\log(1+\mu(A_{\ell,\varepsilon})^{-1})} \le \frac{C_0\ell}{\log(1+\mu(A_{\ell,\varepsilon})^{-1})} \tag{2.2.7}
$$

for some constant C_0 independent of ℓ. Moreover it is well known that

$$
\frac{1}{\ell}\sum_{j=1}^{\ell} p_j^2 - \left(\frac{1}{\ell}\sum_{j=1}^{\ell} p_j\right)^2 = \frac{1}{\ell}\sum_{j=1}^{\ell}\left(p_j - \left(\frac{1}{\ell}\sum_{j=1}^{\ell} p_j^2\right)^2\right)
$$

has the same law as $\ell^{-1}\sum_{j=1}^{\ell-1} p_j^2$. By Cramer theorem A.2.3 we have

$$\mu(A_{\ell,\varepsilon}) = \mu\left(\ell^{-1}\sum_{j=1}^{\ell-1} p_j^2 \leq \varepsilon\right) \sim e^{-\ell \inf_{x\leq\varepsilon} I(x)}$$

where I is the large deviations rate function associated to $(p_j^2)_{j=1,\dots,\ell}$. A simple computation shows that $\inf_{x\leq\varepsilon} I(x) = I(\varepsilon)$ goes to $+\infty$ as $\varepsilon \to 0$. Letting first ℓ going to $+\infty$ and then $\varepsilon \to 0$ we get

$$\nu(z_2 - z_1^2 = 0) = 0$$

□

Lemma 2.2.6 *For any function $F \in \mathcal{D}(\Omega)$ and any bounded $\mathcal{F}_{inv}$-measurable function h we have*

$$\int h(r,p)\, \mathcal{A}F(r,p)\, d\nu(r,p) = 0\ .$$

Proof: Clearly it is sufficient to prove the lemma for h in the form $h(\omega) = \pi(p)\rho(r)$ where π (resp. ρ) is a bounded $\mathcal{F}_{inv}$-measurable functions of the p's (resp. of the r's). We use the following approximations similar to (2.2.2) for π and ρ:

$$\pi(p) = \lim_{k\to\infty} \pi_k^{(N)}(p) = \lim_{k\to\infty}\lim_{N\to\infty} \frac{1}{2N+1}\sum_{j=-N}^{N} \tau_j \pi_k(p)$$

$$\rho(r) = \lim_{k\to\infty} \rho_k^{(N)}(r) = \lim_{k\to\infty}\lim_{N\to\infty} \frac{1}{2N+1}\sum_{j=-N}^{N} \tau_j \rho_k(r)$$

where π_k (resp. ρ_k) is a smooth local function measurable w.r.t. the σ-filed $\mathcal{F}_k^p$ (resp. $\mathcal{F}_k^r$) generated by (p_x), $x \in \{-k,\dots,k\}$ (resp. (r_x), $x \in \{-k,\dots,k\}$). In fact the local function π_k (resp. ρ_k) is a smooth approximation of $\nu(\pi|\mathcal{F}_k^p)$ (resp. $\nu(\rho|\mathcal{F}_k^r)$).

Since π_k, ρ_ℓ and F are smooth functions, (2.2.1) implies

$$\int \pi_k^{(N)}\rho_\ell^{(M)}\mathcal{A}F\, d\nu \;=\; -\int F\left[\mathcal{A}\pi_k^{(N)}\,\rho_\ell^{(M)} + \pi_k^{(N)}\mathcal{A}\rho_\ell^{(M)}\right] d\nu$$

Observe that

$$\mathcal{A}(\pi_k^{(N)}) = \frac{1}{2N+1}\sum_{j=-N}^{N}\tau_j\left[\sum_{i\in\mathbb{Z}}(V'(r_{i+1}) - V'(r_i))\partial_{p_i}\pi_k\right]$$

converges ν a.s. as N goes to infinity to

$$\nu\left(\sum_{i\in\mathbb{Z}}(V'(r_{i+1})-V'(r_i))\partial_{p_i}\pi_k|\mathcal{F}_{inv}\right)=\sum_{i\in\mathbb{Z}}\nu\left((V'(r_{i+1})-V'(r_i))|\mathcal{F}_{inv}\right)\nu\left(\partial_{p_i}\pi_k|\mathcal{F}_{inv}\right)=0$$

by lemma 2.2.4. Hence we have

$$\lim_{k\to\infty}\lim_{N\to\infty}\int\pi_k^{(N)}\rho_\ell^{(M)}\mathcal{A}F\,d\nu=-\int F\pi\mathcal{A}\rho_\ell^{(M)}d\nu$$

and similarly we have that $\mathcal{A}\rho_\ell^{(M)}$ converges ν a.s. as M goes to infinity to 0. It follows that

$$\int\pi\rho\mathcal{A}F d\nu=\lim_{\ell\to\infty}\lim_{M\to\infty}\lim_{k\to\infty}\lim_{N\to\infty}\int\pi_k^{(N)}\rho_\ell^{(M)}\mathcal{A}F\,d\nu=0$$

which completes the proof. □

Proof of Theorem 2.2.3.

It follows from lemma 2.2.6 that for every $F(r,p)\in\mathcal{D}(\Omega)$

$$\int\mathcal{A}F(r,p)\,d\nu(r,p|\mathcal{F}_{inv})=0\ . \tag{2.2.8}$$

Choosing in (2.2.8) the function

$$F=(p_j-z_1)\phi(r)$$

with $\phi(r)\in\mathcal{D}(\mathbb{R}^{\mathbb{Z}})$ that we specify later, we obtain by lemma 2.2.4

$$\begin{aligned}0&=\int\left\{\sum_i(p_j-z_1)p_i\left(\partial_{r_i}\phi-\partial_{r_{i+1}}\phi\right)+\left(V'(r_{j+1})-V'(r_j)\right)\phi(r)\right\}\,d\nu(r,p|\mathcal{F}_{inv})\\&=\sum_i\left(\int(p_j-z_1)p_i\nu(dp|\mathcal{F}_{inv})\right)\left(\int\left(\partial_{r_i}\phi-\partial_{r_{i+1}}\phi\right)d\nu(r|\mathcal{F}_{inv})\right)\\&\quad+\int\left(V'(r_{j+1})-V'(r_j)\right)\phi(r)\,d\nu(r|\mathcal{F}_{inv})\\&=\int\left\{\hat\beta^{-1}\left(\partial_{r_j}\phi-\partial_{r_{j+1}}\phi\right)+\left(V'(r_{j+1})-V'(r_j)\right)\phi(r)\right\}\,d\nu(r|\mathcal{F}_{inv})\ .\end{aligned} \tag{2.2.9}$$

Define

$$\psi_\ell(r)=e^{\sum_{i=1}^{\ell}(\hat\beta V(r_i)-\hat\lambda r_i)}$$

where $\hat{\lambda} = \lambda(z_0, \hat{\beta})$. Notice that $\hat{\lambda}$ and $\hat{\beta}$ are just function of $\mathbf{z}$, so we can treat them as constant under $\nu(dr|\mathcal{F}_{inv})$. Choosing

$$\phi(r) = \chi(r)\psi_\ell(r),$$

with $\chi(r)$ a local smooth function, we get for any $j = 1, \dots, \ell - 1$:

$$\int \hat{\beta}^{-1} \left(\partial_{r_j}\chi - \partial_{r_{j+1}}\chi\right) \psi_l(r)\, d\nu(r|\mathcal{F}_{inv}) = 0 \ .$$

We choose now

$$\chi(r) = \chi_b(r) g\left(\sum_{i=1}^{\ell} r_i\right) \chi_0(r_1, \dots, r_{\ell-1}),$$

where χ_b is a local function not depending on $r_1, \dots, r_\ell$, and g is a smooth function on $\mathbb{R}$. Since

$$\partial_{r_j}\chi(r) - \partial_{r_{j+1}}\chi(r) = \chi_b(r) g\left(\sum_{i=1}^{\ell} r_i\right) \left(\partial_{r_j}\chi_0(r) - \partial_{r_{j+1}}\chi_0(r)\right)$$

if $j = 1, \dots, \ell - 1$, we can further condition on $\sum_{k=1}^{\ell} r_k = \ell u$ and on the exterior configuration $\{r_i, i \neq 1, \dots, \ell\}$, and obtain, for all $j = 1, \dots, \ell - 1$,

$$\begin{aligned}\int \big(\partial_{r_j}\chi_0(r) - \partial_{r_{j+1}}\chi_0(r)\big)\psi_l(r) \\ \nu\left(dr_1, \dots, dr_\ell \Big| \sum_{k=1}^{\ell} r_k = \ell u, r_i,\ i \neq 1, \dots, \ell, \mathcal{F}_{inv}\right) = 0\end{aligned} \tag{2.2.10}$$

This is enough to characterize the measure

$$\begin{aligned}\psi_l(r)\nu\left(dr_1, \dots, dr_\ell \Big| \sum_{k=1}^{\ell} r_k = \ell u, r_i,\ i \neq 1, \dots, \ell, \mathcal{F}_{inv}\right) = \\ = e^{-\ell\hat{\lambda}r} \prod_{i=1}^{\ell} e^{\hat{\beta}V(r_i)} \nu\left(dr_1, \dots, dr_\ell \Big| \sum_{k=1}^{\ell} r_k = \ell u, r_i,\ i \neq 1, \dots, \ell, \mathcal{F}_{inv}\right)\end{aligned}$$

as the Lebesgue measure on the hyperplane $\{(r_1, \dots, r_\ell) : \sum_{k=1}^{\ell} r_k = \ell u\}$ (up to a multiplicative constant). In particular it follows that

$$\nu(dr_1, \dots, dr_\ell | r_i,\ i \neq 1, \dots, \ell, \mathcal{F}_{inv}) = \frac{e^{-\sum_{i=1}^{\ell}(\hat{\beta}V(r_i) - \hat{\lambda}r_i)}}{Z(\hat{\lambda}, \hat{\beta})^{\ell}} dr_1 \dots dr_\ell.$$

which implies

$$\nu(dr|\mathcal{F}_{inv}) = \prod_{j\in\mathbb{Z}} \frac{e^{-(\hat{\beta}V(r_i)-\hat{\lambda}r_i)}}{Z(\hat{\lambda},\hat{\beta})} \tag{2.2.11}$$

Similarly, choosing in (2.2.8) the function

$$F = \psi(p)(r_j - z_0)$$

we have

$$0 = \int \left\{ (p_j - p_{j-1})\psi(p) + \sum_i \left(V'(r_{i+1}) - V'(r_i)\right)(r_j - z_0)\partial_{p_i}\psi(p) \right\} \, d\nu(r,p|\mathcal{F}_{inv}) \tag{2.2.12}$$

Since

$$\begin{aligned} &\int V'(r_i)(r_j - z_0)\partial_{p_i}\psi(p) \, d\nu(r,p|\mathcal{F}_{inv}) \\ = &\int d\nu(r|\mathcal{F}_{inv})V'(r_i)(r_j - z_0)\left(\int \partial_{p_i}\psi(p)\nu(dp|\mathcal{F}_{inv})\right) \\ &= \delta_{i,j}\hat{\beta}^{-1}\int \partial_{p_i}\psi(p) \, d\nu(p|\mathcal{F}_{inv}) \end{aligned}$$

and (2.2.12) became

$$\int \left\{ (p_j - p_{j-1})\psi(p) + \beta^{-1}(\partial_{p_j} - \partial_{p_j})\psi(p) \right\} \, d\nu(p|\mathcal{F}_{inv}) = 0 \tag{2.2.13}$$

which is enough to characterise $d\nu(p|\mathcal{F}_{inv})$ as

$$\nu(dp|\mathcal{F}_{inv}) = \prod_{j\in\mathbb{Z}} \frac{e^{-\hat{\beta}(p_i - z_1)^2/2}}{\sqrt{2\pi\hat{\beta}^{-1}}} \tag{2.2.14}$$

and finally we have by lemma 2.2.4

$$\nu(dr,dp|\mathcal{F}_{inv}) = \nu(dr|\mathcal{F}_{inv})\nu(dp|\mathcal{F}_{inv}) = \mu^{gc}_{\mathbf{z}} \tag{2.2.15}$$

□

2.3 Conservative stochastic dynamics

The proof exposed in section 2.2 is based on the assumption that the stationary distribution of the velocity, conditioned on the positions, are convex combination of gaussians. Nowhere we used the non-linearity of the interaction, that in a hamiltonian deterministic dynamics should be the cause of such mixing of velocities. This is a very difficult problem, that we do not even know how to attack mathematically. We choose an easier path here which is to approximate the mixing effect due the non-linearities of the dynamics by adding some stochastic terms to it. The porpouse of this stochastic term is to create this mixing of the velocities so that we can apply the argument of section 2.2. We also would like that the total momentum and total energy is conserved by this stochastic mechanism, and that has a *local* nature. A simple way is to exchange the momentum of each consecutive particles p_j, p_{j+1}, in such way that $p_j + p_{j+1}$ and $p_j^2 + p_{j+1}^2$ are both conserved. Define the exchange operators acting on functions $f : \Omega \to \mathbb{R}$ by

$$(Y_{i,j} f)(r,p) = f(r, p^{j,k}) - f(r,p) \tag{2.3.1}$$

and for consecutive particles

$$Y_i = Y_{i,i+1}$$

We define now the operator

$$\mathcal{S} = \sum_i Y_i \tag{2.3.2}$$

The energy-momentum conservative infinite dynamics is defined as the Markov process on $\Omega = (\mathbb{R}^2)^{\mathbb{Z}}$ generated by the formal generator

$$\mathcal{L} = \mathcal{A} + \gamma \mathcal{S}. \tag{2.3.3}$$

In this section we show the following ergodic property for the infinite stochastic dynamics:

Theorem 2.3.1 *Let ν a translation invariant probability measure, stationary for the dynamics generated by $\mathcal{L}$. Assume that there exist a finite constant C such that*

$$H_\Lambda(\nu|\mu) \le C|\Lambda| \tag{2.3.4}$$

Then ν is a convex combination of grand canonical measures.

The ode describing the evolution are now substiuted by the following stochastic differential equations:

$$\begin{aligned}
dr_j(t) &= p_j(t) - p_{j-1}(t)dt \\
dp_j(t) &= (V'(r_{j+1}(t) - V'(r_j(t)))dt \\
&\quad + \sqrt{\gamma}\,(p_{j+1}(t-) - p_j(t-))\,dN_{j,j+1}(t) + \sqrt{\gamma}\,(p_{j-1}(t-) - p_j(t-))\,dN_{j-1,j}(t), \qquad j \in \mathbb{Z}.
\end{aligned} \tag{2.3.5}$$

where $N(t) = (N_{j,j+1}(t))_{j\in\mathbb{Z}}$ are independent standard Poisson processes.

The existence of the infinite dynamics is done similarly to the deterministic case. To get the approximation by finite dimensional dynamics one defines a dynamics generated by $\mathcal{L}_n = \mathcal{A}_n + \gamma \mathcal{S}_n$, then we prove that this converges to the infinite dynamics in a set of initial conditions that has measure one for any Gibbs measure. Notice that also here all Gibbs measure with null momentum average are stationary for these finite dynamics.

For the set of initial conditions we choose as in the deterministic case the Hilbert space

$$\Omega_a = \left\{ \omega = (r_j, p_j)_{j\in\mathbb{Z}} \in (\mathbb{R}^2)^{\mathbb{Z}} \ : \ \|\omega\|_a^2 = \sum_{j\in\mathbb{Z}} (p_j^2 + r_j^2) e^{-a|j|} < \infty \right\}, \quad a > 0$$

equipped with the norm $\|\cdot\|_a$. The set Ω_a has measure one with respect to any Gibbs measure. In the following lemma, the expectation $\mathbb{E}$ is the probability measure corresponding to the sequence of independent Poisson processes $N = (N_{j,j+1})_{j\in\mathbb{Z}}$. We also introduce the Banach space $\mathcal{H}_a$ composed of all predictable Ω_a-valued processes ω on the time interval $[0, T]$ with norm

$$N(\omega) = \left[\mathbb{E} \left(\sup_{t\in[0,T]} \|\omega(t)\|_a^2 \right) \right]^{1/2}$$

Lemma 2.3.2 *For any $\sigma \in \Omega_a$, there exists a unique stochastic process $\omega(\cdot, \sigma) = (r_i(\cdot), p_i(\cdot))_{i\in\mathbb{Z}}$ belonging to $\mathcal{H}_a$ and satisfying (2.3.5) with initial condition $\omega(0, \sigma) = \sigma$. The application $\sigma \in \Omega_a \to \omega(\cdot, \sigma) \in \mathcal{H}_a$ is continuously differentiable and the derivatives satisfy the linearized equations associated to (2.3.5).*

Proof The proof relies on the classical iteration procedure in Banach spaces. It is standard and we only sketch the proof. Let us write (2.3.5) in the form

$$d\omega(t) = F(\omega(t))dt + B(\omega(t))dN(t) \tag{2.3.6}$$

where $F : \Omega_a \to \Omega_a,\ B : \Omega_a \to \Omega_a$ are suitable functions whose exact expression is not used. Using (2.1.1) it is not difficult to see that the map

$$\begin{array}{rcl} \mathcal{K} : \Omega_a \times \mathcal{H}_a & \to & \mathcal{H}_a \\ (\sigma, \omega) & \to & \sigma + \int_0^{\cdot} F(\omega(s))ds + \int_0^{\cdot} B(\omega(s))dN(s) \end{array}$$

is such that

$$N\left(\mathcal{K}(\sigma,\omega) - \mathcal{K}(\sigma,\omega')\right) \leq \frac{1}{2} N(\omega - \omega')$$

if T is sufficiently small. By Picard's fixed point theorem there exists a unique $\omega \in \mathcal{H}_a$ such that $\mathcal{K}(\sigma,\omega) = \omega$. This establish the existence and uniqueness of $\omega(\cdot,\sigma)$ for short time interval. Iterating the procedure gives the existence (and uniqueness) for all times.

To get the differentiability with respect to initial conditions we observe that $\omega(\cdot,\sigma)$ satisfies

$$\mathcal{K}(\sigma, \omega(\cdot,\sigma)) - \omega(\cdot,\sigma)) = 0 \tag{2.3.7}$$

and that local inversion theorem is valid because of the assumption (2.1.1). This implies the claim. □

Starting from an initial configuration $\omega \in \Omega_a$, conservation of the energy by the dynamics gives the following a priori bound

$$\mathbb{E}_\omega \left[\sum_j e^{-a|j|} \mathcal{E}_j(\omega(t)) \right] \leq C_0 e^{c_1 t} \left[\sum_j e^{-a|j|} \mathcal{E}_j(\omega) \right] \tag{2.3.8}$$

By this way we define a semigroup $(P^t)_{t\geq 0}$ on $C_0(\Omega_a)$

$$\forall f \in B(\Omega_a),\ \forall \sigma \in \Omega_a, \quad (P^t f)(\sigma) = \mathbb{E}_\omega \left[f(\omega(t,\sigma) \right]$$

where $\omega(t,\sigma) = \{r_j(t), p_j(t);\ j \in \mathbb{Z}\}$ is the solution of (2.3.5).

By Itô's formula we have that if f is two times differentiable with bounded derivatives then

$$(P^t f)(\sigma) = f(\sigma) + \int_0^t (P^s \mathcal{L} f)(\sigma) ds \tag{2.3.9}$$

Moreover if $f \in C_0^2(\Omega_a)$ and $t \geq 0$ then by lemma 2.3.2 the function $g = P^t f$ is two times differentiable with bounded derivatives. By (2.3.9) we have the forward Kolmogorov equation

$$(P^h g)(\sigma) - g(\sigma) = \int_0^h (P^s \mathcal{L} g)(\sigma) ds$$

and the function $s \to (P^s \mathcal{L}g)(\sigma)$ is continuous because $\omega(\cdot,\sigma)$ has continuous trajectories and $\mathcal{L}g$ is a bounded function. Therefore, sending $h \to 0$, we have

$$\frac{d}{dh}\Big|_{h=0}((P^h g)(\sigma)) = \frac{d}{dh}\Big|_{h=t}((P^h f)(\sigma)) = (\mathcal{L}g)(\sigma)$$

so that the backward Kolmogorov equation is valid

$$(P^t f)(\sigma) = f(\sigma) + \int_0^t (\mathcal{L}P^s f)(\sigma) ds \tag{2.3.10}$$

Two probability measures μ and ν on Ω such that $\int f d\mu = \int f d\nu$ for all $f \in \mathcal{D}(\Omega)$ are equal. If μ is a stationary state for $(P^t)_t$ then the forward Kolmogorov equation implies that $\int \mathcal{L} f d\mu = 0$ for all $f \in \mathcal{D}(\Omega)$. If $\int \mathcal{L} f d\mu = 0$ for all $f \in \mathcal{D}(\Omega)$ then the backward Kolmogorov equation implies that $\int (P^t f) d\mu = \int f d\mu$ for every $f \in \mathcal{D}(\Omega)$ and hence μ is stationary for $(P^t)_{t\geq 0}$. Hence we have

Lemma 2.3.3 *Stationary states μ satisfying the moment condition*

$$\sup_{j\in\mathbb{Z}} \int \mathcal{E}_j d\mu < +\infty$$

are characterized by the stationary Kolmogorov equation:

$$\int \mathcal{L}\phi(\omega) d\mu(\omega) = 0 \text{ for } \phi \in \mathcal{D}(\Omega)$$

We now prove that the infinite volume dynamics is well approximated by the finite dimensional dynamics $\omega^n(t) = \{r_i^n(t), p_i^n(t), i \in \mathbb{Z}\}$. It is defined by the following stochastic differential equations

$$\begin{aligned}
\dot{r}_i^{(n)}(t) &= p_i^{(n)}(t) - p_{i-1}^{(n)}(t) \qquad i = -n, \dots, n+1 \\
\dot{p}_i^{(n)}(t) &= V'(r_{i+1}^{(n)}(t)) - V'(r_i^{(n)}(t)) \\
&\quad + \mathbf{1}_{\{i\leq n-1\}} \sqrt{\gamma}\,(p_{i+1}(t-) - p_i(t-))\, dN_{i,i+1}(t) + \mathbf{1}_{\{i\geq -n+1\}} \sqrt{\gamma}\,(p_{i-1}(t-) - p_i(t-))\, dN_{i-1,i}(t), \\
&\qquad i = -n, \dots, n.
\end{aligned} \tag{2.3.11}$$

with the coordinates $(q_i(t), p_i(t)) = (q_i(0), p_i(0))$ if $i \notin \{-n, \dots, n\}$. The dynamics is generated by $\mathcal{L}_n = \mathcal{A}_n + \mathcal{S}_n$ where $\mathcal{A}_n$ is defined by

$$\mathcal{A}_n = \sum_{j=-n}^{n} \left\{ p_j(\partial_{r_j} - \partial_{r_{j+1}}) + (V'(r_{j+1}) - V'(r_j))\, \partial_{p_j} \right\} \tag{2.3.12}$$

and $\mathcal{S}_n$ is given by

$$\mathcal{S}_n = \sum_{j=-n}^{n-1} Y_j^2 \tag{2.3.13}$$

Remark that (2.3.8) is also valid for the finite-dimensional dynamics

$$\mathbb{E}_\omega \left[\sum_j e^{-a|j|} \mathcal{E}_j(\omega^{(n)}(t)) \right] \leq C_0 e^{c_1 t} \left[\sum_j e^{-a|j|} \mathcal{E}_j(\omega) \right] \tag{2.3.14}$$

Choose a initial configuration $\omega \in \Omega_a$ and $b > a$. Let us define

$$\delta_n(t) = \mathbb{E}_\omega \left(\|\omega^{(n)}(t) - \omega(t)\|_b^2 \right) = \mathbb{E}_\omega \left(\sum_{i \in \mathbb{Z}} e^{-b|i|} \left(|r_i^{(n)}(t) - r_i(t)|^2 + |p_i^{(n)}(t) - p_i(t)|^2 \right) \right) \tag{2.3.15}$$

where the dynamics $\omega^{(n)}(t)$ and $\omega(t)$ start from the same initial configuration ω.

By Cauchy-Schwarz's inequality and Itô's formula, we have

$$\delta_n(t) \leq C_T \int_0^t ds \delta_n(s) + C_T \sum_{|i| \geq n-2} e^{-b|i|} \mathbb{E}_\omega \left[\mathcal{E}_i(\omega) + \mathcal{E}_i(\omega(t)) + \mathcal{E}_i(\omega^{(n)}(t)) \right], \quad t \in [0, T] \tag{2.3.16}$$

where C_T is a positive constant depending on T and such that C_T goes to zero with T and that can change from line to line. By the a priori bounds (2.3.8, 2.3.14), we have

$$\mathbb{E}_\omega \left[\mathcal{E}_i(\omega) + \mathcal{E}_i(\omega(t)) + \mathcal{E}_i(\omega^{(n)}(t)) \right] \leq C_T e^{a|i|} \left(\sum_{j \in \mathbb{Z}} e^{-a|j|} \mathcal{E}_j(\omega) \right) \tag{2.3.17}$$

so that

$$\delta_n(t) \leq C_T \int_0^t ds \delta_n(s) + \varepsilon_n, \quad \varepsilon_n \leq \frac{C_T}{b-a} e^{-(b-a)n} \left(\sum_{j \in \mathbb{Z}} e^{-a|j|} \mathcal{E}_j(\omega) \right) \tag{2.3.18}$$

By Gronwall's inequality we get

$$\delta_n(t) \leq \varepsilon_n e^{C_T T} \tag{2.3.19}$$

Let P_n the semigroup generated by $\mathcal{L}_n$. Estimate (2.3.19) is enough to prove the following lemma

Lemma 2.3.4 *Let $a > 0$ and $\omega \in \Omega_a$, then*

- $\mathbb{P}_\omega$ *a.s.*, $(r_i^{(n)}(t), p_i^{(n)}(t))$ *converges to* $(r_i(t), p_i(t))$ *as* n *goes to infinity.*
- *For any bounded Lipschitz local function* ϕ *and* $t \in [0,T]$ *there exist constants* $C_n = C_n(a,T,\phi) \to 0$ *as* $n \to \infty$ *such that:*

$$\left|P_n^t\phi(\omega) - P^t\phi(\omega)\right| \le C_n \left(\sum_{j\in\mathbb{Z}} e^{-a|j|}\mathcal{E}_j(\omega)\right)$$

Let μ and ν probability measures on $\Omega = (\mathbb{R}^2)^{\mathbb{Z}}$, and for any $\Lambda \subset \mathbb{Z}$ let $\mathcal{F}_\Lambda$ the ensemble of the measurable functions of $\omega_\Lambda = (r_j, p_j; j \in \Lambda)$ (i.e. functions on Ω that depends only on the variables in Λ).

In the following let $\mu = \mu^{gc}_{\beta_0}$ a grandcanonical Gibbs measure at temperature β_0^{-1}. If ν is translation invariant, denoting $\Lambda_n = \{-n,\dots,n\}$, we have that $H_{\Lambda_n}(\nu|\mu)$ is a superadditive function of n (see proposition B.1.4), and consequently it exists the limit

$$\bar{H}(\nu|\mu) = \lim_{n\to\infty}\frac{1}{2n+1}H_{\Lambda_n}(\nu|\mu) = \sup_n \frac{1}{|\Lambda_n|}H_{\Lambda_n}(\nu|\mu) \tag{2.3.20}$$

For any local measurable function ϕ define the limit

$$\bar{F}(\phi) = \lim_{n\to\infty}\frac{1}{2n+1}\bar{F}_n(\phi), \quad \bar{F}_n(\phi) = \log\int e^{\sum_{i=-n}^{n}\tau_i\phi}\,d\mu \tag{2.3.21}$$

where τ_i is the shift operator on functions on $(\mathbb{R}^2)^{\mathbb{Z}}$.

We recall here proposition B.1.5:

Proposition 2.3.5 *Let* ν *a translation invariant probability on* Ω*, then*

$$\bar{H}(\nu|\mu) = \sup_\phi\left\{\int \phi\,d\nu - \bar{F}(\phi)\right\} \tag{2.3.22}$$

where the supremum is taken over all bounded measurable local functions ϕ*.*

As a consequence we can prove easily the following bound on the average energy density:

$$\int \mathcal{E}_0\,d\nu \le C(1 + H_\Lambda(\nu|\mu)) \tag{2.3.23}$$

Here is the ergodic property for the infinite stochastic dynamics:

Theorem 2.3.6 *Let ν a translation invariant probability measure, stationary for the dynamics generated by $\mathcal{L}$. Assume that there exist a finite constant C such that*

$$H_\Lambda(\nu|\mu) \leq C|\Lambda| \tag{2.3.24}$$

where $\mu = \mu_{\beta_0}$ is a reference grand canonical measure. Then ν is a convex combination of grand canonical measures.

We have seen that for a translation invariant ν, (2.3.24) is equivalent to the condition $\bar{H}(\nu|\mu) \leq C < \infty$.

The proof is divided in two steps. Let us first consider a generic probability mesure ν_*, not necessarily translation invariant, such that $H(\nu_*|\mu) < \infty$, and let us denote by $g = \frac{d\nu_*}{d\mu}$. Let us denote, for any n, the Dirichlet forms:

$$D_n(\nu_*) = \sup_\psi \left\{ -\int \frac{\mathcal{S}_n \psi}{\psi}\, d\nu_* \right\} \tag{2.3.25}$$

where the supremum is carried on the set of positive functions $\psi : \Omega \to (0, +\infty)$ such that $0 < M^{-1} \leq \psi \leq M < +\infty$ for some positive constant M.

Lemma 2.3.7 *Let ν^* be be a probability measure on Ω absolutely continuous w.r.t. μ and such that $D_n(\nu_*) < +\infty$. Then $g = d\nu^*/d\mu$ satisfies*

$$D_n(\nu_*) = \frac{1}{2} \sum_{j=-n}^{n-1} \int (Y_j \sqrt{g})^2\, d\mu\ . \tag{2.3.26}$$

Proof: Let $\psi : \Omega \to (0, +\infty)$ such that $0 < M^{-1} \leq \psi \leq M < +\infty$ for some positive constant M. Observe that $Y_i^2 = -2Y_i$ and that Y_i is a self-adjoint operator in $\mathbb{L}^2(\mu)$. Therefore

$$\begin{aligned}
- & \int \frac{\mathcal{S}_n \psi}{\psi}\, d\nu_* = \frac{1}{2} \sum_{i=-n}^{n-1} \int \frac{Y_i^2 \psi}{\psi} g d\mu = \frac{1}{2} \sum_{i=-n}^{n-1} \int Y_i \psi\, Y_i \left(\frac{g}{\psi} \right) d\mu \\
= & \frac{1}{2} \sum_{i=-n}^{n-1} \int \left[g(p^{i,i+1}) - g(p^{i,i+1}) \frac{\psi(p)}{\psi(p^{i,i+1})} - g(p) \frac{\psi(p^{i,i+1})}{\psi(p)} + g(p) \right] d\mu \\
= & \frac{1}{2} \sum_{i=-n}^{n-1} \int \left[g(p^{i,i+1}) - \sqrt{g}(p^{i,i+1}) \sqrt{g}(p) \left[\frac{(\psi/\sqrt{g})(p)}{(\psi/\sqrt{g})(p^{i,i+1})} + \frac{(\psi/\sqrt{g})(p^{i,i+1})}{(\psi/\sqrt{g})(p)} \right] + g(p) \right] d\mu \\
\leq & \frac{1}{2} \sum_{j=-n}^{n-1} \int (Y_j \sqrt{g})^2\, d\mu
\end{aligned}$$

because $z+1/z \geq 2$ for every positive z. This proves $D_n(\nu^*) \leq \frac{1}{2}\sum_{j=-n}^{n-1} \int (Y_j\sqrt{g})^2 \, d\mu$.

For the other sense of the inequality, let $M > 0$ and consider $\psi_M = M^{-1} + \inf(\sqrt{g}, M)$. We have seen that

$$D_n(\nu^*) \geq \frac{1}{2}\sum_{i=-n}^{n-1} \int \left[g(p^{i,i+1}) - g(p^{i,i+1})\frac{\psi_M(p)}{\psi_M(p^{i,i+1})} - g(p)\frac{\psi_M(p^{i,i+1})}{\psi_M(p)} + g(p) \right] d\mu$$

Observe that $\dfrac{\psi_M(p^{i,i+1})}{\psi_M(p)}$ is positive and converges to $\sqrt{g}(p^{i,i+1})/\sqrt{g}(p)$. By Fatou lemma we get

$$D_n(\nu_*) \geq \frac{1}{2}\sum_{j=-n}^{n-1} \int (Y_j\sqrt{g})^2 \, d\mu$$

which completes the proof. □

A simple consequence of proposition B.2.2 and convexity of the Dirichlet form gives the following

Proposition 2.3.8 *For any probability mesure ν and any n, we have*

$$H(\nu_* P_n^t|\mu) + tD_n(\bar{\nu}_{*,n}^t) \leq H(\nu_*|\mu) \tag{2.3.27}$$

where $\bar{\nu}_{*,n}^t = t^{-1}\int_0^t \nu_* P_n^s ds$.

Because of (2.3.26), if $H(\nu_*|\mu) < +\infty$, then for any $j = -n+1, \dots, n-1$

$$H(\nu_* P_n^t|\mu) + \frac{t}{2}\sum_{j=-n}^{n-1} \int (Y_j\sqrt{\bar{g}_n^t})^2 \, d\mu \leq H(\nu_*|\mu)$$

where $\bar{g}_n^t = \frac{d\bar{\nu}_{*,n}^t}{d\mu}$. In the second term of the above, because is composed by a sum of positive parts, we can restrict this to any $m \leq n-1$:

$$H(\nu_* P_n^t|\mu) + \frac{t}{2}\sum_{j=-m}^{m} \int (Y_j\sqrt{\bar{g}_n^t})^2 \, d\mu \leq H(\nu_*|\mu)$$

By (B.1.2) and (2.3.25), for any choice of function $\phi \in \mathcal{D}(\Omega)$ and local functions $\psi_i \in \mathcal{D}(\Omega)$ (bounded by below by a positive constant)

$$\int P_n^t\phi \, d\nu_* - \log\int e^\phi d\mu - \frac{t}{2}\sum_{j=-m}^{m} \int \frac{Y_i^2\psi_i}{\psi_i} \, d\bar{\nu}_{*,n}^t \leq H(\nu_*|\mu)$$

Now we can finally let $n \to \infty$, and by theorem 2.3.4 we obtain

$$\int P^t \phi \, d\nu_* - \log \int e^{\phi} d\mu - \frac{t}{2} \sum_{j=-m}^{m} \int \frac{Y_i^2 \psi_i}{\psi_i} \, d\bar{\nu}_*^t \leq H(\nu_* | \mu) \tag{2.3.28}$$

where $\bar{\nu}_*^t = t^{-1} \int_0^t \nu_* P^s \, ds$.

Proposition 2.3.9 *Let ν be a translation invariant measure stationary for P^t such that for a finite constant C, $H_\Lambda(\nu|\mu_{\beta_0}^{gc}) \leq C|\Lambda|$ for any finite interval Λ. Then for any n we have $D_n(\nu) = 0$.*

Proof We apply now (2.3.28) to $\nu_* = \nu_*^{(m)} = \nu|_{\Lambda_m} \otimes \mu|_{\Lambda_m^c}$. Notice that $H(\nu_*^{(m)}|\mu) = H_{\Lambda_m}(\nu|\mu)$, and consequently

$$\lim_{m \to \infty} \frac{1}{2m} H(\nu_*^{(m)}|\mu) = \bar{H}(\nu|\mu)$$

Choosing $\phi = \sum_{i=-m}^{m} \tau_i \phi_0$, $\psi_i = \tau_i \psi_0$, where $\phi_0 \in \mathcal{D}(\Omega)$ and $\psi_0 \in \mathcal{D}(\Omega)$ is bounded by below by a positive constant, we obtain

$$\sum_{i=-m}^{m} \int P^t(\tau_i \phi_0) \, d\nu_*^{(m)} - \bar{F}_m(\phi_0) - \frac{t}{2} \sum_{i=-m}^{m} \int \tau_i \frac{Y_0^2 \psi_0}{\psi_0} \, d\bar{\nu}_*^{(m),t} = H(\nu_*^{(m)}|\mu)$$

and all we need to prove is that

$$\lim_{n \to \infty} \frac{1}{2n+1} \sum_{i=-n}^{n} \int P^t(\tau_i \phi_0) \, d\nu_*^{(n)} = \int P^t \phi_0 d\nu = \int \phi_0 d\nu \tag{2.3.29}$$

and

$$\lim_{n \to \infty} \frac{1}{2n+1} \sum_{i=-n}^{n} \int \tau_i \frac{Y_0^2 \psi_0}{\psi_0} \, d\bar{\nu}_*^{(n),t} = \int \frac{Y_0^2 \psi_0}{\psi_0} \, d\nu \tag{2.3.30}$$

In fact maximising what we obtained over ϕ_0 and ψ_0 we get

$$-\inf_{\psi_0} \int \frac{Y_0^2 \psi_0}{\psi_0} \, d\nu = 0$$

It is clear that we can repeat the argument substituting Y_j to Y_0, and we obtain

$$-\inf_{\psi_0} \int \frac{Y_j^2 \psi_0}{\psi_0} \, d\nu = 0$$

In the last infimum it is easy to extend the infimum to the set of functions $\psi_0 : \Omega \to (0, +\infty)$ bounded by above and by below by positive constants. Summing up over j we obtain

$$0 \leq D_n(\nu) = -\inf_{\psi} \sum_{j=-n-1}^{n+1} \int \frac{Y_j^2 \psi}{\psi} \, d\nu \leq - \sum_{j=-n-1}^{n+1} \inf_{\psi} \int \frac{Y_j^2 \psi}{\psi} \, d\nu = 0.$$

□

Proof of (2.3.29) and (2.3.30).

The difficulty comes form the fact that $P^t \phi$ is not local.

We approximate again P^t by our local dynamics P^t_ℓ. Observe that by (2.3.23), for any $i = 1, \ldots, n$,

$$\int \mathcal{E}_j(\omega) d(\tau_i \nu_*^{(n)}) \leq \sup_{i \in \mathbb{Z}} \left(\int \mathcal{E}_i d\nu + \int \mathcal{E}_i d\mu \right) \leq K$$

with K independent of n. Then it follows from lemma 2.3.4 that

$$\sup_n \left| \int P^t \phi \; d(\tau_i \nu_*^{(n)}) - \int P^t_\ell \phi \; d(\tau_i \nu_*^{(n)}) \right| \leq K C_\ell \sum_{j \in \mathbb{Z}} e^{-a|j|}$$

with $C_\ell \to 0$ as $\ell \to \infty$.

Now we have that $P^t_\ell \phi$ is a local function, and by definition of $\nu_*^{(n)}$,

$$\frac{1}{2n+1} \sum_{i=-n}^{n} \int P^t_\ell \phi \; d(\tau_i \nu_*^{(n)}) = \frac{1}{2n+1} \sum_{i=-n}^{n} \int P^t_\ell \phi \; d(\tau_i \nu) + C(\ell)/n$$

for some constant $C(\ell) > 0$. Sending first n to infinity and then ℓ we get

$$\lim_{\ell \to \infty} \lim_{n \to \infty} \frac{1}{2n+1} \sum_{i=-n}^{n} \int P^t_\ell \phi \; d(\tau_i \nu_*^{(n)}) = \int P^t \phi \; d\nu = \int \phi d\nu.$$

Proof of (2.3.30) is similar.

□

Theorem 2.3.6 is a consequence of the following proposition

Proposition 2.3.10 *If ν is a probability measure on Ω such that $H_\Lambda(\nu|\mu) \leq C|\Lambda|$ for every finite subset Λ and satisfying $D_n(\nu) = 0$ for any $n \geq 2$, then $\nu(dp|r)$ is exchangeable.*

Proof Let g_n be the density of $\nu|_{\Lambda_n}$ with respect to $\mu|\Lambda_n$ where $\Lambda_n = \{-n, \dots, n\}$. We call $\mathcal{B}_n$ the set of functions $\psi(r,p)$ bounded by below and by above by strictly positive constants and depending on the p's only through $p_i, i \in \Lambda_n$.

The condition $D_n(\nu) = 0$ implies

$$0 = \sup \left\{ - \int \frac{\mathcal{S}_n \psi}{\psi} d\nu|_{\Lambda_n} \; ; \; \psi \in \mathcal{B}_n \right\} \tag{2.3.31}$$

The proof of lemma 2.3.7 shows that the right hand side is equal to

$$\frac{1}{2} \sum_{j=-n}^{n-1} \int \left(Y_j \sqrt{g_n} \right)^2 d\mu|_{\Lambda_n} \tag{2.3.32}$$

Since the sum is composed of positive terms it implies that $g_n(r, p^{j,j+1}) = g_n(r,p)$ a.s. for every $j \in \{-n, \dots, n-1\}$. Since this is true for every $n \geq 2$ we get that $\nu(dp|r)$ is exchangeable.

□

We conclude the proof of Theorem 2.3.6, by observing that ν is separately stationary for $\mathcal{S}$ and $\mathcal{A}$, and then we conclude by applying Theorem 2.2.3.

2.4 Other stochastic dynamics

2.4.1 Energy conserving noise

We can also define a noise $\mathcal{S} = \sum_j X_j^2$ acting on the momenta conserving only kinetic energy. The construction is similar : for nearest neighbors atoms $j, j+1$ we define the vector field X_j by

$$X_j = p_{j+1} \partial_{p_j} - p_j \partial_{p_{j+1}} \tag{2.4.1}$$

It is tangent to the circle $\{(p_j, p_{j+1}) \in \mathbb{R}^2; \quad p_j^2 + p_{j+1}^2 = 1\}$ so that

$$\mathcal{S} = \sum_j X_j^2 \tag{2.4.2}$$

conserves the kinetic energy. Momentum is not conserved and is in fact eigenvector of $\mathcal{S}$ since $\mathcal{S}(p_j) = -p_j$.

2.4.2 Momentum exchange and momentum flip

One can also consider noise of Poissonian type conserving energy and eventually also momentum. Poissonian energy conserving noise is defined by the following flip operator

$$(\mathcal{S}f)(p) = \sum_j \left[f(p^j) - f(p)\right] \tag{2.4.3}$$

where p^j is the configuration obtained from p by changing the coordinate p_j in $-p_j$.

Poissonian momentum-energy conserving noise is realized by exchange of momenta of nearest neighbor atoms. The generator of this noise is given by

$$(\mathcal{S}f)(p) = \sum_j \left[f(p^{j,j+1}) - f(p)\right] \tag{2.4.4}$$

where $p^{j,j+1}$ is the configuration obtained from p by exchanging the coordinates p_j and p_{j+1}.

Remark that these noise have very poor ergodic properties (which is not the case of the Brownian noises defined before). Nevertheless results of section 2.2 can be applied for them and it implies that the dynamics obtained by adding these noises to the Hamiltonian dynamics is ergodic.

2.5 Bibliographical Notes

The argument for the proof of the ergodicity of the stochastic model is adapted from [11], [10], [5] and [6].

Chapter 3

Hydrodynamic Limit: Hyperbolic Scaling

3.1 Hyperbolic conservation laws

We consider in this chapter the system with periodic boundary conditions ($i \in \mathbb{T}_N$). We will first consider the deterministic system assuming that it is ergodic in the sense of 2.2.1. Then we will consider the stochastic conservative perturbations considered in section 2.3, that will make the dynamic ergodic, and we will show that these perturbations do not modify the macroscopic equations.

Configuration space is $\Omega_N = (\mathbb{R} \times \mathbb{R})^{\mathbb{T}_N}$ and a generic configuration $(r_i, p_i)_{i \in \mathbb{T}_N}$ is denoted by ω. The generator of the dynamics $(\omega(t))_{t \geq 0}$ is given by $\mathcal{A}_N$, the Liouville operator.

The system conserves the following quantities

$$\sum_{i \in \mathbb{T}_N} r_i\text{: length of the chain}$$
$$\sum_{i \in \mathbb{T}_N} p_i \text{ : momentum}$$
$$\sum_{i \in \mathbb{T}_N} \mathcal{E}_i \text{ : energy}$$

The conservation laws can be read locally as

$$(\mathcal{A}_N(r_i), \mathcal{A}_N(p_i), \mathcal{A}_N(\mathcal{E}_i)) = \mathbf{J}_{i-1} - \mathbf{J}_i$$

where $\mathbf{J}_i$ is the instantaneous current between i and $i+1$ given by

$$\mathbf{J}_i = -(p_i,\, V'(r_{i+1}),\, p_i V'(r_{i+1})) \tag{3.1.1}$$

We are interested in the macroscopic behavior of the three conserved quantities $(\sum r_i, \sum p_i, \sum e_i)$ at time Nt, as $N \to \infty$. For this pourpose we define the empirical densities:

$$\begin{aligned} \mathfrak{r}_N(t,G) &= \frac{1}{N} \sum_{i \in \mathbb{T}_N} G(i/N) r_i(Nt) \\ \mathfrak{p}_N(t,G) &= \frac{1}{N} \sum_{i \in \mathbb{T}_N} G(i/N) p_i(Nt) \\ \mathfrak{e}_N(t,G) &= \frac{1}{N} \sum_{i \in \mathbb{T}_N} G(i/N) e_i(Nt) \end{aligned} \tag{3.1.2}$$

where $G(y)$ is a smooth function on $\mathbb{T}$, the circle of length 1.

We start at time 0 with an initial probability distribution on the configuration of the system such that there exist smooth functions $\mathfrak{r}_0, \mathfrak{p}_0, \mathfrak{e}_0$ on $\mathbb{T}$ and

$$\{\mathfrak{r}_N(0,G), \mathfrak{p}_N(0,G), \mathfrak{e}_N(0,G)\} \underset{N\to\infty}{\longrightarrow} \left\{ \int G(y)\mathfrak{r}_0(y)dy, \int G(y)\mathfrak{p}_0(y)dy, \int G(y)\mathfrak{e}_0(y)dy \right\}$$

in probability.

We want to prove that we have the same convergence for $\mathfrak{r}_N(t,G), \mathfrak{p}_N(t,G), \mathfrak{e}_N(t,G)$ to corresponding *smooth profiles* $\mathfrak{r}(t,y), \mathfrak{p}(t,y), \mathfrak{e}(t,y)$ solution of the hyperbolic system of partial differential equations:

$$\begin{aligned} \partial_t \mathfrak{r} &= \partial_y \mathfrak{p} \\ \partial_t \mathfrak{p} &= \partial_y \tau(\mathfrak{r}, \mathfrak{e} - \mathfrak{p}^2/2) \\ \partial_t \mathfrak{e} &= \partial_y \left(\mathfrak{p} \tau(\mathfrak{r}, \mathfrak{e} - \mathfrak{p}^2/2) \right) \end{aligned} \tag{3.1.3}$$

with initial condition $\mathfrak{r}_0, \mathfrak{p}_0, \mathfrak{e}_0$. It is useful to use the notation $\mathfrak{U} = \mathfrak{e} - \mathfrak{p}^2/2$ to denote the corresponding profile of *internal energy*. The function $\tau(r,u) = \lambda(r,u)/\beta(r,u)$ is the tension defined by (1.1.7) and (1.1.8) from the thermodynamical entropy $S(r,u)$ (1.1.4).

We will prove this convergence under some restrictive conditions on the interaction V, and on the solution $\mathfrak{u}(t,y) = (\mathfrak{r}(t,y), \mathfrak{p}(t,y), \mathfrak{e}(t,y))$.

Observe that under the Gibbs measure $\mu^{gc}_{\tau,\bar{p},\beta}$ (with $\tau = \lambda/\beta$) the relation

$$\forall j \in \mathbb{Z}, \quad \int d\mu^{gc}_{\tau,\bar{p},\beta} V'(r_j) = \tau$$

and one has that

$$\tau(\mathfrak{r}, \mathfrak{U}) = \int V'(r_0) \mu^{gc}_{\tau(\mathfrak{r},\mathfrak{U}),\mathfrak{p},\beta(\mathfrak{r},\mathfrak{U})}(dr_0)$$

It follows from these relations that computing the thermodynamic entropy along the solution of (3.1.3) we have

$$\partial_t S\left(\mathfrak{r}(t,y),\mathfrak{U}(t,y)\right) = -\beta\tau\partial_y\mathfrak{p} + \beta\left[\partial_y\left(\mathfrak{p}\tau\right) - \mathfrak{p}\partial_y\tau\right] = 0 \tag{3.1.4}$$

i.e. (3.1.3) is isoentropic. This is strictly dependent on teh smoothness of the solution, i/e/ that we are only considering the equation (3.1.3) in the smooth regime, before apperance of shocks [1].

Let $F : U \subset \mathbb{R}^m \to \mathbb{R}^p$ is a sufficiently differentiable function from the open subset U of $\mathbb{R}^m$, $m \geq 1$. If $p = 1$ we denote the gradient of F at $\mathbf{x} \in U$ by $(DF)(\mathbf{x}) \in \mathbb{R}^m$. If $p \geq 2$ and $F = (F^1, \dots, F^p)$ with each F^i real valued we use the notation $(DF)(\mathbf{x}) = (DF^1(\mathbf{x}), \dots, DF^p(\mathbf{x})) \in M_{n,p}(\mathbb{R})$ for the Jacobian matrix of F at $\mathbf{x}$. The Hessian matrix of F is denoted by D^2F.

To simplify notation we denote

$$\lambda(\mathfrak{u}) = \lambda(\mathfrak{r},\mathfrak{U}), \quad \beta(\mathfrak{u}) = \beta(\mathfrak{r},\mathfrak{U})$$

and

$$\mathbb{S}(\mathfrak{u}) = \mathbb{S}(\mathfrak{r},\mathfrak{p},\mathfrak{e}) = S(\mathfrak{r},\mathfrak{U})$$

By (1.1.7) we have

$$(D\mathbb{S})(\mathfrak{u}) = (-\lambda(\mathfrak{u}), -\beta(\mathfrak{u})\mathfrak{p}, \beta(\mathfrak{u}))$$

and we rewrite (3.1.3) as

$$\partial_t\mathfrak{u} - \partial_y\widehat{\mathbf{J}}(\mathfrak{u}) = 0 \tag{3.1.5}$$

with $\widehat{\mathbf{J}}(\mathfrak{u}) = (\mathfrak{p}, \lambda(\mathfrak{u})/\beta(\mathfrak{u}), \mathfrak{p}\lambda(\mathfrak{u})/\beta(\mathfrak{u}))$, and the isoentropic property reads as

$$(D\mathbb{S})(\mathfrak{u}) \cdot \partial_y[\widehat{\mathbf{J}}(\mathfrak{u})] = 0.$$

It may be useful to use more symmetric notations and call $\Theta(v) = \log\mathcal{Z}(\lambda,\beta p,\beta)$, for $v = (\lambda,\beta p,\beta) \in \mathbb{R}^2 \times (0,\infty)$, and $\Phi(w) = -\mathbb{S}(r,p,\mathcal{E})$ for $w = (r,p,-\mathcal{E}) \in \mathbb{R}^2 \times (-\infty,0)$. By (1.1.4), Φ is the Legendre-Fenchel transform of Θ. Since Θ is convex, lower semicontinuous and not identically equal to infinity Fenchel-Moreau's theorem implies that Θ is the Legendre-Fenchel transform of Φ. Hence we have

$$\Theta(v) = \sup_w\{v \cdot w - \Phi(w)\}, \qquad \Phi(w) = \sup_v\{v \cdot w - \Theta(v)\}$$

[1] Shocks should make this time derivative positive in some sense. This means that proving such convergence in the presence of schocks would imply to obtain, in this hyperbolic scace-time limit, irreversible adiabatic transformation that increase thermodynamic entropy, i.e. the second principle of thermodynamics. But at the moment even the problem of uniqueness of such solutions is mathematically open

We have that

$$(D\Phi)(w) = (\lambda, \beta p, \beta), \quad (D\Theta)(v) = (r(\lambda,\beta), p, -(u(\lambda,\beta) + p^2/2))$$

are never equal to 0. Hence $\Theta : \mathbb{R}^2 \times (0,\infty) \to \mathbb{R}^2 \times (-\infty, 0)$ and $\Phi : \mathbb{R}^2 \times (-\infty, 0) \to \mathbb{R}^2 \times (0,\infty)$ are diffeomorphisms, one inverse of the other and

$$D\Phi(D\Theta(v)) = v, \qquad D\Theta(D\Phi(w)) = w,$$

Every couple v, w are said in *duality* if

$$v = D\Phi(w), \qquad w = D\Theta(v), \quad v \in \mathbb{R}^2 \times (0,+\infty), \quad w \in \mathbb{R}^2 \times (-\infty, 0)$$

and then they verify immediately the relations

$$\Phi(w) + \Theta(v) = w \cdot v, \quad D^2\Theta(v) = D^2\Phi(w)^{-1}$$

For $\mathfrak{u} = (\mathfrak{r}, \mathfrak{p}, \mathfrak{e})$ we define

$$\tilde{\mathfrak{u}} = (\mathfrak{r}, \mathfrak{p}, -\mathfrak{e}), \quad \tilde{\mathbf{J}}(\tilde{\mathfrak{u}}) = (\mathfrak{p}, \lambda(\mathfrak{u})/\beta(\mathfrak{u}), -\mathfrak{p}\lambda(\mathfrak{u})/\beta(\mathfrak{u}))$$

For $v = (\lambda, \beta p, \beta)$ define

$$\Sigma(v) = v \cdot \tilde{\mathbf{J}}(D\Theta(v)) = \lambda p = \frac{v_1 v_2}{v_3} \tag{3.1.6}$$

then

$$D\Sigma(v) = \tilde{\mathbf{J}}(D\Theta(v)) \tag{3.1.7}$$

Let $\mathfrak{v}(t,x)$ the dual of $\tilde{\mathfrak{u}}(t,x)$ where $\mathfrak{u}(t,x)$ is the solution of (3.1.5). Then $\mathfrak{v}(t,x)$ solves the *symmetric* system

$$\partial_t[D\Theta(\mathfrak{v})] = \partial_y(D\Sigma(\mathfrak{v})) \tag{3.1.8}$$

Proposition 3.1.1

$$\partial_t \mathfrak{v}(t,x) = D\tilde{\mathbf{J}}(\tilde{\mathfrak{u}})\partial_y \mathfrak{v} \tag{3.1.9}$$

Proof Equation (3.1.8) can be rewritten as

$$(D^2\Theta)\partial_t \mathfrak{v} = (D^2\Sigma)\partial_y \mathfrak{v}$$

Since $D^2\Theta(\mathfrak{v}(t,x))^{-1} = (D^2\Phi)(\tilde{\mathfrak{u}}(t,x))$, we have

$$\partial_t \mathfrak{v} = (D^2\Phi)(D^2\Sigma)\partial_y \mathfrak{v}$$

Differentiating (3.1.7) we have

$$D^2\Sigma = (D^2\Theta)(D\tilde{\mathbf{J}}(\tilde{\mathfrak{u}}))$$

and substituting we obtain

$$\partial_t \mathfrak{v} = (D\tilde{\mathbf{J}}(\tilde{\mathfrak{u}}))\partial_y \mathfrak{v}$$

□

On V we assume that has at most quadratic growth for $r \to \infty$, i.e.

$$|V'(r)|^2 \leq CV(r), \qquad |r| \geq R \tag{3.1.10}$$

for some constant R and C.

We also assume that initial profile and solution $\mathfrak{u}(t, y)$ of (3.1.3) are smooth, i.e. the theorem is valid up to appearance of the first shock.

3.2 Local Gibbs states

By (1.1.7), given a macroscopic profile $\{\mathfrak{u}(y) = (\mathfrak{r}(y), \mathfrak{p}(y), \mathfrak{e}(y)), y \in \mathbb{T}\}$ such that $\mathfrak{U}(y) = \mathfrak{e}(y) - \mathfrak{p}(y)^2/2 > 0$, there is a unique corresponding profile of parameters $(\tau(y), \lambda(y), \beta(y))$ defined by

$$\lambda(y) = -\partial_r S\left(\mathfrak{r}(y), \mathfrak{U}(y)\right), \quad \beta(y) = \partial_u S\left(\mathfrak{r}(y), \mathfrak{U}(y)\right)$$

We can define then an inhomogeneous product probability measure on the configuration space Ω_N

$$g^N_{\mathfrak{u}(\cdot)} = \prod_{i \in \mathbb{T}_N} \frac{\exp[\beta(i/N)(-\mathcal{E}_i + \mathfrak{p}(i/N)p_i) + \lambda(i/N)r_i]}{\mathcal{Z}(\lambda(i/N), \beta(i/N)\mathfrak{p}(i/N), \beta(i/N))} \tag{3.2.1}$$

Let $\psi(p, r)$ a local function of the configuration p, r (like $\psi = p_0 V'(r_1)$ etc). If N is large enough, we can define ψ on the configuration on $\mathbb{T}_N$ without ambiguities. We denote by τ_i the spatial shift on configurations (i.e. $\tau_i\psi = p_i V'(r_{i+1})$ in the above example). We will use the same notation τ_i in the case $i \in \mathbb{Z}$ or $i \in \mathbb{T}_N$.

It is elementary (see proposition 3.3.2) to prove the law of large numbers for a local function ψ as

$$\frac{1}{N} \sum_{i \in \mathbb{T}_N} G(i/N)\tau_i\psi \underset{N\to\infty}{\longrightarrow} \int_{\mathbb{T}} G(y)\tilde{\psi}(\mathfrak{u}(y))\, dy \qquad \text{in } \mathbb{L}^1(g^N_{\mathfrak{u}(\cdot))d\mathbf{r}d\mathbf{p}}).$$

where

$$\tilde{\psi}(\mathfrak{u}) = <\psi>_{\mathfrak{u}}$$

is the grand-canonical expectation.

Our goal will be in proving that the distribution at time Nt on the system, i.e. the solution of the forward equation

$$\partial_t f_N(t,p,r) = N\mathcal{A}_N^* f_N(t,p,r)$$

is close enough to $g^N_{\mathfrak{u}(t,\cdot)}$, with $\mathfrak{u}(t,y)$ solution of (3.1.3), such that they share the same laws of large numbers. This vague assertion are usually called "local equilibrium". We will make this more precise. We will measure the distance between $f_N(t)$ and $g^N_{\mathfrak{u}(t,\cdot)}$ with their relative entropy.

In the following we will use the symmetrized notations introduced in the previous section. So to the (smooth) solution $\mathfrak{u}(t,y)$ of (3.1.5), there corresponds the dual solution $\mathfrak{v}(t,y)$ of the symmetrized equation (3.1.8) and we denote the corresponding local Gibbs measure by $g^N_{\mathfrak{u}(t,\cdot)}\, d\mathbf{r}d\mathbf{p}$ by $g^N_t\, d\mathbf{r}d\mathbf{p}$ that can be written as

$$g_t^N(\omega) = \prod_{i\in\mathbb{T}_N} e^{\mathfrak{v}(t,i/N)\cdot\xi_i - \Theta(\mathfrak{v}(t,i/N))}, \qquad \xi_i = (r_i, p_i, -\mathcal{E}_i) \tag{3.2.2}$$

3.3 Relative Entropy

We start with an upper bound for the mean energy. Because total energy is conserved by the dynamics we have

$$\int \sum_{i\in\mathbb{T}_N} \mathcal{E}_i\, f_t^N\, d\mathbf{r}d\mathbf{p} = \int \sum_{i\in\mathbb{T}_N} \mathcal{E}_i\, f_0^N\, d\mathbf{r}d\mathbf{p}$$

By assumption on the initial state, this last quantity converges as N goes to infinity to $\int_{\mathbb{T}} \mathfrak{e}_0(y)dy < +\infty$. Since $(V')^2 \le CV$ for some positive constant C, we get

Lemma 3.3.1 *There exists a positive constant C such that*

$$\int N^{-1}\sum_{i\in\mathbb{T}_N} \mathcal{E}_i\, f_t^N\, d\mathbf{r}d\mathbf{p} \le C, \quad \int N^{-1}\sum_{i\in\mathbb{T}_N} (V')^2(r_i)\, f_t^N\, d\mathbf{r}d\mathbf{p} \le C$$

We use the following simplified notation for the relative entropy

$$H_N(t) = H(f_N(t)d\mathbf{r}d\mathbf{p}\,|\,g_t^N d\mathbf{r}d\mathbf{p}) = \int f_N(t)\log\left(\frac{f_N(t)}{g^N_{\mathfrak{u}(t,\cdot)}}\right)\, d\mathbf{r}\; d\mathbf{p} \tag{3.3.1}$$

Proposition 3.3.2 *Assume that*

$$\lim_{N\to\infty} \frac{H_N(t)}{N} = 0$$

then for any bounded local function ψ *and continuous* $G(y)$

$$\mathbb{E}_{f_N(t)}\left(\left|\frac{1}{N}\sum_i G(i/N)\tau_i\psi - \int_{\mathbb{T}} G(y)\tilde{\psi}(\mathfrak{u}(t,y))\,dy\right|\right) \underset{N\to\infty}{\longrightarrow} 0$$

Proof. To simplify we assume the local function ψ depends only on the configuration through $\omega_0 = (p_0, r_0)$. Observe that since $\tilde{\psi}(\mathfrak{u}(t,\cdot))$ is continuous we have

$$\limsup_{N\to\infty} \mathbb{E}_{f_N(t)}\left(\left|\int_{\mathbb{T}} G(y)\tilde{\psi}(\mathfrak{u}(t,y))\,dy - \frac{1}{N}\sum_{i\in\mathbb{T}_N} G(i/N)\tilde{\psi}(\mathfrak{u}(t,i/N))\right|\right) = 0$$

Similarly since G is continuous and ψ is bounded, we have

$$\begin{aligned}
&\left|\frac{1}{N}\sum\nolimits_{i\in\mathbb{T}_N} G(i/N)\tau_i\psi - \frac{1}{N}\sum\nolimits_{i\in\mathbb{T}_N} G(i/N)\left(\frac{1}{2\ell+1}\sum\nolimits_{|j-i|\le\ell}\tau_j\psi\right)\right| \\
&= \left|\frac{1}{N}\sum\nolimits_{j\in\mathbb{T}_N}\tau_j\psi\left(G(j/N) - \frac{1}{2\ell+1}\sum\nolimits_{|i-j|\le\ell} G(i/N)\right)\right| \\
&\le \frac{C(\ell,G,\psi)}{N}
\end{aligned}$$

where $C(\ell, G, \psi)$ is a finite constant depending on ℓ, G and ψ. Hence we are left to prove

$$\limsup_{\ell\to\infty}\limsup_{N\to\infty}\mathbb{E}_{f_N(t)}\left(\frac{1}{N}\sum_{i\in\mathbb{T}_N}\left|\frac{1}{2\ell+1}\sum_{|j-i|\le\ell}\tau_j\psi - \tilde{\psi}(\mathfrak{u}(t,i/N))\right|\right) = 0 \qquad (3.3.2)$$

By entropy inequality, for every $\eta > 0$ the expectation in (3.3.2) is bounded above by

$$\frac{1}{\eta N}H_N(t) + \frac{1}{\eta N}\log\mathbb{E}_{g^N_{\mathfrak{u}(t,\cdot)}}\left[\exp\left\{\eta\sum_{i\in\mathbb{T}_N}\left|\frac{1}{2\ell+1}\sum_{|j-i|\le\ell}\tau_j\psi - \tilde{\psi}(\mathfrak{u}(t,i/N))\right|\right\}\right]$$

Since $e^{|x|} \le e^x + e^{-x}$, we can forget the modulus in the last exponential. In the sequel we will choose η as a function of ℓ. By assumption $H_N(t)/N$ goes to 0 as N

goes to infinity. Hence we have to show

$$\limsup_{\ell\to\infty}\limsup_{N\to\infty}\frac{1}{\eta N}\log\mathbb{E}_{g^N_{\mathfrak{u}(t,\cdot)}}\left[\exp\left\{\eta\sum_{i\in\mathbb{T}_N}\frac{1}{2\ell+1}\sum_{|j-i|\le\ell}\tau_j\psi\;-\tilde{\psi}(\mathfrak{u}(t,i/N))\right\}\right]=0 \tag{3.3.3}$$

Let us introduce the box $\Lambda_\ell=\{-\ell,\dots,\ell\}$ of length $2\ell+1$. We assume without loss of generality that $2\ell+1$ divides N and we decompose $\mathbb{T}_N$ as follows

$$\mathbb{T}_N=\cup_{j\in\Lambda_\ell}B(j),\quad B(j)=\{j+(2\ell+1)q;\,q=0,\dots N/(2\ell+1)-1\} \tag{3.3.4}$$

Since ψ depends only on ω_0, for each $j\in\Lambda_\ell$ fixed, the random variables

$$X_i^j=\frac{1}{2\ell+1}\sum_{|k-i|\le\ell}\tau_k\psi,\quad i\in B(j)$$

are independent under the product measure $g^N_{\mathfrak{u}(t,\cdot)}$. We have

$$\sum_{i\in\mathbb{T}_N}\frac{1}{2\ell+1}\sum_{|k-i|\le\ell}\tau_k\psi=\sum_{j\in\Lambda_\ell}\left(\sum_{i\in B(j)}\frac{1}{2\ell+1}\sum_{|k-i|\le\ell}\tau_k\psi\right)=\sum_{j\in\Lambda_\ell}\left(\sum_{i\in B(j)}X_i^j\right)=\sum_{j\in\Lambda_\ell}Y_j \tag{3.3.5}$$

By generalized Hölder's inequality we have

$$\log\mathbb{E}_{g^N_{\mathfrak{u}(t,\cdot)}}\left[e^{\eta\sum_{j\in\Lambda_\ell}Y_j}\right]\le\frac{1}{2\ell+1}\sum_{j\in\Lambda_\ell}\log\mathbb{E}_{g^N_{\mathfrak{u}(t,\cdot)}}\left[e^{\eta(2\ell+1)Y_j}\right]$$

and by independence (for fixed j) of the X_i^j's, we get

$$\begin{aligned}&\frac{1}{\eta N}\log\mathbb{E}_{g^N_{\mathfrak{u}(t,\cdot)}}\left[\exp\left\{\eta\sum_{i\in\mathbb{T}_N}\frac{1}{2\ell+1}\sum_{|j-i|\le\ell}\tau_j\psi\;-\tilde{\psi}(\mathfrak{u}(t,i/N))\right\}\right]\\&\le\frac{1}{\eta(2\ell+1)N}\sum_{i\in\mathbb{T}_N}\log\mathbb{E}_{g^N_{\mathfrak{u}(t,\cdot)}}\left[e^{\eta\sum_{|k-i|\le\ell}\left\{\tau_k\psi-\tilde{\psi}(\mathfrak{u}(t,i/N))\right\}}\right]\end{aligned} \tag{3.3.6}$$

As N goes to infinity this sum converges to

$$\frac{1}{\eta(2\ell+1)}\int_{\mathbb{T}}\log\mathbb{E}_{g_{\mathfrak{u}(t,x)}}\left[e^{\eta\sum_{|k|\le\ell}\left\{\tau_k\psi-\tilde{\psi}(\mathfrak{u}(t,x))\right\}}\right]$$

By the standard inequalities

$$e^x\le1+|x|+\frac{x^2}{2}e^{|x|},\quad\log(1+|x|)\le|x|$$

we get that the previous integral is bounded above by

$$\frac{1}{2\ell+1}\int_{\mathbb{T}} \mathbb{E}_{g_{\mathfrak{u}(t,x)}}\left[\left|\sum_{|k|\le\ell}\left\{\tau_k\psi - \tilde{\psi}(\mathfrak{u}(t,x))\right\}\right|\right] + 2\eta\|\psi\|_\infty^2(2\ell+1)\exp(2\eta(2\ell+1)\|\psi\|_\infty) \tag{3.3.7}$$

We choose $\eta = (2\ell+1)^{-1}\varepsilon$ with $\varepsilon > 0$ going to 0 after ℓ. By the law of large numbers and the dominated convergence theorem (ψ is bounded), (3.3.7) goes to zero. □

Proposition 3.3.3

$$\frac{d}{dt}H_N(t) = -\int \left[(N\mathcal{A}_N + \partial_t)\log g^N_{\mathfrak{u}(t,\cdot)}\right] f_N(t)\, d\mathbf{r}\, d\mathbf{p}$$

Proof. To simplify notations, let us denote $f_t = f_N(t)$, and $g_t = g^N_{\mathfrak{u}(t,\cdot)}$. Then

$$\begin{aligned}\frac{d}{dt}H_N(t) &= \int (\partial_t f_t)\log(f_t/g_t)d\mathbf{r}\, d\mathbf{p} + \int \partial_t f_t d\mathbf{r}\, d\mathbf{p} - \int \partial_t(\log g_t) f_t d\mathbf{r}\, d\mathbf{p}\\ &= \int f_t N\mathcal{A}_N \log(f_t) d\mathbf{r}\, d\mathbf{p} - \int f_t[N\mathcal{A}_N + \partial_t]\log(g_t)d\mathbf{r}\, d\mathbf{p}\\ &= -\int f_t[N\mathcal{A}_N + \partial_t]\log(g_t)d\mathbf{r}\, d\mathbf{p}\end{aligned}$$

□

We compute now $[N\mathcal{A}_N + \partial_t]\log(g_t)$. Observe that with the notations we have introduced we can write

$$\log g_t = \sum_{i\in\mathbb{T}_N}\left[\mathfrak{v}(t,i/N)\cdot\xi_i - \Theta(\mathfrak{v}(t,i/N)\right] \tag{3.3.8}$$

with $\xi_i = (r_i, p_i, -\mathcal{E}_i)$.

$$\begin{aligned}N\mathcal{A}_N\log(g_t) &= \sum_{i\in\mathbb{T}_N} N\left[\mathfrak{v}\left(t,\frac{i+1}{N}\right) - \mathfrak{v}\left(t,\frac{i}{N}\right)\right]\cdot\tilde{\mathbf{J}}^a_i\\ &= \sum_{i\in\mathbb{T}_N}(\partial_y\mathfrak{v})(t,i/N)\cdot\tilde{\mathbf{J}}^a_i + R^a_N(t)\end{aligned} \tag{3.3.9}$$

where $\tilde{\mathbf{J}}^a_i$ is defined by

$$\tilde{\mathbf{J}}^a_i = (p_{i+1}, V'(r_i), -p_{i+1}V'(r_i))$$

By lemma 3.3.1 and the smoothness of $\mathfrak{v}$ we have that R_N^a/N is small in the sense

$$\lim_{N\to\infty} \int_0^t ds \int d\mathbf{r} d\mathbf{p}\, f_s^N \left(N^{-1} R_N^a(s)\right) = 0 \tag{3.3.10}$$

By the isoentropic property of the solution $\mathfrak{u}(t,y)$, we have

$$\int_{\mathbb{T}} \partial_y \mathfrak{v}(t,y) \cdot \tilde{\mathbf{J}}(\tilde{\mathfrak{u}}(t,y))\, dy = -\int_{\mathbb{T}} \mathfrak{v}(t,y) \cdot \partial_y(\tilde{\mathbf{J}}(\tilde{\mathfrak{u}}))\, dy = \int_{\mathbb{T}} (D\mathbb{S})(\mathfrak{u}) \cdot (\partial_y \widehat{\mathbf{J}})(\mathfrak{u}) dy = 0$$

so also

$$\frac{1}{N} \sum_i (\partial_y \mathfrak{v})(t, i/N) \cdot \tilde{\mathbf{J}}(\tilde{\mathfrak{u}}(t,i/N)) \longrightarrow 0$$

We have then obtained that

$$N\mathcal{L}_N \log(g_t) = -\sum_i (\partial_y \mathfrak{v})(t,i/N) \cdot \left[\tilde{\mathbf{J}}_i^a - \tilde{\mathbf{J}}(\tilde{\mathfrak{u}}(t,i/N))\right] + R_N(t)$$

with R_N/N small in the sense (3.3.10).

We compute now $\partial_t \log g_t^N$:

$$\partial_t \log g_t^N = \sum_i \left[(\partial_t \mathfrak{v})(t,i/N) \cdot \xi_i - \partial_t \Theta(\mathfrak{v}(t,i/N))\right]$$

then

$$\partial_t \Theta(\mathfrak{v}(t,\cdot)) = D\Theta(\mathfrak{v}(t,\cdot)) \cdot \partial_t \mathfrak{v}(t,\cdot) = \tilde{\mathfrak{u}}(t,\cdot) \cdot \partial_t \mathfrak{v}(t,\cdot)$$

which gives

$$\partial_t \log g_t^N = \sum_i \left[(\partial_t \mathfrak{v})(t,i/N) \cdot (\xi_i - \tilde{\mathfrak{u}}(t,i/N))\right] \tag{3.3.11}$$

Recall that by proposition 3.1.1

$$(\partial_t \mathfrak{v})(t,y) = (D\tilde{\mathbf{J}})(\tilde{\mathfrak{u}}(t,y)) \partial_y \mathfrak{v}(t,y) \tag{3.3.12}$$

Resuming we have obtained that

$$\begin{aligned} &-(N\mathcal{L}_N + \partial_t) \log g_t^N \\ &= -\sum_{i\in\mathbb{T}_N} \partial_y \mathfrak{v}(t,i/N) \cdot \left[\tilde{\mathbf{J}}_i^a - \tilde{\mathbf{J}}(\tilde{\mathfrak{u}}(t,i/N)) - (D\tilde{\mathbf{J}})(\tilde{\mathfrak{u}}(t,i/N))(\xi_i - \tilde{\mathfrak{u}}(t,i/N))\right] + R_N(t) \end{aligned} \tag{3.3.13}$$

We first need to do some cutoff in order to deal after only with bounded variables. Let $A_{i,l} = \{|\mathcal{E}_i| \le l\}$, and define $\tilde{\mathbf{J}}^a_{i,l} = \tilde{\mathbf{J}}^a_i \mathbf{1}_{A_{i,l}}$ and $\xi_{i,l} = \xi_i \mathbf{1}_{A_{i,l}}$. By the properties of V, we have that $\tilde{\mathbf{J}}^a_{i,l}$ and $\xi_{i,l}$ are bounded.

Then, by entropy inequality, for any $\nu > 0$ sufficiently small

$$\begin{aligned}\int d\mathbf{r}d\mathbf{p} f_t^N \sum_i (\partial_y \mathfrak{v})(t, i/N) \cdot \tilde{\mathbf{J}}^a_i \mathbf{1}_{A^c_{i,l}} \\ \le \frac{1}{\nu} \sum_i \log\left(1 + \int_{A^c_{i,l}} e^{\nu \partial_y \mathfrak{v}(t,i/N)\cdot \tilde{\mathbf{J}}^a_i + \mathfrak{v}(t,i/N)\cdot \xi_i - \Theta(\mathfrak{v}(t,i/N))}\right) + \frac{H_N(t)}{\nu} \\ = \frac{N o(l)}{\nu} + \frac{H_N(t)}{\nu}\end{aligned}$$

with $o(l)$ that tends to 0 as $l \to \infty$.

We introduce now some averaging on a *microscopic* block of size k. We will let $k \to \infty$ **after** $N \to \infty$. To simplify notations we assume k divides N and k is even. We denote $\Lambda_k(y) = \{x \in \mathbb{T}_N; |y - x| \le (k-1)/2\}$ the box of length k centered around y and we introduce the *microscopic* averaged profiles

$$\tilde{\mathfrak{u}}_{N,k}(i) = \frac{1}{k} \sum_{j \in \Lambda_k(i)} \xi_j, \quad \xi_j = (r_j, p_j, -\mathcal{E}_j) \tag{3.3.14}$$

First observe that, using the smoothness of $\partial_y \mathfrak{v}$we can bound the difference

$$\sum_{i \in \mathbb{T}_N} \partial_y \mathfrak{v}(t, i/N) \cdot \left[\tilde{\mathbf{J}}^a_{i,l} - \frac{1}{k} \sum_{j \in \Lambda_k(i)} \tilde{\mathbf{J}}^a_{j,l}\right] \le C_1 k l$$

Similarly we have

$$\sum_{i \in \mathbb{T}_N} \partial_y \mathfrak{v}(t, i/N) \cdot (D\tilde{\mathbf{J}})(\tilde{\mathfrak{u}}(t, i/N)) \left[\xi_i - \frac{1}{k} \sum_{j \in \Lambda_k(i)} \xi_j\right] \le C_1 \frac{k}{N} \sum_{i \in \mathbb{T}_N} \mathcal{E}_i$$

In section 3.4 we will prove that

$$\lim_{l \to \infty} \lim_{k \to \infty} \lim_{N \to \infty} \int_0^t ds \int d\mathbf{r}d\mathbf{p} f_s^N(\mathbf{r}, \mathbf{p}) \frac{1}{N} \sum_{i \in \mathbb{T}_N} \left| \frac{1}{k} \sum_{j \in \Lambda_k(i)} \tilde{\mathbf{J}}^a_{j,l} - \tilde{\mathbf{J}}(\tilde{\mathfrak{u}}_{N,k}(i)) \right| = 0 \tag{3.3.15}$$

Then we have to deal with

$$N^{-1}\sum_{i=1}^{N}\partial_y\mathfrak{v}(t,i/N)\cdot\Big[\tilde{\mathbf{J}}(\tilde{\mathfrak{u}}_{N,k}(i))-\tilde{\mathbf{J}}(\tilde{\mathfrak{u}}(t,i/N))-(D\tilde{\mathbf{J}})(\tilde{\mathfrak{u}}(t,i/N))(\tilde{u}_{N,k}(i)-\tilde{\mathfrak{u}}(t,i/N))\Big] \tag{3.3.16}$$

for any positive constant A.

Here again, we use the decomposition (3.3.4). We rewrite (3.3.16) as a sum of $(k+1)/2$ terms, each term indexed by ℓ being the sum of N/k averages in disjoint microscopic boxes of length k

$$\begin{aligned}
-(NL+\partial_t)g_t^N &= \sum_{\ell=0}^{(k-1)/2}\sum_{j=1}^{N/k}\mathbf{G}(t,y_j^\ell/N)\cdot\mathbf{\Omega}(\tilde{\mathfrak{u}}_{N,k}(y_j^\ell);\tilde{\mathfrak{u}}(t,y_j^\ell/N))+R_{N,k,l}(t)\\
&\mathbf{\Omega}(\mathbf{w},\mathbf{u})=\tilde{\mathbf{J}}(\mathbf{w})-\tilde{\mathbf{J}}(\mathbf{u})-(D\tilde{\mathbf{J}})(\mathbf{u})(\mathbf{w}-\mathbf{u})\\
&\mathbf{G}(t,y)=-\partial_y\mathfrak{v}(t,y)
\end{aligned} \tag{3.3.17}$$

and

$$\lim_{l\to\infty}\lim_{k\to\infty}\lim_{N\to\infty}\frac{1}{N}\int_0^T\int R_{N,k,l}(t)f_s^N d\mathbf{r}d\mathbf{p}=0$$

Using again the entropy inequality (B.1.2), we are left to prove that for $\eta>0$ small enough

$$\lim_{k\to\infty}\lim_{N\to\infty}\frac{1}{k}\sum_{\ell=0}^{(k-1)/2}\left\{\frac{1}{N}\log\int e^{\eta k\sum_{j=1}^{N/k}\mathbf{G}(t,y_j^\ell/N)\cdot\Omega(\tilde{\mathfrak{u}}_{N,k}(y_j^\ell);\tilde{\mathfrak{u}}(t,y_j^\ell/N))}g_t^N\,dpdr\right\}=0 \tag{3.3.18}$$

Since we have arranged the sum over j's on disjoint blocks, that are independently distributed by g_t^N, the left hand side of (3.3.18) is equal to

$$\lim_{k\to\infty}\lim_{N\to\infty}\frac{1}{k}\sum_{\ell=0}^{(k-1)/2}\left\{\frac{k}{N}\sum_{j=1}^{N/k}\frac{1}{k}\log\int e^{\eta k\mathbf{G}(t,y_j^\ell/N)\cdot\mathbf{\Omega}(\tilde{\mathfrak{u}}_{N,k}(y_j^\ell);\tilde{\mathfrak{u}}(t,y_j^\ell/N))}g_t^N\,dpdr\right\}$$

One shows this limit is equal to 0 by using the large deviation properties of the product measure g_t^N, that locally is almost homogeneous. In fact by using the smoothness for the various functions involved, we can substitute, in the previous expression, the inhomogeneous g_t^N with a product homogeneous measure $g_{\mathfrak{u}(t,y_j^\ell/N)}$, with a prize small in k/N and uniform on ℓ and we are left with

$$\lim_{k\to\infty}\lim_{N\to\infty}\frac{1}{k}\sum_{\ell=0}^{(k-1)/2}\left\{\frac{k}{N}\sum_{j=1}^{N/k}\frac{1}{k}\log\int e^{\eta k\mathbf{G}(t,y_j^\ell/N)\cdot\mathbf{\Omega}(\tilde{\mathfrak{u}}_k;\tilde{\mathfrak{u}}(t,y_j^\ell/N))}g_{\mathfrak{u}(t,y_j^\ell/N)}\,dpdr\right\}=0$$

where $\tilde{\mathfrak{u}}_k = k^{-1}\sum_{|x|\le k/2}\xi_x$.

The limit in N results in an integral over $\mathbb{T}$ because we have a Riemann sum and the functions involved are smooth. Observe also the limit in N is independent of ℓ. Then by applying the Laplace-Varadhan's theorem A.4.1 for this product measures one obtains

$$\lim_{k\to\infty}\lim_{N\to\infty}\frac{1}{k}\sum_{\ell=0}^{(k-1)/2}\left\{\frac{k}{N}\sum_{j=1}^{N/k}\frac{1}{k}\log\int e^{\eta k\mathbf{G}(t,y_j^\ell/N)\cdot\boldsymbol{\Omega}(\tilde{\mathfrak{u}}_k;\tilde{\mathfrak{u}}(t,y_j^\ell/N))}g_{\mathfrak{u}(t,y_j^\ell/N)}\,dpdr\right\}$$
$$=\frac{1}{2}\int_{\mathbb{T}}dy\ \sup_{\mathfrak{w}}\left\{\eta\mathbf{G}(t,y)\cdot\Omega(\mathfrak{w},\tilde{\mathfrak{u}}(t,y))-I(\mathfrak{w},\tilde{\mathfrak{u}}(t,y))\right\} \tag{3.3.19}$$

where $I(\mathfrak{w},\tilde{\mathfrak{u}}(t,y))$ is the rate function of $(\xi_x)_x$ as $(r_x,p_x)_x$ are distributed according to the homogenous product measure $g_{\mathfrak{u}(t,y)}(\mathbf{r},\mathbf{p})d\mathbf{r}d\mathbf{p}$. From now we omit the dependance in (t,y) of the involved functions $\mathfrak{u},\tilde{\mathfrak{u}},\mathfrak{v}$. Recall (3.2.2) and that $\tilde{\mathfrak{u}}$ and $\mathfrak{v}$ are in duality then we have

$$\begin{aligned} I(\mathfrak{w},\tilde{\mathfrak{u}}) &= \sup_{\mathbf{x}}\left\{\mathbf{x}\cdot\mathbf{w}-\log\left(\int e^{\mathbf{x}\cdot\xi}e^{\mathfrak{v}\cdot\xi-\Theta(\mathfrak{v})}d\mathbf{r}d\mathbf{p}\right)\right\}\\ &= \sup_{\mathbf{x}}\left\{\mathbf{x}\cdot\mathbf{w}-\Theta(\mathfrak{v}+\mathbf{x})+\Theta(\mathfrak{v})\right\}\\ &= \Theta(\mathfrak{v})-\mathfrak{v}\cdot\mathfrak{w}+\Phi(\mathfrak{w}) \end{aligned}$$

where the last equality follows from the equality between the Fenchel-Legendre transform of Θ and the function Φ.

Hence we have

$$I(\mathfrak{w},\tilde{\mathfrak{u}})=\Phi(\mathfrak{w})+\Theta(\mathfrak{v})-\mathfrak{w}\cdot\mathfrak{v} \tag{3.3.20}$$

Notice that $I(\tilde{\mathfrak{u}},\tilde{\mathfrak{u}})=0$ and that

$$(D_{\mathfrak{w}}I)(\mathfrak{w},\tilde{\mathfrak{u}})=D\Phi(\mathfrak{w})-D\Phi(\tilde{\mathfrak{u}}) \tag{3.3.21}$$

so also $D_{\mathfrak{w}}I(\tilde{\mathfrak{u}},\tilde{\mathfrak{u}})=0$. Furthermore I is strictly convex in $\mathfrak{w}$:

$$(D^2_{\mathfrak{w}}I)(\mathfrak{w},\tilde{\mathfrak{u}})=(D^2\Phi)(\mathfrak{w})>0 \tag{3.3.22}$$

Since $\boldsymbol{\Omega}(\tilde{\mathfrak{u}},\tilde{\mathfrak{u}})=0$ and

$$D_{\mathfrak{w}}\boldsymbol{\Omega}(\mathfrak{w},\tilde{\mathfrak{u}})=(D\tilde{\mathbf{J}})(\mathfrak{w})-(D\tilde{\mathbf{J}})(\tilde{\mathfrak{u}}) \tag{3.3.23}$$

we also have $(D_{\mathfrak{w}}\boldsymbol{\Omega})(\tilde{\mathfrak{u}},\tilde{\mathfrak{u}})=0$.

Lemma 3.3.4 *For $\eta > 0$ small enough*

$$\eta \mathbf{G}(t,y) \cdot \mathbf{\Omega}(\mathfrak{w}, \tilde{\mathfrak{u}}(t,y)) \le I(\mathfrak{w}, \tilde{\mathfrak{u}}(t,y)), \qquad \forall \mathfrak{w}$$

Proof This follows from condition (3.1.10) on V (exercise) □

Consequently for η small enough

$$\sup_{\mathfrak{w}} \{\eta \mathbf{G}(t,y) \cdot \mathbf{\Omega}(\mathfrak{w}, \tilde{\mathfrak{u}}(t,y)) - I(\mathfrak{w}, \tilde{\mathfrak{u}}(t,y))\} = 0 \tag{3.3.24}$$

and we have finally proved that

$$\frac{d}{dt} H_N(t) \le C H_N(t) + \tilde{R}_{N,k,l}(t)$$

with $\lim_{l\to\infty} \lim_{k\to\infty} \lim_{N\to\infty} \int_0^t N^{-1} \tilde{R}_{N,k,l}(s)\ ds = 0$. By Gronwall's inequality we obtain

$$\lim_{N\to\infty} \frac{H_N(t)}{N} = 0$$

and by proposition 3.3.2 the hydrodynamic limit follows.

3.4 Proof of one block lemma

We now prove lemma 3.3.15, which is a weak form of local equilibrium. It is now that we use the stochastic perturbation of the dynamics. Thanks to the characterization of the infinite volume ergodic measures of chapter 2, the proof is very simple.

We define the space time average of the distribution:

$$\bar{f}^N = \frac{1}{tN} \sum_{i=1}^{N} \int_0^t \tau_i f_s^N\ ds$$

and $\bar{f}_k^N$ its projection on $\{(r_i, p_i) \in \mathbb{R}^{2(k+1)};\quad i \in \Lambda_k\}$ where $\Lambda_k = \{-[k/2]-1, \dots, [k/2]+1\}$. We also denote $d\nu^N = \bar{f}^N \prod_{i\in\mathbb{T}_N} dr_i dp_i$ and $d\nu_k^N = \bar{f}_k^N \prod_{i\in\Lambda_k} dr_i dp_i$ the corresponding probability measures on $\mathbb{R}^N$ on $\mathbb{R}^{2(k+1)}$.

Lemma 3.4.1 *For each fixed k, the sequence of probability measure $(\nu_k^N)_{N\ge k}$ is tight.*

Proof

It is enough to prove that there exists a $C_k < \infty$ independent on N such that

$$\int \sum_{i \in \Lambda_k} \left[p_i^2/2 + V(r_i) \right] d\nu_k^N \leq C_k$$

Since entropy is decreasing and convex and because of the initial condition we have

$$H(\nu^N | \mu_{0,0,1}^{gc}) \leq C_0 N$$

Consider the partition of $\{0, \ldots, N-1\}$ into $p = N/|\Lambda_k|$ consecutive dijoint boxes of length $|\Lambda_k|$: $\{0, \ldots, N-1\} = \cup_{j=1}^{p} \Lambda_k(j)$. By translation invariance of ν_N, we have

$$H_{\Lambda_k}(\nu^N | \mu_{0,0,1}^{gc}) = H_{\Lambda_k(j)}(\nu^N | \mu_{0,0,1}^{gc}), \quad j = 1, \ldots, p$$

By the superadditivity property B.1.4 of entropy we have

$$H(\nu^N | \mu_{0,0,1}^{gc}) \geq \sum_{j=1}^{p} H_{\Lambda_k(j)}(\nu^N | \mu_{0,0,1}^{gc}) = p H_{\Lambda_k}(\nu^N | \mu_{0,0,1}^{gc})$$

Hence we get

$$H_{\Lambda_k}(\nu_k^N | \mu_{0,0,1}^{gc}) \leq C_0 |\Lambda_k| \tag{3.4.1}$$

and by entropy inequality it follows

$$\int \sum_{i \in \Lambda_k} \left[p_i^2/2 + V(r_i) \right] d\nu_k^N \leq C_k$$

□

For any k let ν_k be a limit point of the sequence $(\nu_k^N)_{N \geq 1}$. The sequence of probability measures $(\nu_k)_{k \geq 1}$ forms a consistent family and by Kolmogorov's theorem there exists a unique probability measure ν on $(\mathbb{R} \times \mathbb{R})^{\mathbb{Z}}$ such that the restriction of ν on $\{(r_i, p_i) \in \mathbb{R}^{2(k+1)}; \quad i \in \Lambda_k\}$ is ν_k. One has easily that ν is invariant by translations. Moreover, by lower semicontinuity of entropy and (3.4.1) there exists a constant C_0 such that for any $k \geq 1$,

$$H_{\Lambda_k}(\nu_k | \mu_{0,0,1}^{gc}) \leq C_0 |\Lambda_k| \tag{3.4.2}$$

It remains to show the following lemma

Lemma 3.4.2 *For any bounded smooth local function $F(r,p)$, we have*

$$\int \mathcal{L} F \, d\nu = 0$$

Proof Let F be a bounded smooth local function with support included in $(\mathbb{R}\times\mathbb{R})^{\Lambda_k}$. We have

$$\int \mathcal{L}F\, d\nu = \int \mathcal{L}F\, d\nu_k = \lim_{N\to\infty}\int \mathcal{L}F\, d\nu_k^N \tag{3.4.3}$$

Define $G = N^{-1}\sum_{x=0}^{N-1}\tau_x F$. By Ito's formula

$$\begin{aligned} N^{-1}\left\{\int d\mathbf{r}d\mathbf{p}G(\mathbf{r},\mathbf{p})f_t^N(\mathbf{r},\mathbf{p}) - \int d\mathbf{r}d\mathbf{p}G(\mathbf{r},\mathbf{p})f_0^N(\mathbf{r},\mathbf{p})\right\} \\ = \int_0^t ds\int d\mathbf{r}d\mathbf{p}(\mathcal{L}G)(\mathbf{r},\mathbf{p})f_s^N(\mathbf{r},\mathbf{p}) \\ = t\int d\mathbf{r}d\mathbf{p}(\mathbf{r},\mathbf{p})(\mathcal{L}F)(\mathbf{r},\mathbf{p})\bar{f}^N(\mathbf{r},\mathbf{p}) \\ = t\int d\nu_k^N(\mathbf{r},\mathbf{p})(\mathcal{L}F)(\mathbf{r},\mathbf{p}) \end{aligned}$$

Since F (and hence G) is bounded the right side of (3.4.4) goes to 0 as N goes to infinity and it follows that

$$\int d\nu(\mathbf{r},\mathbf{p})(\mathcal{L}F)(\mathbf{r},\mathbf{p}) = 0 \tag{3.4.4}$$

□

By theorem 2.2.3, ν is convex combination of Gibbs measures $\mu^{gc}_{\tau,\bar{p},\beta}$. Then we have

$$\begin{aligned} \limsup_{k\to\infty}\limsup_{N\to\infty}\sup_{j=0,\dots,N/k}\int d\nu_k^N\left|\frac{1}{k}\sum_{|i-kj|<k/2}\tilde{\mathbf{J}}_i^a + \tilde{\mathbf{J}}(\mathfrak{u}_{N,k}(y_j))\right|\mathbf{1}_{\left|\tilde{\mathfrak{u}}_{N,k}(y_j)\right|\le A} \\ \le \limsup_{k\to\infty}\sup_{B_k\in\mathcal{B}}\sup_{\nu\in\mathcal{G}}\int d\nu\left|\frac{1}{k}\sum_{i\in B_k}\tilde{\mathbf{J}}_i^a - \tilde{\mathbf{J}}\left(\frac{1}{k}\sum_{i\in B_k}\xi_i\right)\right|\mathbf{1}_{\frac{1}{k}\sum_{i\in B_k}|\xi_i|\le A} \end{aligned}$$

where $\mathcal{B}$ is the set of boxes $i+\Lambda_k$, $i\in\mathbb{Z}$, and $\mathcal{G}$ the set of Gibbs measures $\mu^{gc}_{\tau,\bar{p},\beta}$. Observe that we can forget the supremum over $\mathcal{B}$ since Gibbs measures are translation invariant. By taking the conditional expectation with respect to $k^{-1}\sum_{i\in B_k}\xi_i$ and thanks to the indicator function we are left to prove

$$\limsup_{k\to\infty}\sup_{|\mathbf{x}|\le A}\int d\mu_{\mathbf{x}}^{k,mc}\left|\frac{1}{k}\sum_{i=0}^{k-1}\tilde{\mathbf{J}}_i^a - \tilde{\mathbf{J}}(\mathbf{x})\right| = 0 \tag{3.4.5}$$

Here again we divide the box $\Lambda_k(k/2)$ in q disjoint boxes $(\Lambda_\ell^j)_{j=1,\dots,q}$ of length ℓ (assuming that ℓ divides k) and we use the fact that under $\mu_{\mathbf{x}}^{k,mc}$ the distribution of $(\xi_i)_{i\in\Lambda_\ell^j}$ is independent of j. Then we have to show

$$\lim_{\ell\to\infty}\lim_{k\to\infty}\sup_{|\mathbf{x}|\le A}\int d\mu_{\mathbf{x}}^{k,mc}\left|\frac{1}{\ell}\sum_{i=0}^{\ell-1}\tilde{\mathbf{J}}_i^a-\tilde{\mathbf{J}}(\mathbf{x})\right|=0$$

Then we apply the equivalence of ensembles theorems 1.2.1 and 1.2.2 and we get lemma **??**.

3.5 Some remarks on the hyperbolic scaling

Observe that the proof applies to the harmonic case $V(r)=r^2/2$. In this case

$$s=-\frac{1}{2\pi}\log\frac{\beta}{2\pi}$$

and

$$\mathfrak{e}=\frac{\mathfrak{r}^2+\mathfrak{u}^2}{2}+\beta^{-1}$$

and equations (3.1.3) take the form

$$\begin{aligned}\partial_t\mathfrak{r}&=\partial_y\mathfrak{p}\\ \partial_t\mathfrak{p}&=\partial_y\mathfrak{r}\\ \partial_t\mathfrak{e}&=\partial_y\left(\mathfrak{p}\mathfrak{r}\right)\end{aligned}\tag{3.5.1}$$

i.e. $\mathfrak{r}(t,y)$ satisfies linear wave equation $\partial_{tt}\mathfrak{r}=\partial_{yy}\mathfrak{r}$, temperature profile $T(y)=\beta^{-1}(y)$ stays constant in time and energy evolves by

$$\partial_t e=\partial_y(\partial_t\mathfrak{r}^2/2)$$

If we take solution of the form $\mathfrak{r}(t,y)=\mathfrak{r}_0(y+t)$, then the energy is given by

$$\mathfrak{e}(t,y)=\mathfrak{r}_0(y+t)^2+\beta^{-1}(y).$$

This *coherent* macroscopic evolution of the energy is due to the microscopic noise (even if the parameter γ of the strength of the noise is not present). In fact in the deterministic harmonic chain ($\gamma=0$), energy is *dispersed* and does not have such macroscopic evolution. Without noise the energy of each Fourier mode k is conserved, and this energy moves with speed $\omega'(k)$, where $\omega(k)=2|\sin(2\pi k)|$ is the dispersion relation of the system.

3.6 Bibliographical notes

The relative entropy method was introduced by H. T. Yau in [15], where was used in the diffusive scaling of the gradient Ginzgurg-Landau model. The method was then used in [12] for the Euler dynamics for a compressible gas. This exposition is largely inspired to [12]. The advantage to work on this lattice case, with respect to the gas dynamics of [12], is that we can work here with quadratic cinetic energies, while in [12] were assumed bounded velocities. A clear exposition of the method for scalar hyperbolic equations (one conserved quantity) can be found in the book of Kipnis-Landim [8], applied to the asymmetric zero range process.

Chapter 4

Equilibrium Fluctuations

4.1 Static Fluctuations

We look in this chapter to the evolution of the fluctuations of the conserved quantities for the system in equilibrium. It will be easier here to consider the infinite system on $\mathbb{Z}$, with initial conditions distributed by the Gibbs measure $\mu_{\lambda,\bar{p},\beta}$, with $\lambda = -(D_r s)(\bar{r},\bar{p},\bar{e})$, and $\beta = (D_e s)(\bar{r},\bar{p},\bar{e})$. With the symmetric notations introduced in the previous chapter we denote $\bar{v} = (\lambda, \beta p, \beta) = D\phi(\bar{u})$, where $\bar{u} = (\bar{r},\bar{p},-\bar{e})$, and

$$d\mu_{\lambda,\bar{p},\beta} = d\mu_{\bar{v}} = \prod_{x\in\mathbb{Z}} e^{\bar{v}\cdot\xi_x - \Theta(\bar{v})} dp_x dr_x$$

with $\xi_x = (r_x, p_x, -e_x)$.

The fluctuations fields are defined as distributions on $\mathbb{R}$ defined by

$$\tilde{\mathfrak{u}}_N(\mathbf{G}) = \frac{1}{\sqrt{N}} \sum_x \mathbf{G}(x/N) \cdot (\xi_x - \bar{u}) \tag{4.1.1}$$

where $\mathbf{G}(y) = (G_1(y), G_2(y), G_3(y))$ is a smooth (vector valued) test function with compact support on $\mathbb{R}$.

Since $\mu_{\bar{v}}$ is a product measure, the standard central limit theorems for independent random variables say that

$$\tilde{\mathfrak{u}}_N \xrightarrow[N\to\infty]{\text{law}} \tilde{\mathfrak{u}}$$

where $\tilde{\mathfrak{u}}$ is a (vector valued) centered Gaussian field on $\mathbb{R}$ with covariance

$$\mathbb{E}(\tilde{\mathfrak{u}}(y) \otimes \tilde{\mathfrak{u}}(y')) \;=\; (D^2\Theta)(\bar{v})\delta(y - y') \tag{4.1.2}$$

i.e.

$$\mathbb{E}(\tilde{\mathfrak{u}}_N(\mathbf{G})\tilde{\mathfrak{u}}_N(\mathbf{F})) \underset{N\to\infty}{\longrightarrow} \int_{\mathbb{R}} \mathbf{G}(y)\cdot(D^2\Theta)(\bar{v})\mathbf{F}(y)\,dy = \sum_{i,j}^{3}(D^2\Theta)(\bar{v})_{i,j}\int G_i(y)F_j(y)\,dy$$

4.2 Evolution of Fluctuations: hyperbolic scaling

We start the infinite system with the equilibrium distribution $\mu_{\bar{v}}$, and we look at the fluctuations fields at the hyperbolic time scaling:

$$\tilde{\mathfrak{u}}_N(Nt,\mathbf{G}) = \frac{1}{\sqrt{N}}\sum_x \mathbf{G}(x/N)\cdot(\xi_x(Nt)-\bar{u})$$

Computing the time evolution of this fluctuation field, with similar computation as done for (3.3.9), we have

$$\begin{aligned}
\tilde{\mathfrak{u}}_N(Nt,\mathbf{G}) - \tilde{\mathfrak{u}}_N(0,\mathbf{G}) &= \int_0^t \frac{1}{\sqrt{N}}\sum_x N\left[\mathbf{G}(\frac{x+1}{N}) - \mathbf{G}(\frac{x}{N})\right]\cdot\mathbf{J}_x(Ns)\,ds \\
&= \int_0^t \frac{1}{\sqrt{N}}\sum_x N\left[\mathbf{G}(\frac{x+1}{N}) - \mathbf{G}(\frac{x}{N})\right]\cdot\left(\mathbf{J}_x(Ns) - \widehat{\mathbf{J}}(\bar{u})\right)\,ds \\
&= \int_0^t \frac{1}{\sqrt{N}}\sum_x \partial_y\mathbf{G}(x/N)\cdot\left(\mathbf{J}_x(Ns) - \widehat{\mathbf{J}}(\bar{u})\right)\,ds + R_N(t)
\end{aligned}$$

where $R_N(t)$ is a term that has small variance as $N\to\infty$ (*This needs to be proven later on*).

We can rewrite this as

$$\begin{aligned}
&\int_0^t \frac{1}{\sqrt{N}}\sum_x \partial_y\mathbf{G}(x/N)\cdot(D\widehat{\mathbf{J}})(\bar{v})\,(\xi_x(Ns)-\bar{u}) \\
&+\int_0^t \frac{1}{\sqrt{N}}\sum_x \partial_y\mathbf{G}(x/N)\cdot\tilde{\Omega}_x(Ns)\,ds + R_N(t)
\end{aligned}$$

with $\tilde{\Omega}_x = \mathbf{J}_x - \widehat{\mathbf{J}}(\bar{u}) - (D\widehat{\mathbf{J}})(\bar{v})\,(\xi_x-\bar{u})$.

The key point here is to prove that space-time variance of $\tilde{\Omega}_x$ is small as $N\to\infty$, in the sense that

$$\lim_{N\to\infty}\mathbb{E}_{\mu_{\bar{v}}}\left(\left[\int_0^t \frac{1}{\sqrt{N}}\sum_x \partial_y\mathbf{G}(x/N)\cdot\tilde{\Omega}_x(Ns)\,ds\right]^2\right) = 0 \qquad (4.2.1)$$

This is sometimes called Boltzmann-Gibbs principle.

A consequence of (4.2.1) is the convergence of $\tilde{\mathfrak{u}}_N(Nt,\cdot) \to \tilde{\mathfrak{u}}(t,\cdot)$, where this is the solution of the linearized equations:

$$\partial_t \tilde{\mathfrak{u}} = (D\widehat{\mathbf{J}})(\bar{u})\ \partial_y \tilde{\mathfrak{u}} \tag{4.2.2}$$

This means that in the hyperbolic scaling, fluctuations of the conserved quantities evolve deterministically following the linearized Euler equation (4.2.2), i.e.

$$\tilde{\mathfrak{u}}(t,\mathbf{G}) = \tilde{\mathfrak{u}}(0, e^{\mathcal{A}^* t}\mathbf{G})$$

where $\mathcal{A} = (D\widehat{\mathbf{J}})(\bar{u})\ \partial_y$ and $A^* = -(D\widehat{\mathbf{J}})(\bar{u})^*\ \partial_y$.

We call these equilibrium fluctuations since the centered gaussian distribution with covariance given by (4.1.2) is stationary for this linearized evolution. In fact computing the covariance

$$\begin{aligned}\mathbb{E}\left(\tilde{\mathfrak{u}}(t,\mathbf{G})\tilde{\mathfrak{u}}(t,\mathbf{F})\right) &= \int e^{\mathcal{A}^* t}\mathbf{G}(y)\cdot D\Theta(\bar{v}) e^{\mathcal{A}^* t}\mathbf{F}(y)\ dy \\ &= \int \mathbf{G}(y)\cdot e^{\mathcal{A}t} D\Theta(\bar{v}) e^{\mathcal{A}^* t}\mathbf{F}(y)\ dy\end{aligned}$$

its time derivative at $t = 0$ is

$$\begin{aligned}&\int \mathbf{G}(y)\cdot(\mathcal{A}D\Theta(\bar{v}) + D\Theta(\bar{v})\mathcal{A}^*)\mathbf{F}(y)\ dy \\ = &\int \mathbf{G}(y)\cdot\left(D\widehat{\mathbf{J}}(\bar{u})\ D\Theta(\bar{v}) - D\Theta(\bar{v})\ D\widehat{\mathbf{J}}(\bar{u})^*\right)\partial_y\mathbf{F}(y)\ dy\end{aligned}$$

By (**??**) we know that $D\widehat{\mathbf{J}}(\bar{u})D\Theta(\bar{v}) = D^2\Sigma(\bar{v})$ that is symmetric, we have:

$$D\widehat{\mathbf{J}}(\bar{u})\ D\Theta(\bar{v}) = D\Theta(\bar{v})\ D\widehat{\mathbf{J}}(\bar{u})^*$$

i.e. $d\mathbb{E}\left(\tilde{\mathfrak{u}}(t,\mathbf{G})\tilde{\mathfrak{u}}(t,\mathbf{F})\right)/dt = 0$.

The Boltzmann-Gibbs principle (4.2.1) is very hard to be proven, even for the stochastically perturbed dynamics, and at the moment is still an open problem.

4.3 Diffusive scaling

Looking at the evolution of the fluctuation field at the diffusive staling (i.e. at time N^2t instead of Nt, is even more difficult. One should first subtract the transport term appearing at the hyperbolic time and look for the evolution of

$$\widetilde{\mathfrak{u}}_N^d(t,\mathbf{G}) = \tilde{\mathfrak{u}}_N(N^2t, e^{-Nt\mathcal{A}^*}\mathbf{G}) \tag{4.3.1}$$

As a matter of fact, for the unpinned one dimensional models, if the stochastic perturbation conserves momentum and energy, we expect these fluctuations to evolve at a different time scale:

$$\tilde{\mathfrak{u}}_N(N^\alpha t, e^{-Nt\mathcal{A}^*}\mathbf{G}) \tag{4.3.2}$$

for some $\alpha < 2$. We will come back on this later on.

If we perturb with noise that conserve only momentum, then we expect diffusive behavior of this fluctuations. Since momentum is not conserved, at the hyperbolic time scale we do not have any evolution, i.e. $\mathcal{A} = 0$ in this case.

Let us look then at the evolution of

$$\begin{aligned} \widetilde{\mathfrak{r}}_N(t, G) &= \frac{1}{\sqrt{N}} \sum_x G(x/N)(r_x(N^2 t) - \bar{r}) \\ \widetilde{\mathfrak{e}}_N(t, G) &= \frac{1}{\sqrt{N}} \sum_x G(x/N)(e_x(N^2 t) - \bar{e}) \end{aligned} \tag{4.3.3}$$

under the dynamics generated by $L = A + \gamma S$, where

$$S = \sum_x (p_x \partial_{p_{x+1}} - p_{x+1}\partial_{p_x})^2$$

Since now momentum is not conserved, we set $\bar{p} = 0$ and the equilibrium parameters are $\bar{u} = (\bar{r}, 0, -\bar{e})$, and $\bar{v} = (\lambda, 0, \beta)$. Also notice that we are not searching for the macroscopic evolution for the momentum fluctuations: since momentum is not conserved these evolves at a much faster scale. On the $N^2 t$ time scale the momentum fluctuations are δ correlated also in time.

Since $J_{1,x} = p_x = -Sp_x$, using (**??**) we can rewrite

$$
\begin{aligned}
\frac{1}{N^{1/2}} \sum_x G(x/N)(r_x(N^2 t) - r_x(0)) &= -N^{1/2} \int_0^t \sum_x G'(x/N)\; p_x(N^2 s)\; ds + R_{4,N}(t) \\
&= -\frac{N^{1/2}}{\gamma} \int_0^t \sum_x G'(x/N)\; \gamma(Sp_x)(N^2 s)\; ds + R_{4,N}(t) \\
&= -\frac{N^{1/2-2}}{\gamma} \int_0^t \sum_x G'(x/N)\; (N^2 L p_x)(N^2 s)\; ds \\
&\quad + \frac{N^{1/2}}{\gamma} \int_0^t \sum_x G'(x/N)\; \gamma(A p_x)(N^2 s)\; ds + R_{4,N}(t) \\
&= \frac{1}{N^{3/2}\gamma} \sum_x G'(x/N)\; (p_x(0) - p_x(N^2 t)) + \int_0^t \frac{1}{N^{1/2}\gamma} \sum_x G'(x/N) p_{x+1}(N^2 s) dw_{x,x+1}(s) \\
&\quad + \frac{1}{N^{1/2}\gamma} \sum_x \int_0^t G''(x/N)\; V'(r_x(N^2 s))\; ds + R_{5,N}(t) \\
&= \frac{1}{N^{1/2}\gamma} \sum_x \int_0^t G''(x/N)\; V'(r_x(N^2 s))\; ds \\
&\quad + \int_0^t \frac{1}{(N\gamma)^{1/2}} \sum_x G'(x/N) p_{x+1}(N^2 s) dw_{x,x+1}(s) + R_{6,N}(t)
\end{aligned}
$$

where $R_{j,N}(t)$ are remainders that can be proven that have small variance as $N \to \infty$. Observe that the quadratic variation of the stochastic integral above is

$$
\int_0^t \frac{1}{N\gamma} \sum_x G'(x/N)^2 p_{x+1}^2(N^2 s)\; ds \underset{N\to\infty}{\longrightarrow} \frac{t}{\gamma\beta} \int G'(y)^2\; dy \tag{4.3.4}
$$

Computing the time evolution of the energy fluctuation field we obtain:

$$
\begin{aligned}
&\frac{1}{N^{1/2}}\sum_x G(x/N)(e_x(N^2t)-e_x(0))\\
&\quad= -N^{1/2}\int_0^t \sum_x G'(x/N)\; j_{x,x+1}(N^2s)\; ds\\
&\qquad+\int_0^t \sqrt{\frac{\gamma}{N}}\sum_x G'(x/N)p_xp_{x+1}(N^2s)dw_{x,x+1}(s)+R_{7,N}(t)\\
&\quad= -N^{1/2}\int_0^t \sum_x G'(x/N)\; j^a_{x,x+1}(N^2s)\; ds\\
&\qquad+\gamma N^{-1/2}\int_0^t \sum_x G''(x/N)p_x^2(N^2s))\; ds\\
&\qquad+\int_0^t \sqrt{\frac{\gamma}{N}}\sum_x G'(x/N)p_xp_{x+1}(N^2s)dw_{x,x+1}(s)+R_{7,N}(t)
\end{aligned}
$$

with $j^a_{x,x+1}=-(p_x+p_{x+1})V'(r_x)/2$. We encounter here the difficulty that $j^a_{x,x+1}$ is not a gradient, and apriori the first term of the RHS of the above expression looks big. Let us assume the following:

Assumption 4.3.1 *There exists a sequence of local functions $(h_n)_n$ and a constant $\kappa^a=\kappa^a(\lambda,\beta)$ such that*

$$
\lim_{n\to\infty}\lim_{N\to\infty}\mathbb{E}_{\mu_{\lambda,\beta}}\left(\left(N^{1/2}\int_0^t\sum_x G'(x/N)[j^a_{x,x+1}-\kappa^a(\tau_{x+1}\psi-\tau_x\psi)-\tau_xLh_n](N^2s)\,ds\right)^2\right)=0 \tag{4.3.5}
$$

where ψ is a local function such that $<\psi>_{\lambda,\beta}=\bar{e}$.

It basically means that the space–time variance of $j^a-\kappa^a(\tau_1\psi-\psi)-Lh_n$, in a box of size $N\times N^2$ is small. This permit to perform a second integration by part and obtain:

$$
\begin{aligned}
&\frac{1}{N^{1/2}}\sum_x G(x/N)(e_x(N^2t)-e_x(0))\\
&\quad= N^{-1/2}\int_0^t\sum_x G''(x/N)(\kappa^a\tau_x\psi+\gamma p_x^2)(N^2s)\;ds\\
&\qquad+\sqrt{\frac{\gamma}{N}}\int_0^t\sum_x G'(x/N)\;\left(\sum_z[Y_z\tau_xh_n]dw_{z,z+1}(s)+p_xp_{x+1}(N^2s)dw_{x,x+1}(s)\right)\\
&\qquad-N^{-3/2}\sum_x G'(x/N)(\tau_xh_n(N^2t)-\tau_xh_n(0))+R_{8,N}(t).
\end{aligned}
$$

The quadratic variation of the stochastic integral in the above expression gives, as $N \to \infty$

$$Dt \int G'(y)^2 \, dy$$

where we will precise later D.

Resuming we have obtained

$$\begin{pmatrix} \widetilde{\mathfrak{r}}_N(t,G_1) \\ \widetilde{\mathfrak{e}}_N(t,G_2) \end{pmatrix} - \begin{pmatrix} \widetilde{\mathfrak{r}}_N(0,G_1) \\ \widetilde{\mathfrak{e}}_N(0,G_2) \end{pmatrix} = N^{-1/2} \int_0^t \sum_x \mathbf{G}''(x/N) \cdot (\mathfrak{J}_x(N^2 s) - \bar{\mathfrak{J}}(\bar{u})) \, ds \\ + \mathbf{M}_N(t, D\mathbf{G}) + R_{9,N}(t)$$

with

$$\mathfrak{J}_x = \begin{pmatrix} \gamma^{-1} V'(r_x) \\ \kappa^a \psi + \gamma p_x^2 \end{pmatrix}, \qquad \bar{\mathfrak{J}}(\bar{u}) = < \mathfrak{J}_0 >_{\bar{v}} = \begin{pmatrix} \lambda/\beta \\ (\kappa^a + \gamma)\bar{e} \end{pmatrix}$$

and $R_{9,N}(t)$ a remainder with a small variance as $N \to \infty$.

We need now a Boltzmann-Gibbs principle similar to (4.2.1):

$$\lim_{N\to\infty} \mathbb{E}_{\mu_{\bar{v}}} \left(\left[\int_0^t \frac{1}{\sqrt{N}} \sum_x \partial_y \mathbf{G}''(x/N) \cdot \widetilde{\Omega}_x(N^2 s) \, ds \right]^2 \right) \; = \; 0 \qquad (4.3.6)$$

with

$$\widetilde{\Omega}_x = \mathfrak{J}_x(N^2 s) - \bar{\mathfrak{J}}(\bar{u}) - D\bar{\mathfrak{J}}(\bar{u}) \begin{pmatrix} r_x - \bar{r} \\ e_x - \bar{e} \end{pmatrix}$$

We call $D\bar{\mathfrak{J}}(\bar{u}) = \mathcal{D}$ the diffusion matrix.

After proving some compactness of the law of these fluctuation fields (as distributional valued stochastic processes), we have the convergence in law to the system of sde:

$$d\widetilde{\mathfrak{u}}(t, \mathbf{G}) = \widetilde{\mathfrak{u}}(t, \mathcal{D}\mathbf{G}'') \, dt \; + \; d\mathbf{W}(t, B\mathbf{G}') \qquad (4.3.7)$$

where B is a matrix realted to $\mathcal{D}$ that can be computed...

As we se many steps of this program are still open, In the harmonic case $V(r) = r^2/2$ all this can be proven rigorously (cf. [7]). In this case the equations are

$$\begin{aligned} \partial_t \widetilde{\mathfrak{r}} &= \frac{1}{\gamma} \partial_y^2 \widetilde{\mathfrak{r}} \; + \; \sqrt{\frac{1}{\gamma\beta}} \partial_y W_1, \\ \partial_t \widetilde{\mathfrak{e}} &= \frac{1+\gamma^2}{2\gamma} \partial_y^2 \widetilde{\mathfrak{e}} \; + \; \frac{1-\gamma^2}{2\gamma} \bar{r} \, \partial_y^2 \widetilde{\mathfrak{r}} + \sqrt{\frac{2}{\gamma\beta}} \partial_y W_1 \; + \; \frac{\sqrt{1+\gamma^2}}{\sqrt{\gamma}\beta} \partial_y W_2, \end{aligned} \qquad (4.3.8)$$

Chapter 5

Conductivity and Green-Kubo Formulas

5.1 Diffusivity

With the notation settled in the previous chapters, let us consider the Hamiltonian of the infinite system:

$$\mathcal{H} = \sum_{x\in\mathbb{Z}^d} \left(\frac{p_x^2}{2} + V(r_x)\right) = \sum_{x\in\mathbb{Z}^d} \mathcal{E}_x \tag{5.1.1}$$

and the corresponding hamiltonian dynamics perturbed by noise that change p_x into $-p_x$ with rate γ, independently for each particle, i.e. the generator is given by

$$L = \mathcal{A} + \gamma S \tag{5.1.2}$$

with

$$Sf(r,p) = \sum_x \left(f(r,p^x) - f(r,p)\right) \tag{5.1.3}$$

where $p^x_y = p_y$ if $y \neq x$, and $p^x_x = -p_x$. Since momentum is not conserved, the equilibrium stationary measure are given by

$$d\mu^{gc}_{\tau,0,\beta} = \prod_{x\in\mathbb{Z}} \frac{e^{-\beta(\mathcal{E}_x - \tau r_x)}}{Z(\beta\tau,\beta)\sqrt{2\pi\beta^{-1}}} dr_x dp_x \ . \tag{5.1.4}$$

Recall that

$$u(\lambda,\beta) = -\frac{\partial \log\left(Z(\lambda,\beta)\sqrt{2\pi/\beta}\right)}{\partial\beta} = \int V(r)\frac{e^{\lambda r - \beta V(r)}}{Z(\lambda,\beta)}\, dr + \frac{1}{2\beta} = \int \mathcal{E}_j \; d\mu^{gc}_{\tau,\beta} \tag{5.1.5}$$

Then the energy static variance is given by

$$\chi_e(\lambda, \beta) = -\partial_\beta u =< \mathcal{E}_0^2 >_{\lambda,\beta} - u(\lambda, \beta)^2 \tag{5.1.6}$$

Now we perturb the equilibrium measure by *adding* some energy at particle 0, defining a new probability measure

$$d\mu' = \frac{E_0}{u(\lambda, \beta)} d\mu^{gc}_{\tau,0,\beta} \tag{5.1.7}$$

and observe that

$$< \mathcal{E}_x >' = u(\lambda, \beta) + \frac{\chi_e}{u}\ \delta(x)_0 \tag{5.1.8}$$

If we start the dynamics with this measure, that is not stationary, we expect the perturbation *diffuse*:

$$< \mathcal{E}_x(t) >' \sim u(\lambda, \beta) + \frac{\chi_u}{u}\ \frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}}. \tag{5.1.9}$$

for *large* x and t (in a diffusive scaling). Since

$$< \mathcal{E}_x(t) >' = \frac{< \mathcal{E}_x(t)\mathcal{E}_0(0) >}{< \mathcal{E}_0 >}$$

this suggest the following definition for D:

$$D(t) = \frac{1}{\chi_e} \sum_x x^2 \left(< \mathcal{E}_x(t)\mathcal{E}_0(0) > - < \mathcal{E}_0 >^2 \right) \tag{5.1.10}$$

and

$$D = D(\lambda, \beta) = \lim_{t\to\infty} \frac{1}{2t} D(t). \tag{5.1.11}$$

It is common to define $S(x, t) =< \mathcal{E}_x(t)\mathcal{E}_0(0) > - < \mathcal{E}_0 >^2$, and its Fourier trasform $\hat{S}(k, t)$ is called *structure function*. If $S(x, t) \geq 0$, one can see $\chi_e^{-1} S(x, t)$ as a probability transition, and the sense of the asymptotic is

$$\frac{\epsilon}{\chi_e} S\left([\epsilon^{-1}x], \epsilon^{-2}t\right) \underset{\epsilon\to 0}{\longrightarrow} \frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}}$$

D is called **thermal diffusivity**. The **thermal conductivity** is defined as

$$\kappa = \frac{\chi_e}{T^2} D = \chi_e \beta^2 D \tag{5.1.12}$$

Oserve in fact that

$$\frac{\chi_e}{T^2} = -\partial_\beta u(\lambda, \beta)\beta^2 = \partial_T u(\lambda, T^{-1}).$$

We will prove later that the limit defining D in (5.1.15) exists. But first we prove the following Green-Kubo formula for D, under the assumption that such limit exists.

Proposition 5.1.1 *It the limit in (5.1.15) exists and is finite, then*

$$D = \frac{2}{\chi_e} \int_0^\infty \sum_x < j_{x,x+1}(t) j_{0,1}(0) > dt. \tag{5.1.13}$$

Proof. Observe that $S(x,t) = S(-x,t)$, and that $S(x,0) = \chi_e \delta_0(x)$. Consequently

$$\sum_x x^2 S(x,t) = \sum_x x^2 \left[S(x,t) - S(x,0) \right]$$
$$= \frac{1}{2} \sum_x x^2 \left[S(x,t) + S(-x,t) - 2S(x,0) \right]$$

and using stationarity and translation invariance, this last quantity is equal to

$$-\frac{1}{2} \sum_x x^2 < (\mathcal{E}_x(t) - \mathcal{E}_x(0))(\mathcal{E}_0(t) - \mathcal{E}_0(0)) >$$
$$= -\frac{1}{2} \sum_x x^2 < (J_{x-1,x}(t) - J_{x,x+1}(t))(J_{-1,0}(t) - J_{0,1}(t)) >$$

where $J_{x,x+1}(t) = \int_0^t j_{x,x+1}(s) ds$, with $j_{x,x+1} = p_x V'(r_{x+1})$. After a summation by part this is equal to

$$-\frac{1}{2} \sum_x (2x+1) < J_{x,x+1}(t))(J_{-1,0}(t) - J_{0,1}(t)) >$$

and by translation invariance and another summation by part it is equal to

$$\sum_x < J_{-x-1,-x}(t) J_{0,1}(t)) >= \sum_x < J_{x,x+1}(t) J_{0,1}(t) >$$
$$= 2 \sum_x \int_0^t ds \int_0^s d\tau < j_{x,x+1}(s) j_{0,1}(\tau) >$$
$$= 2 \sum_x \int_0^t ds \int_0^s d\tau < j_{x,x+1}(s-\tau) j_{0,1}(0) >=$$
$$= 2 \sum_x \int_0^t ds \int_0^s d\tau < j_{x,x+1}(\tau) j_{0,1}(0) >$$

Dividing by $2\chi_e t$ and taking the limit as $t \to \infty$, we obtain (5.1.13). □

Before proving the convergence in (5.1.15), we prove that the noise perturbation imply that thermal conductivity is finite. The proof of the convergence will be in the snext section.

Proposition 5.1.2

$$\sup_{t\geq 0} \frac{D(t)}{2t} \quad \leq \quad \frac{16 < V'(r_0)^2 >}{\beta \chi_e \gamma} \tag{5.1.14}$$

Proof. From the calculation in the proof of proposition 5.1.1, we have

$$D(t) = \frac{1}{\chi_e} \sum_x < J_{x,x+1}(t) J_{0,1}(t) >= \lim_{N\to\infty} \frac{1}{2N\chi_e} \left\langle \left(\int_0^t \sum_{|x|\leq N} j_{x,x+1}(s)\, ds \right)^2 \right\rangle \tag{5.1.15}$$

By the general estimate for variance of Markov processes in stationary state:

$$\left\langle \left(\int_0^t \sum_{|x|\leq N} j_{x,x+1}(s)\, ds \right)^2 \right\rangle \leq \frac{16t}{\gamma} \left\langle \sum_{|x|\leq N} j_{x,x+1}, (-S)^{-1} \sum_{|x|\leq N} j_{x,x+1} \right\rangle \tag{5.1.16}$$

and since $Sp_x = -2p_x$, we have $(-S)^{-1} \sum_{|x|\leq N} j_{x,x+1} = \frac{1}{2} \sum_{|x|\leq N} j_{x,x+1}$, and then, ising independence of the velocities, the RHS of (5.1.16) is equal to

$$\frac{8t}{\gamma} \left\langle (\sum_{|x|\leq N} j_{x,x+1})^2 \right\rangle = \frac{16tN}{\gamma} \left\langle j_{0,1}^2 \right\rangle = \frac{16tN}{\gamma\beta} \left\langle V'(r_0)^2 \right\rangle .$$

□

We can repeat the same argument with the other conserved quantity, i.e. $\sum_x r_x$. If we start with the perturbed equilibrium measure

$$d\mu'' = \frac{r_0}{r(\lambda,\beta)} d\mu^{gc}_{\lambda,\beta} \tag{5.1.17}$$

Then defining the static variance of the stretch

$$\chi_r(\lambda,\beta) = \partial_\lambda r(\lambda,\beta) =< r_0^2 > - r(\lambda,\beta)^2 \tag{5.1.18}$$

We obtain that this perturbation will diffuse with variance given by

$$\begin{aligned} D_r &= \lim_{t\to\infty} \frac{1}{2t\chi_r} \sum_x x^2 \left[< r_x(t) r_0(0) > - < r_0 >^2 \right] \\ &= \frac{1}{\chi_r} \int_0^\infty \sum_x < p_x(t) p_0(0) > \; dt \end{aligned} \tag{5.1.19}$$

With the same arguments one could show that $D_r < +\infty$, but in fact it can be computed explicitely and we obtain (exercise):

$$D_r = \frac{1}{\gamma \chi_r} = \frac{1}{\gamma} \partial_r \lambda(r,u) \tag{5.1.20}$$

In order to complete the diffusion matrix, we can consider respectively the time evolution of

$$< r_x(t) >' = \frac{< r_x(t)\mathcal{E}_0(0) >}{< \mathcal{E}_0 >} \tag{5.1.21}$$

and

$$< \mathcal{E}_x(t) >'' = \frac{< r_0(0)\mathcal{E}_x(t) >}{< \mathcal{E}_0 >} \tag{5.1.22}$$

and obtain

$$\begin{aligned} D_{r,e} &= \lim_{t\to\infty} \frac{1}{2t\chi_{r,e}} \sum_x x^2 \left[< r_x(t)\mathcal{E}_0(0) > -ru\right] \\ D_{e,r} &= \lim_{t\to\infty} \frac{1}{2t\chi_{r,e}} \sum_x x^2 \left[< r_0(0)\mathcal{E}_x(t) > -ru\right] \end{aligned} \tag{5.1.23}$$

By a simple time-reversal argument and the translatin invariance it is easy to prove the so called Onsager relation:

$$D_{r,e} = D_{e,r} \tag{5.1.24}$$

and by similar arguments as above it can be written as

$$\frac{1}{\chi_{r,e}} \int_0^\infty \sum_x \langle j_{x,x+1}(t) p_0(0) \rangle \, dt = \frac{1}{\chi_{r,e}} \int_0^\infty \sum_x \langle j_{0,1}(0) p_x(t) \rangle \, dt \tag{5.1.25}$$

5.2 Proof of convergence in the Green-Kubo formula

Chapter 6

Non-equilibrium stationary states: linear response

$$
\begin{aligned}
\dot{r}_1(t) &= p_1(t) \\
\dot{r}_j(t) &= p_j(t) - p_{j-1}(t), \qquad j = 2, \dots, n, \\
\dot{p}_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t) \qquad j = 2, \dots, n-1 \\
dp_1 &= \left(V'(r_2(t)) - V'(r_1(t))\right) dt - p_1(t)dt + \sqrt{\beta}_1 dw_1(t) \\
dp_n &= \left(\tau - V'(r_n(t))\right) dt - p_n(t)dt + \sqrt{\beta}_n dw_n(t)
\end{aligned}
\tag{6.0.1}
$$

that describe the system subject to an external tension (force) τ on the last particle, and attached on the left to a wall ($p_0(t) = 0$ for all t), and with two *Langevin* thermostats attached at the boundaries with different temperatures $T_r = \beta_n^{-1}$ and $T_l = \beta_1^{-1}$.

The unperturbed generator is given by

$$L_0 = \mathcal{A}_\tau + B_1 + B_n \tag{6.0.2}$$

where

$$B_j = \beta_j^{-1} \partial_{p_j}^2 - p_j \partial_{p_j} \tag{6.0.3}$$

and $\mathcal{A}_\tau$ is the correspondig hamiltonian operator

$$
\begin{aligned}
\mathcal{A}_\tau = \sum_{x=2}^{n} \left\{ (p_x - p_{x-1})\, \partial_{r_x} + (V'(r_x) - V'(r_{x-1}))\, \partial_{p_{x-1}} \right\} \\
+ p_1 \partial_{r_1} + (\tau - V'(r_n))\, \partial_{p_n}
\end{aligned}
\tag{6.0.4}
$$

In order to study situation with finite macroscopic thermal conductivity, se add some different stochastic perturbation that are energy preserving. The generator of these persurbation we will denote by γS, with $\gamma > 0$ a positive parameter measuring the strength of the perturbation.

We choose first the simple case of the independent velocity change of sign, given by

$$Sf(r,p) = \sum_{x=1}^{n} \left(f(r,p^x) - f(r,p)\right) \tag{6.0.5}$$

where $p^x_y = p_y$ if $y \neq x$, and $p^x_x = -p_x$.

So we consider the dynamics generated by $L_\gamma = L_0 + \gamma S$.

In appendix SS we prove that a unique stationary probability measure exists and has a density $f_{ss}(r,p)$ with respect the Lebesgue measure on $(\mathbb{R} \times \mathbb{R})^n$. We want to study here the conductivity properties of this stationary measure, in the asymptotic $n \to \infty$.

If $T_l = T_r = T = \beta^{-1}$, then by direct computation one can see that

$$f_{ss} = \prod_{x=1}^{n} \frac{e^{-\beta(\mathcal{E}_x - \tau r_x)}}{Z(\beta\tau,\beta)\sqrt{2\pi\beta^{-1}}} \tag{6.0.6}$$

If $T_l \neq T_r$, f_{ss} cannot be computed explicitely, and the pourpouse of this chapetr in to study the main properties of this stationary state. We will denote with $< \cdot >_s$ the expectation with respect do the stationary probability measure, omitting the dependence on n, T_l, T_r, γ when not necessary to be specified.

An immediate consequence of stationarity is that for any $x = 1, \dots, n$:

$$\begin{aligned} < p_x >_s &= 0 \\ < V'(r_x) >_s &= \tau \\ < j_{x,x+1} >_s &= - < p_x V'(r_{x+1}) >= J_s \end{aligned} \tag{6.0.7}$$

where J_s is the average stationary current of energy flowing from left to right. Notice that J_s is also the energy current at the boundaries, i.e. the stationary average energy exchanged with the thermostats:

$$J_s = T_l - < p_1^2 >_s = < p_n^2 > - T_r \tag{6.0.8}$$

6.1 Entropy production

A simple entropy production argument shows that the sign of J is the same as $T_l - T_r$, i.e. energy flows from the hot to the cold reservoir.

By stationarity, and the skewsymmetry of $\mathcal{A}$, we have

$$
\begin{aligned}
0 &= - < L_\gamma \log f_{ss} >_s \\
&= \gamma \sum_x \int f_{ss}(r,p) \log \frac{f_{ss}(r,p)}{f_{ss}(r,p^x)} drdp - \int f_{ss}(r,p)\left(B_1 + B_n\right) \log f_{ss}(r,p) drdp
\end{aligned}
$$

where we denote $drdp = \prod_{y=1}^n dr_y dp_y$.

By explicit calculation we have (for $j = 1$ and $j = n$):

$$
\begin{aligned}
&- \int f_{ss}(r,p) B_j \log f_{ss}(r,p) drdp \\
&\quad = T_j \int \frac{(\partial_{p_j}(f_{ss}/g_{T_j}))^2}{f_{ss}/g_{T_j}} drdp + T_j^{-1}\left(T_j - < p_j^2 >_s\right) \\
&\qquad\qquad = \mathcal{D}_j + \left(\delta_1(j) T_l^{-1} - \delta_n(j) T_n^{-1}\right) J_s
\end{aligned}
$$

And by (6.0.8) we obtain

$$
0 = \gamma \sum_{x=1}^n H(f_{ss}|f_{ss}^x) + \mathcal{D}_1 + \mathcal{D}_n + \left(T_l^{-1} - T_r^{-1}\right) J_s \tag{6.1.1}
$$

i.e.

$$
\left(T_r^{-1} - T_l^{-1}\right) J_s = \gamma \sum_{x=1}^n H(f_{ss}|f_{ss}^x) + \mathcal{D}_1 + \mathcal{D}_n \geq 0. \tag{6.1.2}
$$

This non-negative quantity is also called *entropy production* of the stationary state.

6.2 Conductivity: linear response

We apply now first order perturbation theory to study the stationary energy flow J_s for small difference of temperature $T_l - T_r = \delta T$. To simplify notations, let us set $T_l = T$ and $T_r = T - \delta T$.

We define conductivity of the finite system the limit (when exists)

$$
\kappa_n = \kappa_n(T, \tau, \gamma) = \lim_{\delta T \to 0} \frac{n J_s}{\delta T}. \tag{6.2.1}
$$

We will compute this limit, by a first order expansion of J_s in δT. It is convenient to introduce a local Gibbs measure with a temperature profile given by the linear interpolation

$$
T_x = -\frac{\delta T}{n-1} x + T + \frac{\delta T}{n-1}.
$$

i.e. the inhomogeneous product probability density

$$g = \prod_{x=1}^{n} \frac{e^{-\beta_x(\mathcal{E}_x - \tau r_x)}}{Z(\tau\beta_x, \beta_x)} \tag{6.2.2}$$

where $\beta_x = T_x^{-1}$. This product probability density in the 0 order approximation of the stationary probability density f_{ss}, and we are interested in the developpement:

$$f_{ss} = g + u\ \delta T + o(\delta T) \tag{6.2.3}$$

It is convenient to work using g as reference measure. Let uf define $\tilde{f}_{ss} = f_{ss} g^{-1}$. Then $\tilde{f}_{ss}$ is solution of the equation

$$\tilde{L}_\gamma^* \tilde{f}_{ss} = 0 \tag{6.2.4}$$

where $\tilde{L}_\gamma^*$ is the adjoint of L_γ with respect to the measure $gdrdp$.

Observe that B_1, B_n and S are symmetric with respect to $gdrdp$.

The adjoint or $\mathcal{A}$ with respect $gdrdp$ is given by

$$\begin{aligned} \mathcal{A}^* &= -\mathcal{A} - \sum_{x=1}^{n-1} (\beta_{x+1} - \beta_x)(j_{x,x+1} + \tau p_x) \\ &= -\mathcal{A} + \frac{\delta T}{T^2 n} \sum_{x=1}^{n-1} (j_{x,x+1} + \tau p_x) + o(\delta T) \end{aligned} \tag{6.2.5}$$

So we can write

$$\begin{aligned} \tilde{L}_\gamma^* &= -\mathcal{A} + \frac{\delta T}{T^2 n} \sum_{x=1}^{n-1} (j_{x,x+1} + \tau p_x) + \gamma S + B_{1,T} + B_{n,T+\delta T} + o(\delta T) \\ &= -\mathcal{A} + \frac{\delta T}{T^2 n} \sum_{x=1}^{n-1} (j_{x,x+1} + \tau p_x) + \gamma S + B_{1,T} + B_{n,T} + \delta T \partial_p^2 + o(\delta T) \\ &= \tilde{L}_\gamma^{*,T} + \delta T \partial_p^2 + o(\delta T) \end{aligned}$$

where $\tilde{L}_\gamma^{*,T}$ is the adjoint, with respect to the homogeneous Gibbs measure at temperature T, of the generator of the dynamics with thermostats at equal temperature T, i e

$$L_\gamma^T = \mathcal{A} + \gamma S + B_{1,T} + B_{n,T}. \tag{6.2.6}$$

A formal expansion of $\tilde{f}_{ss}$ in δT:

$$\tilde{f}_{ss} = 1 + \tilde{u}\ \delta T + o(\delta T) \tag{6.2.7}$$

gives that $\tilde{u}(r,p)$ must satisfy the equation

$$\tilde{L}_\gamma^{*,T}\tilde{u} = -\frac{1}{T^2 n}\sum_{x=1}^{n-1}\left(j_{x,x+1}+\tau p_x\right) = \frac{1}{T^2 n}\sum_{x=1}^{n-1} p_x\left(V'(r_{x+1})-\tau\right) \tag{6.2.8}$$

Since the right hand side of (6.3.8) is antisymmetric for a global change of sign $p \to -p$, defining $\check{u}(r,p) = \tilde{u}(r,-p)$, we have that $\check{u}$ satisfies the equation

$$L_\gamma^T \check{u} = \frac{1}{T^2 n}\sum_{x=1}^{n-1}\left(j_{x,x+1}+\tau p_x\right) \tag{6.2.9}$$

We can now compute the average energy curet at the first order in δT:

$$J_s = \langle j_{y,y+1}\rangle_s = \delta T \int j_{y,y+1}\ \tilde{u}\ g\ dr\ dp + o(\delta T) \tag{6.2.10}$$

and since $j_{y,y+1}$ is antisymmetric in p, this is equal to

$$\begin{aligned}
J_s &= -\delta T \int j_{y,y+1}\ \check{u}\ g\ dr\ dp + o(\delta T)\\
&= \frac{\delta T}{T^2 n}\sum_{x=1}^{n-1}\int j_{y,y+1}\left[(-L_\gamma^T)^{-1}\left(j_{x,x+1}+\tau p_x\right)\right] g\ dr\ dp + o(\delta T)\\
&= \frac{\delta T}{T^2 n}\sum_{x=1}^{n-1}\int_0^\infty dt \int j_{y,y+1}\left[e^{tL_\gamma^T}\left(j_{x,x+1}+\tau p_x\right)\right] g\ dr\ dp + o(\delta T)\\
&= \frac{\delta T}{T^2 n}\sum_{x=1}^{n-1}\int_0^\infty dt\ \langle j_{y,y+1}(0)\left(j_{x,x+1}(t)+\tau p_x(t)\right)\rangle_{T,\gamma} + o(\delta T)
\end{aligned} \tag{6.2.11}$$

where $< \cdot >_{T,\gamma}$ is the expectation for the dynamics generated by L_γ^T in equilibrium.

Using the noisy part of the dynamics, we can further compute this thermal conductivity, by observing that

$$\sum_{x=1}^{n-1} p_x = \frac{1}{2\gamma}\left(V'(r_n)-V'(r_1)\right) - \frac{1}{2\gamma}L_\gamma^T\sum_{x=1}^{n-1}p_x - \frac{1}{\gamma}p_1 \tag{6.2.12}$$

that gives

$$\begin{aligned}
\frac{\delta T}{T^2 n}\sum_{x=1}^{n-1}\int_0^\infty dt\ \langle j_{y,y+1}(0)\tau p_x(t)\rangle_{T,\gamma} &= \frac{\tau\delta T}{T^2 n 2\gamma}\int_0^\infty dt\ \langle j_{y,y+1}(0)\left(V'(r_n(t))-V'(r_1(t))\right)\rangle_{T,\gamma}\\
&\quad + \frac{\tau\delta T}{T^2 n 2\gamma}\sum_{x=1}^{n-1}\langle j_{y,y+1}(0)p_x(0)\rangle_{T,\gamma} + \frac{\tau\delta T}{T^2 n\gamma}\langle j_{y,y+1}(0)p_1(0)\rangle_{T,\gamma}\\
&= \frac{\tau\delta T}{T^2 n 2\gamma}\int_0^\infty dt\ \langle j_{y,y+1}(0)\left(V'(r_n(t))-V'(r_1(t))\right)\rangle_{T,\gamma} + \frac{\tau^2\delta T}{2nT\gamma}
\end{aligned}$$

if we choose $y \neq 1$.

So we have obtained the following formula for the conductivity:

$$\begin{aligned}\kappa_n =& \frac{1}{T^2}\sum_{x=1}^{n-1}\int_0^\infty dt\, \langle j_{y,y+1}(0) j_{x,x+1}(t)\rangle_{T,\gamma} + \frac{\tau^2}{2T\gamma} \\ &+ \frac{\tau}{2T^2\gamma}\int_0^\infty dt\, \langle j_{y,y+1}(0)\left(V'(r_n(t)) - V'(r_1(t))\right)\rangle_{T,\gamma}\end{aligned} \tag{6.2.13}$$

The challenging (open) problem is to prove and identify the limit for $n \to \infty$ of the conductivity. This should be given by

$$\lim_{n\to\infty} \kappa_n = \frac{1}{T^2}\sum_{x\in\mathbb{Z}}\int_0^\infty dt\, \langle j_{0,1}(0) j_{x,x+1}(t)\rangle_{T,\gamma} + \frac{\tau^2}{2T\gamma} \tag{6.2.14}$$

where now the dynamics is the infinite one in equilibrium. Notice that the first term is connected to the diffusivity D_e of the energy, while the second correspond to the off-diagonal $D_{e,r}$ term in the diffusivity matrix (5.1.23).

6.3 Unpinned model

The above analysis will change little if the chain is not attached to a wall on the right hand side, but a constant force acts on the first particle, of equal strength τ but of opposite signe to the one attached on the right end.

More interesting situation if the forces differ, $\tau_l \neq \tau_r$ and study the behaviour for small difference in the first order. Of course the center of mass of the system will move of a speed that we will determine in the stationary state.

The generator is now given by $L = \mathcal{A}_{\tau_l,\tau_r} + \gamma S + B_1 + B_n$, where

$$\begin{aligned}\mathcal{A}_{\tau_l,\tau_r} = \sum_{x=2}^{n}(p_x - p_{x-1})\,\partial_{r_x} + \sum_{x=2}^{n-1}\left(V'(r_{x+1}) - V'(r_x)\right)\partial_{p_x} \\ - \left(\tau_l - V'(r_2)\right)\partial_{p_1} + \left(\tau_r - V'(r_n)\right)\partial_{p_n}\end{aligned} \tag{6.3.1}$$

Notice that now does not appear the coordinate r_1.

We skip for the moment all problem connected to the existece of a stationary state, and assume its uniqueness.

Then, using similar notation as above we have the following relations for the average velocity of the system:

$$V_s =< p_x >_s =< V'(r_2) >_s - \tau_l = \tau_r - < V'(r_n >_s \qquad \forall x = 1, \dots, n \tag{6.3.2}$$

If $\tau_r = \tau_l + \delta\tau$, then for small $\delta\tau$ we have $V_s = \tilde{V}_0 \delta\tau + o(\delta\tau)$.

Since, for $x \neq 1, n$

$$Lp_x = -2\gamma p_x + V'(r_{x+1}) - V'(r_x) \tag{6.3.3}$$

it is easy to prove here that $\tilde{V}_0 = (2\gamma)^{-1}$, independent of tension and temperature!

Also it is easy to see that there is a linear profile of tension defined by $\tilde{\tau}_x =< V'(r_x) >$ that satisfies

$$n(\tilde{\tau}_x - \tilde{\tau}_{x+1}) = V_s \tag{6.3.4}$$

Let us see now the influence of the tension gradient on the thermal conductivity. Let τ_x the linear interpolation profile between τ_l and $\tau_r = \tau_l + \delta\tau$. We use now as reference measure

$$g = \prod_{x=1}^{n} \frac{e^{-\beta_x(\mathcal{E}_x - \tau_x r_x)}}{Z(\tau_x \beta_x, \beta_x)} \tag{6.3.5}$$

The corresponding adjoint of the Hamiltonian operator is

$$\begin{aligned} \mathcal{A}^* &= -\mathcal{A} - \sum_{x=1}^{n-1} (\beta_{x+1} - \beta_x)\, j_{x,x+1} + (\beta_{x+1}\tau_{x+1} - \beta_x \tau_x)\, p_x \\ &= -\mathcal{A} + \frac{\delta T}{T^2 n} \sum_{x=1}^{n-1} (j_{x,x+1} + \tau p_x) + \frac{\delta\tau}{nT} \sum_{x=1}^{n-1} p_x + o(\delta T, \delta\tau) \end{aligned} \tag{6.3.6}$$

We now expand $\tilde{f}_{ss}$, the stationary probability density with respect to g, at the linear order in δT and $\delta\tau$:

$$\tilde{f}_{ss} = 1 + \tilde{u}\delta T + \tilde{v}\delta\tau + o(\delta T, \delta\tau) \tag{6.3.7}$$

where $\tilde{u}$ and $\tilde{v}$ are solution of

$$\begin{aligned} \tilde{L}_{\gamma}^{*,T} \tilde{u} &= -\frac{1}{T^2 n} \sum_{x=1}^{n-1} (j_{x,x+1} + \tau p_x) \\ \tilde{L}_{\gamma}^{*,T} \tilde{v} &= -\frac{1}{nT} \sum_{x=1}^{n-1} p_x \end{aligned} \tag{6.3.8}$$

And for current and velocity we have at the first order:

$$\begin{aligned} J_s =< j_{y,y+1} >_s &= \delta T \int j_{y,y+1}\, \tilde{u}\, g_T\, drdp + \delta\tau \int j_{y,y+1}\, \tilde{v}\, g_T\, drdp \\ &= \frac{\delta T}{n}\kappa_n^e + \frac{\delta\tau}{n}\kappa_n^{e,r} \end{aligned}$$

$$\begin{aligned} V_s =< p_y >_s &= \delta T \int p_y\, \tilde{u}\, g_T\, drdp + \delta\tau \int p_y\, \tilde{v}\, g_T\, drdp \\ &= \frac{\delta T}{n}\kappa_n^{r,e} + \frac{\delta\tau}{n}\kappa_n^{r} \end{aligned}$$

and it is easy to prove the Onsager relation $\kappa_n^{r,e} = \kappa_n^{e,r}$.

Chapter 7

Kinetic limits

We denote with $\hat{v}(k)$, $k \in \mathbb{T} = [0, 1]$, the Fourier transform of a function v on $\mathbb{Z}$,

$$\hat{v}(k) = \sum_{z \in \mathbb{Z}} e^{-2\pi i k z} v(z), \tag{7.0.1}$$

and with $\tilde{f}(z)$, $z \in \mathbb{Z}$, the inverse Fourier transform of a function f on $\mathbb{T}$,

$$\tilde{f}(z) = \int_{\mathbb{T}} dk \; e^{2\pi i k z} f(k). \tag{7.0.2}$$

The function $\omega(k) = \sqrt{\hat{\alpha}(k)}$ is called *dispersion relation.*

it is convenient to introduce the complex valued field $\psi : \mathbb{Z} \to \mathbb{C}$ defined as

$$\psi(y, t) = \frac{1}{\sqrt{2}} \big((\tilde{\omega} * q)_y(t) + i p_y(t) \big). \tag{7.0.3}$$

Observe that $|\psi(y)|^2 = \frac{1}{2} p_y^2 + \frac{1}{2} \sum_{y' \in \mathbb{Z}} \alpha(y - y') q_y q_{y'} = e_y$ is the energy of particle y and conservation of total energy is equivalent to the conservation of the ℓ_2-norm. For every $t \geq 0$ the evolution of ψ is given by the stochastic differential equations,

$$\begin{aligned} d\psi(y, t) = & - i (\tilde{\omega} * \psi)(y, t) dt + \frac{1}{2} \varepsilon \gamma \beta * (\psi - \psi^*)(y, t) dt \\ & + \sqrt{\frac{\varepsilon \gamma}{3}} \sum_{k = -1, 0, 1} \big(Y_{y+k} \tfrac{1}{2} (\psi - \psi^*)(y, t) \big) dw_{y+k}(t), \end{aligned} \tag{7.0.4}$$

where β is defined through

$$(\beta * f)(z) = \frac{1}{6} \Delta (4 f(z) + f(z - 1) + f(z + 1)). \tag{7.0.5}$$

The Fourier trasform is then

$$\hat{\psi}(k,t) = \frac{1}{\sqrt{2}}\omega(k)\hat{q}(k,t) + i\hat{p}(k,t) \tag{7.0.6}$$

and its time evolution is given by

$$\begin{aligned} d\hat{\psi}(k,t) =& - i\omega(k)\hat{\psi}(k,t)dt - \gamma\hat{\beta}(k)\left(\hat{\psi}(k,t) - \hat{\psi}(k,t)^*\right)dt \\ &+ \sqrt{\gamma}\int R(k,k')\left(\hat{\psi}(k-k',t) - \hat{\psi}(k-k',t)^*\right)\widehat{W}(dk',dt) \end{aligned} \tag{7.0.7}$$

where $\widehat{W}(dk',dt)$ is the white noise on $\mathbb{T}\times\mathbb{R}$, i.e. centered gaussian field with covariance

$$\mathbb{E}\left(\widehat{W}(dk,dt)\widehat{W}(dk',dt')\right) = \delta(k-k')\delta(t-t')dkdt$$

while $\hat{\beta}(k)$ and $R(k,k')$ are explicitely computed after a leghtly calculation, and depend n the type of noise.

Chapter 8

Fourier's law for the energy conserving model

One of the main difficulties in proving Fourier's law and hydrodynamic limit is to establish a *fluctuation-dissipation* relation, i.e. a decomposition of the current of the conserved quantity (here the energy) in a dissipative part (a spatial *gradient*) and a fluctuating part (a *time derivative*). Thanks to the stochastic perturbation one can write here an exact fluctuation-dissipation relation (cf. equation (8.2.14)). Then, in order to obtain Fourier's law, we have to bound (uniformly in the size of the system) the second moment of the positions and velocity at the boundary. In fact we can bound the second moments of all the coordinates, that gives a bound of the expectation of the total energy proportional to the size of the system.

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

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

$$\mathcal{H}_N = \sum_{x=1}^{N-1} e_x, \quad e_x = \frac{(p_x^2 + (r_x - \rho)^2)}{2} \qquad x = 1, \dots, N-2; \quad e_{N-1} = \frac{p_{N-1}^2}{2}. \tag{8.0.1}$$

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

$$
\begin{aligned}
dr_x &= (p_{x+1} - p_x)dt, \qquad x = 1, \dots, N-2 \\
dp_x &= (r_x - r_{x-1})dt - \gamma p_x dt + \sqrt{\gamma}\left(p_{x-1}dw_{x-1,x} - p_{x+1}dw_{x,x+1}\right), \quad x = 2, \dots, N-2 \\
dp_1 &= (r_1 - \rho)dt - \frac{1+\gamma}{2}p_1 dt - \sqrt{\gamma}p_2 dw_{1,2} + \sqrt{T_l}dw_{0,1}, \\
dp_{N-1} &= -(r_{N-2} - \rho)dt - \frac{1+\gamma}{2}p_{N-1}dt + \sqrt{\gamma}p_{N-2}dw_{N-2,N-1} + \sqrt{T_r}dw_{N-1,N},
\end{aligned}
\tag{8.0.2}
$$

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

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

The generator of the evolution has the form

$$
\begin{aligned}
L_N = &\sum_{x=1}^{N-2}(p_{x+1} - p_x)\partial_{r_x} + \sum_{x=2}^{N-2}(r_x - r_{x-1})\partial_{p_x} + r_1\partial_{p_1} - r_{N-2}\partial_{p_{N-1}} \\
&+ \frac{\gamma}{2}\sum_{x=1}^{N-2}X_{x,x+1}^2 + \frac{1}{2}\left(T_l\partial_{p_1}^2 - p_1\partial_{p_1}\right) + \frac{1}{2}\left(T_r\partial_{p_{N-1}}^2 - p_{N-1}\partial_{p_{N-1}}\right)
\end{aligned}
\tag{8.0.3}
$$

where

$$
X_{x,x+1} = p_{x+1}\partial_{p_x} - p_x\partial_{p_{x+1}} \tag{8.0.4}
$$

One can check easily that the Lie algebra generated by these vector fields and the hamiltonian part of L_N has full rank at every point of the state space $\mathbb{R}^{N-1} \times \mathbb{R}^{N-2}$. By Hörmander theorem it follows that this operator is hypoelliptic (cf. thm 22.2.1 in [**?**]), so the stationary measure has a smooth density. We denote with $< \cdot >$ the expectation with respect to the stationary measure (see appendix at the end of the chapter for the existence and uniqueness of the stationary measure).

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

$$
L_N e_x = j_{x-1,x} - j_{x,x+1} \tag{8.0.5}
$$

with the instantaneous current of energy given by

$$
\begin{aligned}
j_{x,x+1} &= -r_x p_{x+1} - \frac{\gamma}{2}(p_{x+1}^2 - p_x^2), \qquad x = 1, \cdots, N-2 \\
j_{0,1} &= \frac{1}{2}(T_l - p_1^2), \qquad j_{N-1,N} = -\frac{1}{2}(T_r - p_{N-1}^2)
\end{aligned}
\tag{8.0.6}
$$

Because of stationarity, for any $x = 1, N-1$ we have

$$< j_{x,x+1} >=< j_{0,1} >=< j_{N-1,N} > \tag{8.0.7}$$

The following theorems are the main results of this chapter.

Theorem 8.0.1 *For any* $\gamma > 0$

$$\lim_{N\to\infty} N < j_{x,x+1} >= \frac{1}{2}\left(\gamma + \gamma^{-1}\right)(T_l - T_r)\,. \tag{8.0.8}$$

Theorem 8.0.2 *For any* $\gamma > 0$

$$\lim_{N\to\infty} \frac{1}{N}\langle \mathcal{H}_N \rangle = \frac{1}{2}(T_l + T_r)\,. \tag{8.0.9}$$

It is easy to see that the averages of the total kinetic and potential energy are equal. It follows then, as corollary of theorem 8.0.9, that the same result is valid for the kinetic and the potential energies, i.e.

$$\lim_{N\to\infty} \frac{1}{N}\sum_{x=1}^{N-1}\left\langle p_x^2 \right\rangle = \lim_{N\to\infty} \frac{1}{N}\sum_{x=1}^{N-2}\left\langle r_x^2 \right\rangle = \frac{1}{2}(T_l + T_r) \tag{8.0.10}$$

Theorem 8.0.3 *For* $\gamma = 1$ *and any bounded function* $G : [0,1] \to \mathbb{R}$, *we have*

$$\lim_{N\to\infty} \left\langle \frac{1}{N}\sum_{x=1}^{N-1} G(x/N) e_x \right\rangle = \int_0^1 G(q)T(q)dq \tag{8.0.11}$$

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

8.1 Entropy production

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

By stationarity we have

$$0 = -2 < L_N \log f_N >= \gamma \sum_{x=1}^{N-2} \int \frac{(X_{x,x+1} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} + T_r \int \frac{(\partial_{p_{N-1}} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} \\ -2 < L_l \log f_N > \tag{8.1.1}$$

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

$$\begin{aligned} -2 < L_l \log f_N > &= -2 \int \frac{f_N}{h} L_l \log \left(\frac{f_N}{h}\right) g_{T_l} d\bar{p}\, d\bar{r} - 2 \int f_N L_l (\log h) g_{T_r} d\bar{p}\, d\bar{r} \\ &= T_l \int \frac{[\partial_{p_1}(f_N/h)]^2}{f_N/h} g_{T_l} d\bar{p}\, d\bar{r} + (T_l^{-1} - T_r^{-1}) \left(T_l - < p_1^2 >\right). \end{aligned} \tag{8.1.2}$$

So by (8.2.16) we have the following bound

$$\gamma \sum_{x=1}^{N-2} \int \frac{(X_{x,x+1} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} + T_r \int \frac{(\partial_{p_{N-1}} f_N)^2}{f_N} g_{T_r} d\bar{p}\, d\bar{r} + T_l \int \frac{[\partial_{p_1}(f_N/h)]^2}{f_N/h} g_{T_l} d\bar{p}\, d\bar{r} \\ = (T_r^{-1} - T_l^{-1}) \left(T_l - < p_1^2 >\right) \tag{8.1.3}$$

In section 8.7.1, we prove that this last expression is bounded by CN^{-1} for some constant C (cf. (8.2.16) and (8.0.6)). This relation also gives us the right sign for the energy current, i.e. if $T_l < T_r$ we have $< j_{x,x+1} >< 0$.

8.2 Some bounds

From (8.0.6) and (8.0.7) we have

$$< p_1^2 > + < p_{N-1}^2 >= T_l + T_r \tag{8.2.1}$$

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

$$< r_1 p_2 >=< r_1 p_1 > \tag{8.2.2}$$

Equation (8.0.7) for $x = 1$ gives

$$< j_{1,2} >= - < r_1 p_2 > -\frac{\gamma}{2} \left(< p_2^2 > - < p_1^2 >\right) \tag{8.2.3}$$

Since this last is equal to $< j_{0,1} >$, using (8.2.2), we obtain

$$\frac{\gamma}{2} < p_2^2 >= - < r_1 p_1 > + \frac{1}{2}(\gamma+1) < p_1^2 > - \frac{1}{2} T_l \tag{8.2.4}$$

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

$$< p_2^2 > \leq C \left(< r_1^2 > + < p_1^2 > \right) \tag{8.2.5}$$

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

$$< p_{N-2}^2 > \leq C(< p_{N-1}^2 > + < r_{N-2}^2 >). \tag{8.2.6}$$

Observe now that

$$L_N(r_1 p_1) = p_1(p_2 - p_1) + r_1^2 - \frac{\gamma+1}{2} p_1 r_1 \tag{8.2.7}$$

so we have the relation

$$< r_1^2 >=< p_1^2 > - < p_1 p_2 > + \frac{\gamma+1}{2} < p_1 r_1 > \tag{8.2.8}$$

and by use of (8.2.4)

$$< r_1^2 >=< p_1^2 > - < p_1 p_2 > + \left(\frac{\gamma+1}{2}\right)^2 < p_1^2 > - \frac{\gamma(\gamma+1)}{4} < p_2^2 > - \frac{\gamma+1}{4} T_l \tag{8.2.9}$$

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

$$< r_1^2 > \leq (1 + \left(\frac{\gamma+1}{2}\right)^2 + \frac{1}{2\alpha}) < p_1^2 > + (\frac{\alpha}{2} - \frac{\gamma(\gamma+1)}{4}) < p_2^2 > \tag{8.2.10}$$

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

$$< r_1^2 > \leq C < p_1^2 > \tag{8.2.11}$$

and an analogous bound is obtained for $< r_{N-2}^2 >$.

Putting all together we have obtained the following lemma:

Lemma 8.2.1 *There exists a constant C depending only on γ and linearly on T_l and T_r such that*

$$< r_1^2 > + < p_1^2 > + < p_2^2 > + < r_{N-2}^2 > + < p_{N-1}^2 > + < p_{N-2}^2 > \leq C(T_l + T_r) \tag{8.2.12}$$

The bulk dynamics is only apparently non-gradient since defining

$$h_x = \frac{1}{2\gamma} p_{x+1}(r_x + r_{x+1}) + \frac{1}{4} p_{x+1}^2, \quad x = 1, \dots, N-3 \tag{8.2.13}$$

permits to rewrite

$$j_{x,x+1} = -\nabla \left(\frac{1}{2\gamma} r_x^2 + \frac{\gamma}{2} p_x^2 + \frac{1}{2\gamma} p_x p_{x+1} + \frac{\gamma}{4} \nabla(p_x^2) \right) + L h_x, \quad x = 1, \dots, N-3. \tag{8.2.14}$$

where the discrete gradient ∇ of a discrete function w is defined by $(\nabla w)(x) = w(x+1) - w(x)$. Using again (8.0.7) we have

$$\begin{aligned} < j_{0,1} > &= \frac{1}{N-3} \sum_{x=1}^{N-3} < j_{x,x+1} > \\ &= -\frac{1}{N-3} \Bigg(\frac{1}{2\gamma} < r_{N-2}^2 > + \frac{\gamma}{2} < p_{N-2}^2 > + \frac{1}{2\gamma} < p_{N-2} p_{N-1} > \\ &+ \frac{\gamma}{4} (< p_{N-1}^2 > - < p_{N-2}^2 >) - \frac{1}{2\gamma} < r_1^2 > - \frac{\gamma}{2} < p_1^2 > - \frac{1}{2\gamma} < p_2 p_1 > - \frac{\gamma}{4} (< p_2^2 > - < p_1^2 >) \Bigg) \end{aligned} \tag{8.2.15}$$

and by (8.2.12) we obtain that there exists a constant C depending only on T_l, T_r and γ such that

$$| < j_{x,x+1} > | \leq \frac{C}{N}, \qquad x = 0, \dots, N-1. \tag{8.2.16}$$

8.3 Fourier's law

Proposition 8.3.1 *For $x = 1$ and $N-2$ we have*

$$\lim_{N \to \infty} < p_x p_{x+1} >= 0 \tag{8.3.1a}$$

$$\lim_{N \to \infty} < r_x p_{x+1} >= 0 \tag{8.3.1b}$$

$$\lim_{N \to \infty} < (p_x^2 - p_{x+1}^2) >= 0 \tag{8.3.1c}$$

Proof. Let us prove the case $x = 1$, for $x = N-2$ the proof is similar. By (8.1.3), (8.2.16) and (8.2.12)

$$\begin{aligned} < r_1 p_2 >=< r_1 p_1 >= \int r_1 p_1 (f_N/h) g_{T_l} d\bar{p}\, d\bar{r} = T_l \int r_1 \partial_{p_1} (f_N/h) g_{T_l} d\bar{p}\, d\bar{r} \\ \leq T_l < r_1^2 >^{1/2} \left(\int \frac{[\partial_{p_1}(f_N/h)]^2}{f_N/h} g_{T_l} \right)^{1/2} d\bar{p}\, d\bar{r} \leq \frac{C}{\sqrt{N}} \end{aligned} \tag{8.3.2}$$

The proof for $< p_1 p_2 >$ is similar.

Now by (8.2.16) for $x = 1$ we have

$$\lim_{N\to\infty} < (p_1^2 - p_2^2) >= 0 \tag{8.3.3}$$

□

Then by (8.2.8) we have

$$\lim_{N\to\infty} < r_1^2 >= \lim_{N\to\infty} < p_1^2 >= T_l \tag{8.3.4}$$

and similarly

$$\lim_{N\to\infty} < r_{N-2}^2 >= \lim_{N\to\infty} < p_{N-1}^2 >= T_r \tag{8.3.5}$$

By (8.2.15) it follows that

$$\lim_{N\to\infty} N < j_{x,x+1} >= \frac{1}{2}\left(\gamma + \gamma^{-1}\right)(T_l - T_r) \tag{8.3.6}$$

i.e. the law of Fourier.

8.4 Average Energy

We first state the following equipartition result:

Proposition 8.4.1

$$\left\langle \sum_{x=1}^{N-1} p_x^2 \right\rangle = \left\langle \sum_{x=1}^{N-2} r_x^2 \right\rangle \tag{8.4.1}$$

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

$$L_N\left(\sum_{x=1}^{N-1} q_x p_x\right) = \sum_{x=1}^{N-1} p_x^2 - \sum_{x=1}^{N-2} r_x^2 - \gamma \sum_{x=2}^{N-2} q_x p_x - \frac{1+\gamma}{2}(q_1 p_1 + q_{N-1} p_{N-1}) \tag{8.4.2}$$

Since $L_N q_x^2 = 2 q_x p_x$, (8.4.1) follows. □

We prove now theorem 8.0.2. *proof* We claim there exists a constant $C > 0$ independent of N such that

$$\left\langle \frac{\mathcal{H}_N}{N} \right\rangle \leq C \tag{8.4.3}$$

Define

$$\phi(x) = \frac{1}{2\gamma} < r_x^2 > + \frac{\gamma}{4}\left(< p_x^2 > + < p_{x+1}^2 >\right) + \frac{1}{2\gamma} < p_x p_{x+1} > . \tag{8.4.4}$$

By (8.0.5) and (8.2.14), we have

$$\Delta\phi(x) = 0, \qquad x = 2, \dots, N-3 \tag{8.4.5}$$

Here, $(\Delta w)(x) = w(x+1) + w(x-1) - 2w(x)$ is the usual discrete Laplacian of the function $w(x)$. By (8.2.12) and the maximum principle, it follows that there exists a constant C independent of N such that

$$|\phi(x)| \leq C, \qquad x = 1, \dots, N-2 \tag{8.4.6}$$

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

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-2} \phi(x) = \frac{1}{2}(\gamma + \gamma^{-1})(T_r + T_r) \tag{8.4.7}$$

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

$$p_x p_{x+1} = \frac{1}{3\gamma}\nabla\left((r_x + r_{x-1})p_{x-1}\right) + \frac{1}{3\gamma} L_N \left(\frac{1}{2}(r_x + r_{x-1})^2 + p_x p_{x-1}\right) \tag{8.4.8}$$

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

$$\sum_{x=2}^{N-3} < p_x p_{x+1} >= \frac{1}{3\gamma}\left(< (r_{N-2} + r_{N-3})p_{N-3} > - < (r_2 + r_1)p_1 >\right) \tag{8.4.9}$$

Now we also have that

$$L_N(p_1 p_2) = -\frac{5\gamma + 1}{2} p_1 p_2 + r_2 p_1 + L_N\left(\frac{r_1^2}{2}\right) \tag{8.4.10}$$

which implies, by (8.2.12),

$$< r_2 p_1 >= \frac{5\gamma + 1}{2} < p_1 p_2 > \leq C \tag{8.4.11}$$

For the other side we have

$$\begin{aligned} &L_N\left(-\frac{1}{2}(r_{N-2} + r_{N-3})^2 + p_{N-1}p_{N-2}\right) \\ &= r_{N-2}p_{N-2} - p_{N-3}(r_{N-2} + r_{N-3}) - \frac{5\gamma + 1}{2} p_{N-1}p_{N-2} \end{aligned} \tag{8.4.12}$$

so that

$$< p_{N-3}(r_{N-2} + r_{N-3}) >= -\frac{5\gamma + 1}{2} < p_{N-1}p_{N-2} > + < r_{N-2}p_{N-2} > \quad (8.4.13)$$

and again by (8.2.12) this quantity is bounded in absolute value by a constant independent of N. So we can conclude that

$$\left| \sum_{x=1}^{N-3} < p_x p_{x+1} > \right| \leq C \quad (8.4.14)$$

with C a constant independent of N. It follows by (8.4.14) and (8.4.7) that

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-2} \left[\frac{1}{2\gamma} < r_x^2 > + \frac{\gamma}{4} \left(< p_x^2 > + < p_{x+1}^2 > \right) \right] = \frac{1}{2}(\gamma + \gamma^{-1})(T_r + T_r) \quad (8.4.15)$$

The by using (8.4.1) we finally get (8.0.9) and (8.0.10). □

8.5 Energy profile for $\gamma = 1$

From the results of the previous section we have that

$$\lim_{N\to\infty} \phi([Nq]) = \frac{1}{2}(\gamma + \gamma^{-1})T(q) \quad (8.5.1)$$

If $\gamma = 1$ we have

$$\begin{aligned} \phi(x) =& \frac{1}{2} < r_x^2 > + \frac{1}{4}(< (p_{x+1}^2 > + < p_x^2 >) + \frac{1}{2} < p_x p_{x+1} > \\ =& < e_x > + \psi(x) \end{aligned} \quad (8.5.2)$$

with

$$\psi(x) = \frac{1}{2} < p_x p_{x+1} > + \frac{1}{4}(< (p_{x+1}^2 > - < p_x^2 >)$$

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

Then, in order to prove (8.0.11), we are left to prove

$$\lim_{N\to\infty} \frac{1}{N} \sum_{x=1}^{N-2} G(x/N)\psi(x) = 0 \quad (8.5.3)$$

Because of (8.4.8), $\psi(x) = \nabla\xi(x)$ with ξ a bounded function, so (8.5.3) follows by summation by part.

8.6 Green-Kubo formula

In this section, we compute the thermal conductivity defined by the Green-Kubo formula κ^{GK} and we show it is given by the conductivity defined in the non-equilibrium setting. Let us define

$$C_N(t) = (2T^2tN)^{-1}\mathbb{E}_\beta\left(\left[\int_0^t \mathfrak{J}(s)ds\right]^2\right)$$

Since starting from μ_β the process is stationary we have

$$C_N(t) = \frac{1}{T^2tN}\int_0^t ds\int_0^s du\mathbb{E}_\beta\left[\mathfrak{J}(u),\mathfrak{J}(0)\right]$$

performing two integration by parts, one obtains that the Laplace transform $\mathfrak{L}_N(\lambda)$ of $tC_N(t)$ is equal to

$$\mathfrak{L}_N(\lambda) = \frac{1}{\lambda^2NT^2}\int_0^\infty dte^{-\lambda t}\mathbb{E}_\beta\left[\mathfrak{J}(t),\mathfrak{J}(0)\right]$$

This last quantity is equal to

$$\frac{1}{\lambda^2T^2N} < \mathfrak{J}, (\lambda - L)^{-1}\mathfrak{J} >$$

By the fluctuation-dissipation equation, we have

$$(\lambda - L)^{-1}\mathfrak{J} = \frac{\mathfrak{J}}{\lambda+\gamma}$$

so that $\mathfrak{L}_N(\lambda)$ is given by

$$\mathfrak{L}_N(\lambda) = \frac{< \mathfrak{J}, \mathfrak{J} >}{T^2N\lambda^2(\lambda+\gamma)}$$

One computes easily $< \mathfrak{J}, \mathfrak{J} >$ and after inversion of the Laplace transform, one gets

$$C_N(t) = \frac{1}{\gamma}\left(1 - \frac{1}{\gamma t}(1-e^{-\gamma t})\right)$$

One concludes that the thermal conductivity defined by the Green-Kubo formula is given by

$$\kappa^{GK} = \gamma^{-1} + \gamma$$

It is the value obtained in theorem 8.0.1.

8.7 Appendix

In this section, we prove existence and uniqueness of the stationary measure $< \cdot >$ for any left temperature T_l and right temperature T_r. Recently, [3], [14] proved existence and uniqueness of the stationary measure for a nonharmonic chain with reservoirs at the boundaries.

8.7.1 Existence

Let us denote by $\Omega = \{\omega = (p_1, \ldots, p_{N-1}, r_1, \ldots, r_{N-2}) \in \mathbb{R}^{2N-3}\}$ the configuration space and by $(\omega_s)_{s\geq 0}$ the Markov process with generator (8.0.3).

Lemma 8.7.1 *If ω_0 is a configuration with finite energy: $\mathcal{H}_N(\omega_0) < +\infty$ then there exists a constant $C > 0$ such that*

$$\forall t \geq 0, \qquad \mathbb{E}_{\omega_0}\left[\frac{1}{t+1}\int_0^t \mathcal{H}_N(\omega_s)ds\right] \leq C \tag{8.7.1}$$

proof By (8.0.5) and(8.0.6), we have

$$L_N \mathcal{H}_N = j_{0,1} - j_{N-1,N} \tag{8.7.2}$$

It follows that

$$\mathbb{E}_{\omega_0}(\mathcal{H}_N(\omega_t)) - \mathcal{H}_N(\omega_0) = \int_0^t \mathbb{E}_{\omega_0}(T_l - p_1^2(s))ds + \int_0^t \mathbb{E}_{\omega_0}(T_r - p_{N-1}^2(s))ds \tag{8.7.3}$$

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

$$\forall t \geq 0, \qquad \mathbb{E}_{\omega_0}\left(\frac{\mathcal{H}_N(\omega_t)}{t+1}\right) \leq C \tag{8.7.4}$$

Using the preceding bound, we can repeat the estimates of section with $< . >$ replaced by the average $t^{-1}\int_0^t \mathbb{E}_{\omega_0}$. The only difference is that we have to take in account the boundary terms depending on t. In the sequel, C is a constant independant of t which can change from line to line. By (8.7.3) and (8.7.4), we know that

$$\frac{1}{t+1}\int_0^t \mathbb{E}_{\omega_0}(p_1^2(s) + p_{N-1}^2(s))ds \leq C \tag{8.7.5}$$

Since $L_N r_1^2 = 2(r-1p_2 - r_1p_1)$, we have

$$\frac{1}{t+1}\left[\mathbb{E}_{\omega_0}(r_1^2(t) - r_1^2(0))\right] = \frac{2}{t+1}\int_0^t \mathbb{E}_{\omega_0}(r_1(s)p_2(s) - r_1(s)p_1(s))ds \qquad (8.7.6)$$

By (8.7.4), the modulus of the left hand-side is bounded by a constant independant of t. Similary as what is done in (8.2.3) and (8.2.4), and using (8.7.4) to bound the boundary terms, we have

$$\left|\frac{1}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}\left[\frac{\gamma}{2}p_2^2(s) + r_1(s)p_1(s) - \frac{1}{2}(\gamma+1)p_1^2(s)\right]\right| \le C \qquad (8.7.7)$$

By Schwarz's inequality, we conclude

$$\frac{1}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}(p_2^2(s)) \le \frac{C}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}(r_1^2(s) + p_1^2(s)) + C \qquad (8.7.8)$$

This estimate is the equivalent to the estimate (8.2.6). In the same way, we can obtain the equivalent of lemma 1, meaning

$$\frac{1}{t+1}\int_0^t ds\mathbb{E}_{\omega_0}(r_1^2(s) + p_1^2(s) + p_2^2(s) + r_{N-2}^2(s) + p_{N-1}^2(s) + p_{N-2}^2(s)) \le C \quad (8.7.9)$$

Let us now define the function

$$\phi(t,x) = \frac{1}{t+1}\int_0^t \mathbb{E}_{\omega_0}\left[\frac{1}{2\gamma}r_x^2(s) + \frac{\gamma}{4}\left(p_x^2(s) + p_{x+1}^2(s)\right) + \frac{1}{2\gamma}p_x(s)p_{x+1}(s)\right] \quad (8.7.10)$$

Similary as section 8.4, one can prove there exists functions $(\theta_x)_{x=2,\dots,N-3}$ such that $\theta_x(\omega) \le C\mathcal{H}_N$ and satisfying

$$\Delta\phi(t,x) = \frac{1}{t+1}\mathbb{E}_{\omega_0}(\theta_x(\omega_t)) - \frac{1}{t+1}\theta_x(\omega_0) \qquad (8.7.11)$$

and we obtain

$$|\Delta\phi(t,x)| \le C \qquad (8.7.12)$$

Moreover, by (8.7.10), $|\phi(t,2)| \le C, \qquad |\phi(t,N-1)| \le C$. By the maximum principle, it follows that

$$|\phi(t,x)| \le C \qquad (8.7.13)$$

Using equation (8.4.8) and the bound (8.7.4), it is easy to show

$$\frac{1}{t+1}\int_0^t \mathbb{E}_{\omega_0}\left[\sum_{x=1}^{N-3} p_x(s)p_{x+1}(s)\right] \le C \qquad (8.7.14)$$

It follows by (8.7.13) and the preceding inequality that

$$\mathbb{E}_{\omega_0}\left[\frac{1}{t+1}\int_0^t \mathcal{H}_N(\omega_s)ds\right] \leq C \tag{8.7.15}$$

□

The proof of the invariant measure is now standard. Let us denote by $(T_t)_{t\geq 0}$ the semi-group corresponding to the diffusion (A.3.1) and let ω_0 be an arbitrary configuration with finite energy. We consider the following family μ_t of probabilities on Ω:

$$\mu_t = \frac{1}{t}\int_0^t \delta_{\omega_0} T_s ds \tag{8.7.16}$$

where δ_{ω_0} is the Dirac mass on the configuration ω_0. By lemma 8.7.1, the sequence of probability measures $(\mu_t)_{t>0}$ is tight. Let μ^* a limit point of the family $(\mu_t)_{t>0}$. A simple checking shows that μ^* is an invariant probability measure of the diffusion (A.3.1).

8.7.2 Uniqueness

Lemma 8.7.2 *Assume $T_l = T_r = 0$. If μ is an invariant measure for the diffusion (A.3.1) then μ is the Dirac mass supported by the configuration $\omega = (0, \ldots, 0)$.*

proof We repeat the computations of section 8.7.1 with $T_l = T_r = 0$. (8.2.1) shows that μ a.s., $p_1 = p_{N-1} = 0$ and (8.2.8) gives $r_1 = 0$ μ a.s. . By (8.2.4), it follows that μ a.s. $p_2 = 0$. Since $L_N r_2^2 = 2(r_2p_3 - r_2p_2)$, $\mu(r_2p_3) = 0$. But $\mu(j_{2,3}) = \mu(j_{0,1})$ and this last term is equal to zero since $\mu(p_1^2) = 0$. Since $j_{2,3} = -r_2p_3 - \frac{\gamma}{2}(p_3^2 - p_2^2)$, we get still $\mu(p_3^2) = 0$. In the same way, we have

$$\mu \qquad \text{a.s.} \qquad p_1 = p_2 = p_3 = p_{N-1} = p_{N-2} = p_{N-3} = 0 \tag{8.7.17}$$

By (8.4.4), (8.4.5) and (**??**), we obtain

$$\mu(\mathcal{H}_N) = 0 \tag{8.7.18}$$

and the lemma is proved. □

Let μ_1 and μ_2 two invariant probability measures for (A.3.1) with temperature on the left T_l and temperature on the right T_r. We consider the following coupling. We note the diffusion satisfying (A.3.1) with initial condition distributed according to μ_1 (resp. μ_2) by $(\omega_t^1)_{t\geq 0}$ (resp $(\omega_t^2)_{t\geq 0}$) and driven by the same Wiener processes

$w_{x,x+1}(t), x = 0, \ldots, N-1$. By linearity, the process $(\omega_t^1 - \omega_t^2)_{t \geq 0}$ is solution of (A.3.1) with $T_l = T_r = 0$. By lemma 8.7.2, we have the following weak convergence

$$\lim_{t \to \infty} \frac{1}{t} \mathbb{E}\left[F(\omega_s^2 - \omega_s^2)\right] ds = F(\mathbf{0}) \tag{8.7.19}$$

for any continuous function $F : \Omega \to \mathbb{R}$ such that $|F(\omega)| \leq C\mathcal{H}_N$, $C > 0$. Here $\mathbf{0}$ is the null configuration.

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

$$|F(\omega) - F(\tilde{\omega})| \leq C\sqrt{\mathcal{H}_N(\omega - \tilde{\omega})} \tag{8.7.20}$$

We have

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

By (8.7.19), this last term goes to 0 as t goes to infinity. It follows easily that $\mu_1 = \mu_2$.

Appendix A

Large Deviations

A.1 Introduction

As Dembo and Zeitouni point out in the introduction to their monograph on the subject [1], there is no real theory of large deviations, but a variety of tools that allow analysis of small probability.

To give an idea of what we mean with *large deviations*, let us consider a sequence of independent identical distributed real valued random variables $X_1, X_2, \ldots, X_n$ such that $\mathbb{E}(X_j^2) = 1$, and $\mathbb{E}(X_j) = 0$. Let $\hat{S}_n = \frac{1}{n}\sum_i X_i$ the empirical sum. The weak law of large numbers says that for any $\delta > 0$,

$$\mathbb{P}(|\hat{S}_n| \geq \delta) \underset{n\to\infty}{\longrightarrow} 0 \tag{A.1.1}$$

The central limit theorem is a refinement that says

$$\mathbb{P}(\sqrt{n}\hat{S}_n \in [a,b]) \underset{n\to\infty}{\longrightarrow} \frac{1}{\sqrt{2\pi}}\int_a^b e^{-x^2/2}dx \ . \tag{A.1.2}$$

In the case $X_j \sim \mathcal{N}(0,1)$, we have $\hat{S}_n \sim N(0, 1/n)$, and we can compute explicitly

$$\mathbb{P}(|\hat{S}_n| \geq \delta) = 1 - \frac{1}{\sqrt{2\pi}}\int_{-\delta\sqrt{n}}^{\delta\sqrt{n}} e^{-x^2/2}dx \ .$$

therefore (**exercise**)

$$\frac{1}{n}\log \mathbb{P}(|\hat{S}_n| \geq \delta) \underset{n\to\infty}{\longrightarrow} -\frac{\delta^2}{2} \tag{A.1.3}$$

Equation (A.1.3) is an example of a large deviation statement.

A.2 Cramér's Theorem in $\mathbb{R}$

Let $\{X_n\}$ a sequence of i.i.d. random variables on $\mathbb{R}$ with common probability distribution $\alpha(dx)$. We define the moment generating function

$$M(\lambda) = \mathbb{E}\left[e^{\lambda X_1}\right] \tag{A.2.1}$$

and let us assume that there exists $\lambda^* > 0$ such that $M(\lambda) < \infty$ if $|\lambda| < \lambda^*$. Notice that, since $|x| \leq \lambda^{-1}(e^{\lambda x} + e^{-\lambda x})$ for any $\lambda > 0$, this condition implies that X_1 is integrable and we denote $m = \mathbb{E}(X_1) \in \mathbb{R}$. It is easy to see that $m = M'(0)$. We are interested in the *logarithmic moment generating function*

$$\mathcal{Z}(\lambda) = \log \mathbb{E}\left[e^{\lambda X_1}\right] \tag{A.2.2}$$

By Jensen's inequality, we have $\mathcal{Z}(\lambda) \geq \lambda m > -\infty$. Let $\mathcal{D}_{\mathcal{Z}} = \{\lambda : \mathcal{Z}(\lambda) < +\infty\}$. Under our hypothesis, $0 \in \mathcal{D}_{\mathcal{Z}}^o$ (the interior of $\mathcal{D}_{\mathcal{Z}}$).

Lemma A.2.1 *1. $\mathcal{Z}(\cdot)$ is convex.*

2. $\mathcal{Z}(\cdot)$ is continuously differentiable in $\mathcal{D}_{\mathcal{Z}}^o$ and

$$\mathcal{Z}'(\lambda) = \frac{\mathbb{E}(X_1 e^{\lambda X_1})}{M(\lambda)} \qquad \lambda \in \mathcal{D}_{\mathcal{Z}}^o.$$

Proof:

1. For any $\alpha \in [0,1]$, it follows by Hölder inequality

$$\mathbb{E}(e^{(\alpha\lambda_1 + (1-\alpha)\lambda_2)X_1}) \leq M(\lambda_1)^\alpha M(\lambda_2)^{1-\alpha}$$

and consequently

$$\mathcal{Z}(\alpha\lambda_1 + (1-\alpha)\lambda_2) \leq \alpha\mathcal{Z}(\lambda_1) + (1-\alpha)\mathcal{Z}(\lambda_2)$$

2. The function $f_\epsilon(x) = (e^{(\lambda+\epsilon)x} - e^{\lambda x})/\epsilon$ converges pointwise to $xe^{\lambda x}$, and $|f_\epsilon(x)| \leq e^{\lambda x}(e^{\delta|x|} - 1)/\delta \leq e^{\lambda x}(e^{\delta x} + e^{-\delta x})/\delta = h(x)$, for every $|\epsilon| \leq \delta$. For any $\lambda \in \mathcal{D}_{\mathcal{Z}}^o$, there exists a $\delta > 0$ small enough such that $\mathbb{E}(h(X_1)) \leq M(\lambda+\delta) + M(\lambda-\delta) < +\infty$. Then the result follows by the dominated convergence theorem.

□

Using the same argument one can prove that $\mathcal{Z}(\cdot) \in \mathcal{C}^\infty(\mathcal{D}^o_{\mathcal{Z}})$. Computing the second derivative we obtain

$$\mathcal{Z}''(\lambda) = \frac{\mathbb{E}(X_1^2 e^{\lambda X_1})}{M(\lambda)} - \left(\frac{\mathbb{E}(X_1 e^{\lambda X_1})}{M(\lambda)} \right)^2 \geq 0$$

Observe that $\mathcal{Z}''(0) = \mathrm{Var}(X_1)$. To avoid the trivial deterministic case, we assume that $\mathrm{Var}(X_1) > 0$. It follows that $\mathcal{Z}''(\lambda) > 0$ for any $\lambda \in \mathcal{D}^o_{\mathcal{Z}}$, i.e. $\mathcal{Z}(\cdot)$ is strictly convex.

We define the rate function as the Fenchel-Legendre transform of $\mathcal{Z}$

$$I(x) = \sup_{\lambda \in \mathbb{R}} \{\lambda x - \mathcal{Z}(\lambda)\} \tag{A.2.3}$$

It is immediate to see that I is convex (as supremum of linear functions), hence continuous, and that $I(x) \geq 0$. Furthermore we have that $I(m) = 0$. In fact by Jensen's inequality $M(\lambda) \geq e^{\lambda m}$ for any $\lambda \in \mathbb{R}$, so that

$$\lambda m - \mathcal{Z}(\lambda) \leq 0$$

and it is equal to 0 for $\lambda = 0$. We conclude that $I(m) = 0$.

Consequently m is a minimum of the convex positive function $I(x)$. It follows that $I(x)$ is nondecreasing for $x \geq m$ and nonincreasing for $x \leq m$.

Observe that if $x > m$ and $\lambda < 0$

$$\lambda x - \mathcal{Z}(\lambda) \leq \lambda m - \mathcal{Z}(\lambda)$$

that implies

$$I(x) = \sup_{\lambda \geq 0} \{\lambda x - \mathcal{Z}(\lambda)\} \qquad x > m \tag{A.2.4}$$

Similarly one obtains

$$I(x) = \sup_{\lambda \leq 0} \{\lambda x - \mathcal{Z}(\lambda)\} \qquad x < m \tag{A.2.5}$$

Here are other important properties of $I(\cdot)$:

Lemma A.2.2 *$I(x) \to +\infty$ as $|x| \to \infty$, and its level sets are compact.*

Proof: If $x > m \vee 0$, for any positive $\lambda \in \mathcal{D}_{\mathcal{Z}}$,

$$\frac{I(x)}{x} \geq \lambda - \frac{\mathcal{Z}(\lambda)}{x}$$

and $\lim_{x\to+\infty} \mathcal{Z}(\lambda)/x = 0$, so we have $\lim_{x\to+\infty} I(x)/x \geq \lambda$. Consequently its level sets $\{x : I(x) \leq a\}$ are bounded, and closed by continuity of I. □

We want to prove the following theorem:

Theorem A.2.3 (Cramer) *For any set $A \subset \mathbb{R}$,*

$$-\inf_{x\in A^o} I(x) \leq \liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \in A) \leq \limsup_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \in A) \leq -\inf_{x\in \bar{A}} I(x)$$

were A^o is the interior of A and $\bar{A}$ is the closure of A.

A.2.1 Properties of Legendre transforms

We denote $\mathcal{D}_I = \{x \in \mathbb{R} : I(x) < \infty\}$.

Lemma A.2.4

The function I is convex in $\mathcal{D}_I$, strictly convex in $\mathcal{D}_I^0$ and $I \in C^\infty(\mathcal{D}_I^o)$. Furthermore for any $\bar{x} \in \mathcal{D}_I^o$ there exists a unique $\bar{\lambda} \in \mathcal{D}_{\mathcal{Z}}^o$ such that

$$\bar{x} = \mathcal{Z}'(\bar{\lambda})$$

and

$$\bar{\lambda} = I'(\bar{x})$$

Furthermore $I(\bar{x}) = \bar{\lambda}\bar{x} - \mathcal{Z}(\bar{\lambda})$.

We will say that $\bar{x}$ and $\bar{\lambda}$ are in duality if the conditions of the above lemma are satisfied.

Proof: The function $F_x(\lambda) = \lambda x - \mathcal{Z}(\lambda)$ has a maximum for $\lambda = \bar{\lambda}$. This is because it is concave and $\partial_\lambda F_x(\bar{\lambda}) = 0$. It follows that $I(\bar{x}) = \bar{\lambda}\bar{x} - \mathcal{Z}(\bar{\lambda})$ and that $\mathcal{Z}(\lambda) = \sup_x \{\lambda x - I(x)\}$. By the same argument $G_\lambda(x) = \lambda x - I(x)$ is maximized by $\bar{x}$. □

A.2.2 Proof of Cramer's theorem

Upper bound

Let us start with A a closed interval of the form $J_x = [x, +\infty)$ and let $x > m$. Then the exponential Chebycheff's inequality gives for any $\lambda > 0$

$$\mathbb{P}(\hat{S}_n \geq x) \leq e^{-n\lambda x}\mathbb{E}[e^{\sum_{i=1}^n \lambda X_i}] = e^{-n\lambda x} M(\lambda)^n$$

Since $\lambda > 0$ is arbitrary, we can optimize the bound and obtain for $x > m$

$$\frac{1}{n}\log \mathbb{P}(\hat{S}_n \geq x) \leq -\sup_{\lambda>0}\{\lambda x - \mathcal{Z}(\lambda)\} = -I(x) \tag{A.2.6}$$

where we use (A.2.4) in the last equality. Similarly for $x < m$ we obtain

$$\frac{1}{n}\log \mathbb{P}(\hat{S}_n \leq x) \leq -\sup_{\lambda<0}\{\lambda x - \mathcal{Z}(\lambda)\} = I(x) \tag{A.2.7}$$

Consider now an arbitrary closed set $C \subset \mathbb{R}$. If $m \in C$, then $\inf_{x\in C} I(x) = 0$ and the upper bound is trivial.

If $m \notin C$, let (x_1, x_2) be the largest open interval around m such that $C \cap (x_1, x_2) = \emptyset$, i.e.

$$C \subseteq (-\infty, x_1] \cup [x_2, +\infty)$$

(if $x_1 = -\infty$ then $C \subseteq [x_2, +\infty)$ and if $x_2 = +\infty$ then $C \subseteq (-\infty, x_1]$). Observe that $x_1 < m < x_2$. Consequently

$$\mathbb{P}(\hat{S}_n \in C) \leq \mathbb{P}(\hat{S}_n \geq x_2) + \mathbb{P}(\hat{S}_n \leq x_1) \leq 2\max\{\mathbb{P}(\hat{S}_n \geq x_2), \mathbb{P}(\hat{S}_n \leq x_1)\}$$

and using (A.2.6) and (A.2.7)

$$\frac{1}{n}\log \mathbb{P}(\hat{S}_n \in C) \leq -\min\{I(x_2), I(x_1)\} + \frac{1}{n}\log 2 \tag{A.2.8}$$

and from the monotonicity of $I(x)$ on $(-\infty, x_1]$ and $[x_2, +\infty)$

$$\inf_{x\in C} I(x) \geq \min\{I(x_2), I(x_1)\}$$

which concludes the upper bound.

Lower bound

Given an open set G, it is enough to prove that for any $x \in G$

$$\liminf_{n\to\infty} \frac{1}{n}\log \mathbb{P}(\hat{S}_n \in G) \geq -I(x)\ .$$

To this end, it is enough to prove that for any x and any $\delta > 0$,

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \in (x-\delta, x+\delta)) \geq -I(x) \ .$$

Clearly it is enough to consider x such that $I(x) < \infty$. Assume α has finite support and that $\alpha((-\infty,0)) > 0, \alpha((0,\infty)) > 0$. Then $\mathcal{Z}$ is finite everywhere ($\mathcal{D}_{\mathcal{Z}} = \mathcal{D}^o_{\mathcal{Z}} = \mathbb{R}$) and there exists a unique $\lambda_0 \in \mathcal{D}^o_{\mathcal{Z}}$ such that

$$I(x) = \lambda_0 x - \mathcal{Z}(\lambda_0) \qquad \text{and} \qquad x = \mathcal{Z}'(\lambda_0)$$

Assuming $x \geq m$, we have that $\lambda_0 \geq 0$.

Let us define the probability law on $\mathbb{R}$

$$\alpha_{\lambda_0}(dy) = \frac{e^{\lambda_0 y}}{M(\lambda_0)} \alpha(dy)$$

Notice that

$$\int y \ \alpha_{\lambda_0}(dy) = \mathcal{Z}'(\lambda_0) = x$$

Noting $A_{n,\delta} = \{(x_1,\ldots,x_n) : (x_1+\cdots+x_n)/n \in (x-\delta, x+\delta)\} \subset \mathbb{R}^n$, then for $\delta_1 < \delta$

$$\begin{aligned}
\mathbb{P}(\hat{S}_n \in (x-\delta, x+\delta)) &\geq \int_{A_{n,\delta_1}} \alpha(dx_1)\ldots\alpha(dx_n) \\
= M(\lambda_0)^n &\int_{A_{n,\delta_1}} e^{-\lambda_0(x_1+\cdots+x_n)} \alpha_{\lambda_0}(dx_1)\ldots\alpha_{\lambda_0}(dx_n) \\
&\geq M(\lambda_0)^n e^{-n\lambda_0(x+\delta_1)} \int_{A_{n,\delta_1}} \alpha_{\lambda_0}(dx_1)\ldots\alpha_{\lambda_0}(dx_n)
\end{aligned}$$

By the law of large numbers, for any $\delta_1 > 0$

$$\int_{A_{n,\delta_1}} \alpha_{\lambda_0}(dx_1)\ldots\alpha_{\lambda_0}(dx_n) \underset{n\to\infty}{\longrightarrow} 1$$

so that

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \in (x-\delta, x+\delta)) \geq -\left[\lambda_0(x+\delta_1) - \mathcal{Z}(\lambda_0)\right] = -I(x) - \lambda_0\delta_1$$

Since $\delta_1 < \delta$ is arbitrary, we can let $\delta_1 \to 0$ and it gives the result. If $x < m$, we have $\lambda_0 < 0$, and in the steps of the above we will have $x - \delta_1$ instead of $x + \delta_1$.

Assume now α is of unbounded support with $\alpha((-\infty,x)) > 0, \alpha((x,\infty)) > 0$. Let $A_0 > 0$ be such that $\alpha([-A_0,x)) > 0, \alpha((x,A_0]) > 0$. For any $A \geq A_0$ let β

be the law of X_1 conditioned on $\{|X_1| \le A\}$, and β_n the law of $\hat{S}_n$ conditioned on $\{|X_i| \le A,\, i = 1, \dots, n\}$. Then, for all $n \ge 1$ and every $\delta > 0$,

$$\alpha_n((x-\delta, x+\delta)) = \beta_n((x-\delta, x+\delta))\,\{\alpha([-A, A])\}^n$$

The preceding result applies for β_n. Note

$$\mathcal{Z}^A(\lambda) = \log \int_{-A}^{A} e^{\lambda y} \alpha(dy),$$

and observe that the logarithmic generating function of β is given by

$$\mathcal{Z}^A(\lambda) - \log \alpha([-A, A]) \;\ge\; \mathcal{Z}^A(\lambda)$$

It follows that

$$\liminf_{n\to\infty} \frac{1}{n} \log \alpha_n((x-\delta, x+\delta)) \ge \inf_{\lambda\in\mathbb{R}} \left\{\mathcal{Z}^A(\lambda) - \lambda x\right\} \tag{A.2.9}$$

Let us define

$$I^*(x) = \limsup_{A\to\infty} \left[\sup_{\lambda\in\mathbb{R}} \left\{\lambda x - \mathcal{Z}^A(\lambda)\right\}\right]$$

then we have

$$\liminf_{n\to\infty} \frac{1}{n} \log \alpha_n((x-\delta, x+\delta)) \ge -I^*(x) \tag{A.2.10}$$

Observe that $\mathcal{Z}^A(\cdot)$ is nondecreasing in A, $\mathcal{Z}^A(0) \le \mathcal{Z}(0) = 0$, and thus $-I^*(x) \le 0$. Moreover the assumption $\alpha([-A_0, x)) > 0, \alpha((x, A_0]) > 0$ implies

$$\lambda x - \mathcal{Z}^A(\lambda) \ge -\inf\left\{\log \alpha[-A_0, x)\,,\, \log \alpha(x, A_0]\right\}$$

Therefore we have $-I^*(x) > -\infty$. The level sets $\{\lambda;\, \mathcal{Z}^A(\lambda) - \lambda x \le -I^*(x)\}$ are non-empty, compact sets that are nested with respect to A. Then it exists λ_0 in their intersection and $-I(x) \le \mathcal{Z}(\lambda_0) - \lambda_0 x = \lim_{A\to\infty} \mathcal{Z}^A(\lambda_0) - \lambda_0 x \le -I^*(x)$. By (A.2.10) we get

$$\liminf_{n\to\infty} \frac{1}{n} \log \alpha_n((x-\delta, x+\delta)) \ge -I(x)$$

The proof for an arbitrary probability law α is completed by observing that if either $\alpha((-\infty, x))$ or $\alpha((x, \infty)) = 0$ then $\mathcal{Z}(\cdot)$ is a monotone function with $\inf_{\lambda\in\mathbb{R}}\{\mathcal{Z}(\lambda) - \lambda x\} = \log \alpha(\{x\})$. Then we have

$$\alpha_n((x-\delta, x+\delta)) \ge \alpha_n(\{x\}) = \alpha(\{x\})^n$$

and

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \in (x-\delta, x+\delta)) \ge -I(x)$$

□

Remark A.2.5 *Notice that the proof contains the non-asymptotic bound* (A.2.8), *i.e.*

$$\forall n \geq 1, \quad \mathbb{P}(\hat{S}_n \in C) \leq 2e^{-n \inf_{x \in C} I(x)} \tag{A.2.11}$$

also called Chernoff's bound.

Remark A.2.6 *The lower bound was obtained by using the change of variable in conjunction with the law of large numbers for the new probabilities. One can get better bound by using the central limit theorem, and obtain the following corollary*

Corollary A.2.7 *For any $x > m$,*

$$\begin{aligned} \lim_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \geq x) &= -I(x) \qquad \text{if } x > m \\ \lim_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \leq x) &= -I(x) \qquad \text{if } x < m \end{aligned} \tag{A.2.12}$$

Proof: By the central limit theorem

$$\int_{\{x_1+\cdots+x_n/n \in [x, x+\delta_1)\}} \alpha_{\lambda_0}(dx_1)\ldots\alpha_{\lambda_0}(dx_n) \underset{n\to\infty}{\longrightarrow} \frac{1}{2}$$

So in the proof of the lower bound one can substitute $(x-\delta, x+\delta)$ with $[x, x+\delta)$. Since $\mathbb{P}(\hat{S}_n \geq x) \geq \mathbb{P}(\hat{S}_n \in [x, x+\delta))$ one obtains

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}(\hat{S}_n \geq x) \geq -I(x)$$

The upper bound follows from the one in theorem A.2.3.

Examples in $\mathbb{R}$

1. Let α be the gaussian distribution

$$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-m)^2/2\sigma^2}\, dx$$

then $I(x) = (x-m)^2/2\sigma^2$. In this case one can compute it directly, since $\hat{S}_n - nm$ has law $\mathcal{N}(0, \sigma^2/n)$.

2. $\alpha = \frac{1}{2}(\delta_0 + \delta_1)$ (Bernoulli). Then $M(\lambda) = \frac{1}{2}(1+e^\lambda)$ and

$$I(x) = x\log x + (1-x)\log(1-x) + \log 2 \qquad \text{if } x \in [0,1]$$

and $I(x) = +\infty$ otherwise.

3. For the exponential law $\alpha(dx) = \beta e^{-\beta x} 1_{x\geq 0}\, dx$, we have $M(\lambda) = \beta/(\beta - \lambda)$ for $-\infty < \lambda < \beta$, otherwise $M(\lambda) = +\infty$. Then

$$I(x) = \beta x - 1 - \log(\beta x) \qquad \text{if } x > 0$$

and $I(x) = +\infty$ if $x \leq 0$.

4. If ξ in a random variable with law $\mathcal{N}(0, 1/\beta)$, then ξ^2 has law $\chi^2(1)$, i.e. a gamma law $\Gamma(1/2, \beta/2)$, which has density

$$\frac{\beta^{1/2}}{\sqrt{2}\Gamma(1/2)} x^{-1/2} e^{-\beta x}$$

Its moment generating function is $M(\lambda) = (\beta/(\beta - 2\lambda))^{1/2}$ if $\lambda < \beta/2$, otherwise equal to $+\infty$. The rate function results

$$I(x) = \frac{1}{2}\{\beta x - \log(\beta x) - 1\} \qquad \text{if } x > 0$$

and $+\infty$ if $x < 0$.

A.3 Cramér's Theorem in $\mathbb{R}^d$

Let $\{\mathbf{X}_n\}$ be a sequence of i.i.d. random variables in $\mathbb{R}^d$, and denote $\alpha(d\mathbf{x})$ the common law. We define as before, for $\mathbf{u} \in \mathbb{R}^d$, the moment generating function and its logarithm

$$M(\mathbf{u}) = \int_{\mathbb{R}^d} e^{\mathbf{u}\cdot\mathbf{x}}\, \alpha(d\mathbf{x}), \qquad \mathcal{Z}(\mathbf{u}) = \log M(\mathbf{u}) \tag{A.3.1}$$

and we denote $\mathcal{D}_{\mathcal{Z}} = \{\mathbf{u} \in \mathbb{R}^d : \mathcal{Z}(\mathbf{u}) < +\infty\}$. We assume that $0 \in \mathcal{D}^o_{\mathcal{Z}}$. Then $M(\mathbf{u})$ is smooth in this open set and $\nabla M(0) = \mathbf{m} = \mathbb{E}(\mathbf{X}_1)$.

The rate function is the Legendre-Fenchel transform of $\mathcal{Z}$:

$$I(\mathbf{x}) = \sup_{\mathbf{u}\in\mathbb{R}^d} \{\mathbf{u}\cdot\mathbf{x} - \mathcal{Z}(\mathbf{u})\} \tag{A.3.2}$$

As in the one dimensional case, it follows immediately from the definition that I is non negative, convex, lower semicontinuous and $I(\mathbf{m}) = 0$. Denoting $\mathcal{D}_I = \{\mathbf{x} : I(\mathbf{x}) < +\infty\}$ we have similar properties as in the one dimensional case:

Lemma A.3.1 *$I(\mathbf{x}) \in \mathcal{C}^\infty({\mathcal{D}_I}^o)$, and $\mathbf{m} \in ({\mathcal{D}_I}^o)$. There exists a diffeomorphism between ${\mathcal{D}_I}^o$ and $\mathcal{D}^o_\lambda$ defined by*

$$\mathbf{u}^* = (\nabla \mathcal{Z})(\mathbf{u}), \quad \mathbf{u} = (\nabla I)(\mathbf{u}^*) \tag{A.3.3}$$

and

$$(\nabla^2 \mathcal{Z})(\mathbf{u}) = \left[\nabla^2 I)(\mathbf{u}^*)\right]^{-1} \tag{A.3.4}$$

Theorem A.3.2 *For any Borel set $A \subset \mathbb{R}^d$,*

$$-\inf_{\mathbf{x}\in A^o} I(\mathbf{x}) \le \liminf_{n\to\infty} \frac{1}{n}\log \mathbb{P}(\hat{S}_n \in A) \le \limsup_{n\to\infty} \frac{1}{n}\log \mathbb{P}(\hat{S}_n \in A) \le -\inf_{\mathbf{x}\in \bar{A}} I(\mathbf{x})$$

were A^o is the interior of A and $\bar{A}$ is the closure of A.

Proof:

The lower bound is proven in the same way as in $d = 1$. Consider $\mathbf{u}^*$ such that $I(\mathbf{u}^*) < +\infty$. To simplify we assume there exists a unique $\mathbf{u} \in \mathcal{D}^o_I$ such that

$$I(\mathbf{u}^*) = \mathbf{u}^* \cdot \mathbf{u} - \mathcal{Z}(\mathbf{u}) \qquad \mathbf{u} = (\nabla I)(\mathbf{u}^*)$$

Then we consider the new probability law on $\mathbb{R}^d$, absolutely continuous with respect to α, defined by

$$\alpha_\mathbf{u}(d\mathbf{x}) = e^{\mathbf{u}\cdot\mathbf{x} - \mathcal{Z}(\mathbf{u})}\, \alpha(d\mathbf{x})$$

Observe that

$$\int \mathbf{x}\alpha_\mathbf{u}(d\mathbf{x}) \; = \; \mathbf{u}^*$$

Noting $A_{n,\delta} = \{(\mathbf{x}_1, \dots, \mathbf{x}_n) : |(\mathbf{x}_1 + \cdots + \mathbf{x}_n)/n - \mathbf{u}^*| \le \delta\} \subset \mathbb{R}^n$, then for any $\delta_1 < \delta$

$$\begin{aligned}
\mathbb{P}(|\hat{\mathbf{S}}_n - \mathbf{u}^*| < \delta) &\ge \int_{A_{n,\delta_1}} \alpha(d\mathbf{x}_1)\dots\alpha(d\mathbf{x}_n) \\
&= M(\mathbf{u})^n \int_{A_{n,\delta_1}} e^{-\mathbf{u}\cdot(\mathbf{x}_1+\cdots+\mathbf{x}_n)} \alpha_\mathbf{u}(d\mathbf{x}_1)\dots\alpha_\mathbf{u}(d\mathbf{x}_n) \\
&= M(\mathbf{u})^n e^{-n\mathbf{u}\cdot\mathbf{u}^*} \int_{A_{n,\delta_1}} e^{-\mathbf{u}\cdot[(\mathbf{x}_1+\cdots+\mathbf{x}_n)-n\mathbf{u}^*]} \alpha_\mathbf{u}(d\mathbf{x}_1)\dots\alpha_\mathbf{u}(d\mathbf{x}_n) \\
&\ge e^{-nI(\mathbf{u}^*)} e^{-n|\mathbf{u}|\delta_1} \int_{A_{n,\delta_1}} \alpha_\mathbf{u}(d\mathbf{x}_1)\dots\alpha_\mathbf{u}(d\mathbf{x}_n)
\end{aligned}$$

The law of large numbers now says that

$$\lim_{n\to\infty} \int_{A_{n,\delta_1}} \alpha_\mathbf{u}(d\mathbf{x}_1)\dots\alpha_\mathbf{u}(d\mathbf{x}_n) = 1$$

and we obtain

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}(|\hat{\mathbf{S}}_n - \mathbf{u}^*| < \delta) \geq -I(\mathbf{u}^*) - |\mathbf{u}|\delta_1$$

and letting $\delta_1 \to 0$ we conclude that for any $\delta > 0$ we have the lower bound

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}(|\hat{\mathbf{S}}_n - \mathbf{u}^*| < \delta) \geq -I(\mathbf{u}^*)$$

The upper bound requires a little more work. Convexity plays a role here.

Let C any Borel set in $\mathbb{R}^d$. Then the exponential Chebicheff inequality implies for any $\mathbf{u} \in \mathbb{R}^d$

$$\mathbb{P}\left(\hat{\mathbf{S}}_n \in C\right) \leq \exp\left[-n \inf_{\mathbf{x}\in C} \mathbf{u}\cdot\mathbf{x}\right] \mathbb{E}\left(e^{n\mathbf{u}\cdot\hat{\mathbf{S}}_n}\right) = \exp\left[-n \inf_{\mathbf{x}\in C} \mathbf{u}\cdot\mathbf{x}\right] M(\mathbf{u})^n$$

and optimizing in $\mathbf{u} \in \mathbb{R}^d$ we obtain

$$\frac{1}{n} \log \mathbb{P}\left(\hat{\mathbf{S}}_n \in C\right) \leq -\sup_{\mathbf{u}\in\mathbb{R}^d} \inf_{\mathbf{x}\in C} \left[\mathbf{u}\cdot\mathbf{x} - \mathcal{Z}(\mathbf{u})\right] \tag{A.3.5}$$

So to conclude we need to exchange "$\sup_{\mathbf{u}\in\mathbb{R}^d}$" with "$\inf_{\mathbf{x}\in C}$". This is immediate if C is a convex set by the following lemma (c.f. [4], chapter 6):

Lemma A.3.3 *Let $g(\mathbf{u}, \mathbf{x})$ be convex and lower semicontinuous in $\mathbf{x}$, concave and uppersemicontinuous in $\mathbf{u}$, then if C is compact and convex*

$$\inf_{\mathbf{x}\in C} \sup_{\mathbf{u}\in\mathbb{R}^d} g(\mathbf{u}, \mathbf{x}) = \sup_{\mathbf{u}\in\mathbb{R}^d} \inf_{\mathbf{x}\in C} g(\mathbf{u}, \mathbf{x}) \tag{A.3.6}$$

Consider now any compact set $K \subset \mathbb{R}^d$,there exists $l > 0$ such that $\inf_{\mathbf{x}\in K} I(\mathbf{x}) = l$. By the ower semicontinuity of $I(\cdot)$, for a fixed $\epsilon > 0$ and any $\mathbf{x}' \in K$, there exists a closed ball $C(\mathbf{x}')$ such that

$$I(\mathbf{x}) \geq l - \epsilon \qquad \forall \mathbf{x} \in C(\mathbf{x}')$$

Since K is compact, there exists a finite subcover $C(\mathbf{x}'_1), \ldots, C(\mathbf{x}'_N)$ extracted from these closed ball. Then

$$\mathbb{P}\left(\hat{\mathbf{S}}_n \in K\right) \leq \sum_{j=1}^{N} \mathbb{P}\left(\hat{\mathbf{S}}_n \in C(\mathbf{x}'_j)\right) \leq N \max_{1\leq j\leq N} \mathbb{P}\left(\hat{\mathbf{S}}_n \in C(\mathbf{x}'_j)\right)$$

$$\leq N \max_{1\leq j\leq N} \exp\left(-n \inf_{C(\mathbf{x}'_j)} I\right) \leq N e^{-n(l-\epsilon)}$$

and

$$\limsup_{n\to\infty} \frac{1}{n} \log \mathbb{P}\left(\hat{\mathbf{S}}_n \in K\right) \leq -(l-\epsilon)$$

Since ϵ is arbitrary, this proves the upper bound for compact sets.

To extend this bound from compact to closed sets, we need to prove the *exponential tightness* of the distribution of $\hat{\mathbf{S}}_n$, i.e.

$$\lim_{\rho\to\infty} \lim_{n\to\infty} \frac{1}{n} \log \mathbb{P}\left(\hat{\mathbf{S}}_n \notin H_\rho\right) = -\infty \tag{A.3.7}$$

where $H_\rho = [-\rho, \rho]^d$ is the centered hypercube of length 2ρ. To prove this observe that, denoting $\hat{S}_n^{(j)}$ is the average of $X_1^{(j)}, \ldots, X_n^{(j)}$, by applying the results obtained in the one-dimensional case, we have

$$\mathbb{P}\left(\hat{\mathbf{S}}_n \notin H_\rho\right) \leq \sum_{j=1}^{d} \mathbb{P}\left(\hat{S}_n^{(j)} \notin (-\rho, \rho)\right) \leq d \max_{j=1,\ldots,d} \exp\left(-n \min\{I^j(\rho), I^j(-\rho)\}\right)$$

where I^j is the rate function for the $j-$marginal distribution of the law α. Then (A.3.7) follows by applying lemma A.2.2.

□

A.4 Generalities on Large Deviations

Let X a complete separable metric space and P_n a family of probability distributions on X. In the previous sections $X = \mathbb{R}^d$ and P_n the distribution of $\hat{S}_n$. We says that $\{P_n\}$ satisfies a large deviation principle with good rate function $I(\cdot)$ if there exists a function $I : X \to [0, \infty]$ such that:

1. $I(\cdot)$ is lower semicontinuous.

2. For each $\ell < \infty$ the set $\{x : I(x) \leq \ell\}$ is compact in X.

3. For each closed set $C \subset X$

$$\limsup_{n\to\infty} \frac{1}{n} \log P_n(C) \leq -\inf_{x\in C} I(x).$$

4. For each open set $G \subset X$

$$\liminf_{n\to\infty} \frac{1}{n} \log P_n(G) \geq -\inf_{x\in G} I(x).$$

Here the adjective *good* refers to properties 1 and 2. The next lemma does not require the rate function I to be good.

Theorem A.4.1 ***Varadhan's Lemma.*** *Let P_n satisfy the large deviation principle with rate function I. Then for any bounded continuous function $F(x)$ on X*

$$\lim_{n\to\infty} \frac{1}{n} \log \int e^{nF(x)} dP_n(x) = \sup_{x\in X}\{F(x) - I(x)\}.$$

Proof.

Upper bound. For any given $\delta > 0$, since F is bounded and continuous, we can find a finite number of closed sets covering X such that the oscillation of $F(\cdot)$ on each of these closed sets is less or equal δ. Then

$$\int e^{nF(x)} dP_n(x) \le \sum_{j=1}^{m} \int_{C_j} e^{nF(x)} dP_n(x) \le \sum_{j=1}^{m} e^{nF_j+\delta} P_n(C_j)$$

where $F_j = \inf_{C_j} F(x)$. It follows

$$\begin{aligned}\limsup_{n\to\infty} \frac{1}{n} \log \int e^{nF(x)} dP_n(x) &\le \sup_{1\le j\le m} [F_j + \delta - \inf_{C_j} I(x)] \\ &\le \sup_{1\le j\le m} \sup_{C_j} [F(x) - I(x)] + \delta \\ &= \sup_{x\in X} [F(x) - I(x)] + \delta\end{aligned}$$

Since δ is arbitrary, we can let it go to 0.

Lower bound. By definition of a supremum for any $\delta > 0$ we can find $y \in X$ such that $F(y) - I(y) \ge \sup_x [F(x) - I(x)] - \delta/2$. Since F is continuous we can find an open neighborhood U of y such that $F(x) \ge F(y) - \delta/2$ for any $x \in U$. Then we obtain

$$\liminf_{n\to\infty} \frac{1}{n} \log \int e^{nF(x)} dP_n(x) \ge \liminf_{n\to\infty} \frac{1}{n} \log \int_U e^{nF(x)} dP_n(x)$$
$$\ge F(y) - \frac{\delta}{2} - \inf_{x\in U} I(x) \ge F(y) - I(y) - \frac{\delta}{2} \ge \sup_x [F(x) - I(x)] - \delta$$

and we conclude from the arbitrariness of δ. □

Theorem A.4.2 ***Contraction Principle.*** *Let P_n satisfy the large deviation principle with rate function I, and $\pi : X \to Y$ a continuous mapping from X to another complete separable metric space Y. Then $\tilde{P}_n = P_n \pi^{-1}$ satisfies a large deviation principle with rate function*

$$\tilde{I}(y) = \inf_{x:\pi(x)=y} I(x),$$
$$\tilde{I}(y) = +\infty \qquad \text{if } \{x : \pi(x) = y\} = \emptyset$$

Proof. Since π is continuous, given any closed set $\tilde{C} \subset Y$, the subset $C = \pi^{-1}(\tilde{C})$ is closed in X. Then

$$\limsup_{n\to\infty} \frac{1}{n} \log \tilde{P}_n(\tilde{C}) = \limsup_{n\to\infty} \frac{1}{n} \log P_n(C) \le -\inf_{x\in C} I(x) = -\inf_{y\in\tilde{C}} \inf_{x:\pi(x)=y} I(x).$$

and similarly for the lower bound. □

A.5 Large deviations for densities

We deal first with the one-dimensional case. If the distribution of $\hat{S}_n$ on $\mathbb{R}$ has a density that we denote by $f_n(x)$, from Cramers theorem we have the intuition that $f_n(x) \sim e^{-nI(x)}$ for large n. We will prove this under some condition on the probability $\alpha(dx)$. It is interesting to notice that we will not use Cramer's theorem in the proof, but the following *local central limit theorem.*

Theorem A.5.1 ***Local central limit theorem.*** *Let $\phi(k)$ the characteristic function of a centered probability measure $\alpha(dx)$ with finite variance σ^2, and assume that $|\phi(k)| < 1$ if $k \neq 0$ and that there exists an integer $r \geq 1$ such that $|\phi|^r$ is integrable. Let $\tilde{g}_n(x)$ the probability density of $(X_1 + \cdots + X_n)/\sqrt{n}$, where X_j are i.i.d. with common law α. Then*

$$\lim_{n\to\infty} \tilde{g}_n(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}.$$

Proof. The characteristic function of α is defined by

$$\phi(k) = \int e^{ixk} \alpha(dx) \tag{A.5.1}$$

The characteristic function of the distribution of $X_1 + \cdots + X_r$ is $\phi^r(k)$ that is integrable. It follows that the probability density $\tilde{g}_n(x)$ exists for any $n \geq r$ (cf. [?], theorem XV.3.3). Then

$$\tilde{g}_n(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ixk} \left[\phi\left(\frac{k}{\sqrt{n}}\right)\right]^n dk$$

and therefore

$$\left| \tilde{g}_n(x) - \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2} \right| \leq \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left| \phi\left(\frac{k}{\sqrt{n}}\right)^n - e^{-k^2\sigma^2/2} \right| dk$$

Given $a > 0$, we split the integral in three parts.

1. Uniformly in $k \in [-a, a]$,

$$\phi\left(\frac{k}{\sqrt{n}}\right)^n = \left(1 - \frac{k^2\sigma^2}{2n} + o\left(\frac{1}{n}\right)\right)^n \underset{n\to\infty}{\longrightarrow} e^{-k^2\sigma^2/2}$$

so that

$$\int_{-a}^{+a} \left| \phi\left(\frac{k}{\sqrt{n}}\right)^n - e^{-k^2\sigma^2/2} \right| dk \to 0$$

2. Observe that it is possible to choose $\delta > 0$ such that

$$|\phi(k)| \leq e^{-k^2\sigma^2/4} \qquad \text{if} \quad |k| \leq \delta.$$

Then for the interval $|k| \in (a, \delta\sqrt{n})$, we can estimate as

$$\int_a^{\delta\sqrt{n}} \left| \phi\left(\frac{k}{\sqrt{n}}\right)^n - e^{-k^2\sigma^2/2} \right| dk \leq \int_a^{\delta\sqrt{n}} 2e^{-k^2\sigma^2/4} dk \leq \int_a^{+\infty} 2e^{-k^2\sigma^2/4} dk$$

that converge to 0 as $a \to \infty$.

3. It remains to estimate the contribution from the interval $(\delta\sqrt{n}, +\infty)$. Since we assumed that $|\phi(k)| < 1$ for $k \neq 0$, and since $|\phi|^k$ is integrable, we have $\phi(k) \to 0$ as $k \to \infty$. Consequently we must have $\sup_{|k|\geq\delta} |\phi(k)| = \eta < 1$, and we can estimate

$$\int_{\delta\sqrt{n}}^{+\infty} \left| \phi\left(\frac{k}{\sqrt{n}}\right)^n - e^{-k^2\sigma^2/2} \right| dk \leq \eta^{n-r} \int_{-\infty}^{+\infty} \left| \phi\left(\frac{k}{\sqrt{n}}\right)\right|^r dk + \int_{\delta\sqrt{n}}^{+\infty} e^{-k^2\sigma^2/2} dk$$
$$= \eta^{n-r}\sqrt{n} \int_{-\infty}^{+\infty} |\phi(k)|^r dk + \int_{\delta\sqrt{n}}^{+\infty} e^{-k^2\sigma^2/2} dk$$

that converges to 0 as $n \to \infty$.

□

Distributions such that their characteristic function $|\phi(k)| < 1$ for $k \neq 0$ are called *non-lattice* ([2], chapter 2). It does not imply they have density.

We assume now that the measure $\alpha(dx)$ satisfies all the assumptions made in section A.2, and furthermore its characteristic function satisfies conditions of the local central limit theorem A.5.1. Then, for $n \geq r$, the distribution of $\hat{S}_n$ on $\mathbb{R}$ has a density that we denote by $f_n(x)$.

Theorem A.5.2 *For any $y \in \mathcal{D}_I^o$ we have*

$$\lim_{n\to\infty} \frac{1}{n} \log f_n(y) = -I(y) \ . \tag{A.5.2}$$

Proof.

Let $\tau_y\alpha$ the translation of the measure α by y. Assume that $m = \int x\alpha(dx) = 0$, otherwise just recenter it and consider $\tau_m\alpha$.

Let $y \in {\mathcal{D}_I}^o$. Then by lemma A.2.4 there exists a unique $\lambda \in {\mathcal{D}_\mathcal{Z}}^o$ such that $y = \mathcal{Z}'(\lambda)$, $\lambda = I'(y)$, and $I(y) = \lambda y - \mathcal{Z}(\lambda)$. Define

$$\tilde{\alpha}(y, dx) = \frac{1}{M(\lambda)} e^{(x+y)\lambda} \tau_y \alpha(dx)$$

Observe that this is a probability distribution with 0 average. In fact

$$\int \tilde{\alpha}(y, dx) = \frac{1}{M(\lambda)} \int e^{z\lambda} \alpha(dz) = 1$$

and

$$\int x\tilde{\alpha}(y, dx) = -y + \frac{1}{M(\lambda)} \int z e^{z\lambda} \alpha(dz) = -y + \mathcal{Z}'(\lambda) = 0$$

So we treat here y as a parameter. Let $X_1^y, \dots, X_n^y$ i.i.d. random variables with law given by $\tilde{\alpha}(y, dx)$.

For $n \geq r$ it exists the density for the distribution of $(X_1^y + \dots + X_n^y)/n$ that we denote by $f_n(x, y)$, and it is equal to

$$f_n(x, y) = \frac{e^{n(x+y)\lambda}}{M(\lambda)^n} f_n(x + y) = e^{n(I(y)+\lambda x)} f_n(x + y)$$

To prove this formula, compute, for a given bounded measurable function $G(\cdot)$:

$$\begin{aligned} \mathbb{E}\left(G((X_1^y + \dots + X_n^y)/n)\right) &= \int_{\mathbb{R}^n} G(\hat{s}_n) e^{n(I(y)+\lambda \hat{s}_n)} \tau_y\alpha(dx_1) \dots \tau_y\alpha(dx_n) \\ &= \int_{\mathbb{R}} G(\hat{s}) e^{n(I(y)+\lambda \hat{s})} f_n(\hat{s} + y) d\hat{s} \end{aligned} \tag{A.5.3}$$

It follows that

$$f_n(y) = e^{-nI(y)} f_n(0, y)$$

To conclude we only need to prove that $(\log f_n(0, y))/n \to 0$ as $n \to \infty$.

Let $\tilde{f}_n(x, y)$ the density of $(X_1^y + \dots + X_n^y)/\sqrt{n}$. Then $f_n(x, y) = \sqrt{n}\tilde{f}_n(\sqrt{n}x, y)$. By the local central limit theorem A.5.1, the result follows immediately. □

For $y \in \mathbb{R}$ define $\nu_y^{(n)}(dx_1, \dots, dx_n)$ the conditional distribution of $(X_1, \dots, X_n)$ on the hyperplane $x_1 + \dots + x_n = ny$. This is defined as the probability measure on $\mathbb{R}^{n-1}$ satisfying the relation

$$\mathbb{E}\left(G(\hat{S}_n)H(X_1, \dots, X_n)\right) = \int_{\mathbb{R}} dy f_n(y) G(y) \int H(x_1, \dots, x_n) \nu_y^{(n)}(dx_1, \dots, dx_n)$$

Lemma A.5.3 *Let F be a bounded continuous function on $\mathbb{R}$ and $y \in \mathcal{D}_I^o$, $\lambda = I'(y)$. For every $\theta \in \mathbb{R}$, the limit*

$$\lim_{n\to\infty} \frac{1}{n} \log \int e^{\theta(F(x_1)+\dots+F(x_n))} \nu_y^{(n)}(dx_1, \dots, dx_n) = G(y, \theta) \tag{A.5.4}$$

exists and G is differentiable at $\theta = 0$ with

$$\frac{\partial G(y, \theta)}{\partial \theta}\bigg|_{\theta=0} = \int F(x) \alpha_\lambda(dx). \tag{A.5.5}$$

Proof Denote by $H_n(y, \theta)$ the function

$$\int e^{\theta(F(x_1)+\dots+F(x_n))} \nu_y^{(n)}(dx_1, \dots, dx_n) = \frac{H_n(y, \theta)}{f_n(y)} \tag{A.5.6}$$

which, by (A.5.3), can be formally written as

$$H_n(y, \theta) = \int_{x_1+\dots+x_n=ny} e^{\theta(F(x_1)+\dots+F(x_n))} \alpha(dx_1) \dots \alpha(dx_n).$$

Let us denote

$$a(\theta) = \int e^{\theta F(x)} \alpha(dx), \qquad M(\lambda, \theta) = \frac{1}{a(\theta)} \int e^{\lambda x + \theta F(x)} \alpha(dx)$$

Then we can compute the Cramér rate function for the law $a(\theta)^{-1} e^{\theta F(x)} \alpha(dx)$, and this is given by

$$I_\theta(y) = I(y, \theta) = \sup_{\bar{\lambda}} \left\{\bar{\lambda} y - \log M(\bar{\lambda}, \theta)\right\}$$

Observe that $\mathcal{D}_{I_\theta} = \mathcal{D}_I$ because F is bounded. If $(Y_1, \dots, Y_n)$ are i.i.d. distributed by $a(\theta)^{-1} e^{\theta F(x)} \alpha(dx)$, then the density of the distribution of $(Y_1 + \dots + Y_n)/n$ is given by $a(\theta)^{-n} H_n(y, \theta)$. Then by applying A.5.2 to this law we obtain

$$\lim_{n\to\infty} \frac{1}{n} \log H_n(y, \theta) = -I(y, \theta) + \log a(\theta).$$

Consequently we have, applying again A.5.2

$$\lim_{n\to\infty}\frac{1}{n}\log\int e^{\theta(F(x_1)+....+F(x_n))}\nu_y^{(n)}(dx_1,\ldots,dx_n)=\lim_{n\to\infty}\frac{1}{n}\log H_n(y,\theta)-\lim_{n\to\infty}\frac{1}{n}\log f_n(y)$$
$$=\log a(\theta)-I(y,\theta)+I(y)\equiv G(y,\theta).$$

Differentiating $G(y,\theta)$ we have

$$\frac{\partial G(y,\theta)}{\partial\theta}=\frac{a'(\theta)}{a(\theta)}-\frac{\partial I(y,\theta)}{\partial\theta}$$

In order to compute this last expression let us set $\lambda^*(y,\theta)=\partial_y I(y,\theta)$. Existence of $\lambda^*(y,\theta)$ is provided by the assumption $y\in\mathcal{D}_I^o$ and the equality between the sets $\mathcal{D}_I$ and $\mathcal{D}_{I_\theta}$. We have

$$I(y,\theta)=\lambda^*y-\log M(\lambda^*,\theta).$$

Then, since $\partial_\lambda\log M(\lambda^*,\theta)=y$, we get

$$\partial_\theta I(y,\theta)=y\partial_\theta\lambda^*-M^{-1}\left(\partial_\theta M+\partial_\lambda M\partial_\theta\lambda^*\right)=-\partial_\theta\log M(\lambda^*,\theta)$$
$$=\partial_\theta\log a(\theta)-M^{-1}\partial_\theta\int e^{\lambda x+\theta F(x)}\alpha(dx)=\frac{a'(\theta)}{a(\theta)}-\int F(x)e^{\lambda^*x+\theta F(x)-\log M(\lambda^*,\theta)}\alpha(dx)$$

So we have

$$\partial_\theta G(y,\theta)=\int F(x)e^{\lambda^*x+\theta F(x)-\log M(\lambda^*,\theta)}\alpha(dx)$$

and sending $\theta\to 0$ we obtain

$$\partial_\theta G(y,0)=\int F(x)e^{\lambda^*(y,0)x-\log M(\lambda^*(y,0),0)}\alpha(dx)=\int F(x)\alpha_\lambda(dx)$$

□

Theorem A.5.4 *For any $y\in\mathcal{D}_I^o$, and any $\epsilon>0$*

$$\lim_{n\to\infty}\nu_y^{(n)}\left(\left|\frac{1}{n}\sum_{j=1}^n F(X_j)-\int F(x)\alpha_\lambda(dx)\right|\geq\epsilon\right)=0 \tag{A.5.7}$$

Proof. Without loosing any generality, let us assume that $\int F(x)\alpha_\lambda(dx)=0$. Consequently $G(\theta,y)=O(\theta^2)$. Then for any $\theta>0$

$$\nu_y^{(n)}\left(\left|\frac{1}{n}\sum_{j=1}^n F(X_j)\right|\geq\epsilon\right)\leq e^{-n\theta\epsilon}\int e^{\theta|\sum_{j=1}^n F(x_j)|}\nu_y^{(n)}(dx_1,\ldots,dx_n)$$
$$\leq e^{-n\theta\epsilon}\int e^{\theta\sum_{j=1}^n F(x_j)}\nu_y^{(n)}(dx_1,\ldots,dx_n)$$
$$+e^{-n\theta\epsilon}\int e^{-\theta\sum_{j=1}^n F(x_j)}\nu_y^{(n)}(dx_1,\ldots,dx_n)$$

and by (A.5.4)

$$\lim_{n\to\infty} \frac{1}{n} \log \nu_y^{(n)} \left(\left| \frac{1}{n} \sum_{j=1}^{n} F(x_j) \right| \geq \epsilon \right) \leq -\theta\epsilon + \max\{G(\theta, y), G(-\theta, y)\}$$

Optimizing the above bound in θ one obtains

$$\lim_{n\to\infty} \frac{1}{n} \log \nu_y^{(n)} \left(\left| \frac{1}{n} \sum_{j=1}^{n} F(x_j) \right| \geq \epsilon \right) \leq -C\epsilon^2$$

for some positive constant C. □

Observe that $\nu_y^{(n)}$ is a symmetric measure, so we have

$$\int F(x_1)\nu_y^{(n)}(dx_1, \ldots, dx_n) = \int \frac{1}{n} \sum_{j=1}^{n} F(x_j)\nu_y^{(n)}(dx_1, \ldots, dx_n) \underset{n\to\infty}{\longrightarrow} \int F(x)\alpha_\lambda(dx)$$

Theorem A.5.5 *Let $F(x_1, \ldots, x_k)$ a bounded continuous function on $\mathbb{R}^k$ and $y \in \mathcal{D}_I^o$, then*

$$\lim_{n\to\infty} \int F(x_1, \ldots, x_k)\nu_y^{(n)}(dx_1, \ldots, dx_n) = \int F(x_1, \ldots, x_k)\alpha_\lambda(dx_1) \ldots \alpha_\lambda(dx_k)$$

Proof. It is enough to consider functions of the form $F(x_1, \ldots, x_k) = F_1(x_1) \ldots F(x_k)$. For simplicity let us prove the case $k = 2$, the generalization to any k is straightforward. Without loosing generality, let us assume that $\int F_j(x)\alpha_\lambda(dx) = 0$. By the exchange symmetry of $\nu_y^{(n)}$ we have

$$\int F_1(x_1)F_2(x_2)\nu_y^{(n)}(dx_1, \ldots, dx_n) = \int \frac{1}{n(n-1)} \sum_{i\neq j} F_1(x_i)F_2(x_j)\nu_y^{(n)}(dx_1, \ldots, dx_n)$$

$$= \int \frac{n^2}{n(n-1)} \left(\frac{1}{n} \sum_i F_1(x_i) \right) \left(\frac{1}{n} \sum_j F_2(x_j) \right) \nu_y^{(n)}(dx_1, \ldots, dx_n) + O\left(\frac{1}{n}\right)$$

and this last expression converges to 0 an $n \to \infty$ by (A.5.7) .

□

The generalization to more dimensions of the above results is quite straightforward and can be left as exercise. Let us state here what the result is in this context.

Let $\alpha(d\mathbf{x})$ a probability measure on $\mathbb{R}^d$ that satisfies conditions used in section A.3. Let us assume that its characteristic function is such that $|\phi(\mathbf{k})| < 1$ for $\mathbf{k} \neq 0$, and such that $|\phi(\mathbf{k})|^r$ is integrable on $\mathbb{R}^d$ for some integer $r \geq 1$. Then, for $n \geq r$ the n-convolution of α has a density and we denote by $f_n(\mathbf{x})$ the density of the distribution of $(\mathbf{X}_1 + \cdots + \mathbf{X}_n)/n$, where $\{\mathbf{X}_j\}$ are i.i.d. with common distribution $\alpha(d\mathbf{x})$.

Theorem A.5.6 *For any* $\mathbf{y} \in \mathcal{D}_I^o$ *we have*

$$\lim_{n\to\infty} \frac{1}{n} \log f_n(\mathbf{y}) = -I(\mathbf{y}) \ . \tag{A.5.8}$$

Example Let $V : \mathbb{R} \to \mathbb{R}_+$ a positive function such that $V(y) \to +\infty$ for $|y| \to +\infty$, and such that

$$Z(\lambda, \beta) = \int e^{-\beta V(y) + \lambda y} dy < \infty \qquad \forall\ \lambda \in \mathbb{R}, \beta > 0.$$

Then we can define the probability density (on $\mathbb{R}^2$)

$$f_{\lambda,\beta}(r,p) = \frac{e^{-\beta(V(r)+p^2/2)+\lambda r}}{\sqrt{2\pi\beta^{-1}}Z(\lambda,\beta)} \tag{A.5.9}$$

Let $\{Y_j = (r_j, p_j)\}$ be a sequence of i.i.d. random variables with common law given by $f_{0,\beta_0}(r,p) dr\, dp$, $\beta_0 > 0$ fixed.

Then the vector valued random variables $\mathbf{X}_j = (r_j,\ (V(r_j) + p_j^2/2))$ clearly has a law $\alpha(d\mathbf{x})$ which is degenerate in $\mathbb{R}^2$ but $\alpha * \alpha$ has a density w.r.t. the Lebesgue measure. Its logarithmic moment generating function is given by

$$\mathcal{Z}(\lambda, \eta) = \log \int e^{\lambda r + \eta(V(r)+p^2/2)} f_{0,\beta}(r,p) dr dp = \log \left(\frac{Z(\lambda, \beta_0 - \eta)}{Z(0,\beta_0)} \sqrt{\frac{\beta_0}{\beta_0 - \eta}} \right)$$

for $\eta < \beta_0$ and $+\infty$ otherwise. The corresponding Legendre transform, for $r \in \mathbb{R}$ and $\mathcal{E} > 0$, is given by

$$\begin{aligned} I(r, \mathcal{E}) &= \sup_{\eta<\beta_0,\lambda} \{\lambda r + \eta\mathcal{E} - \log \mathcal{Z}(\lambda,\eta)\} \\ &= \sup_{\beta>0,\lambda} \left\{ \lambda r - \beta\mathcal{E} - \log\left(\sqrt{2\pi\beta^{-1}} Z(\lambda,\beta)\right)\right\} + \beta_0\mathcal{E} + \log\left(\sqrt{2\pi\beta_0^{-1}} Z(0,\beta_0)\right) \end{aligned}$$

The function defined by

$$S(r,\mathcal{E}) = \inf_{\lambda,\beta>0}\left\{-\lambda r + \beta\mathcal{E} - \log\left(Z(\lambda,\beta)\sqrt{2\pi\beta^{-1}}\right)\right\} \tag{A.5.10}$$

is called *thermodynamic entropy*. So we have obtained

$$I(r,\mathcal{E}) = -S(r,\mathcal{E}) + \beta_0\mathcal{E} + \log Z(0,\beta_0) + \frac{1}{2}\log\frac{2\pi}{\beta_0}$$

Observe that S does not depend on β_0.

The density of the distribution of $\frac{1}{n}\sum_{j=1}^{n}\mathbf{X}_j$ is given by

$$\begin{aligned}
&f_n(r,\mathcal{E})\\
&= \int_{\mathbb{R}^{2n}} \frac{e^{-\beta_0\sum_j \mathcal{E}_j}}{(2\pi\beta_0^{-1})^{n/2}Z(0,\beta_0)^n}\delta\left(\frac{1}{n}\sum_{j=1}^{n}\mathcal{E}_j - \mathcal{E}; \frac{1}{n}\sum_{j=1}^{n} r_j - r\right)\prod_j dr_j dp_j\\
&= \frac{e^{-n\beta_0\mathcal{E}}}{(2\pi\beta_0^{-1})^{n/2}Z(0,\beta_0)^n}\int_{\mathbb{R}^{2n}} \delta\left(\frac{1}{n}\sum_{j=1}^{n}\mathcal{E}_j - \mathcal{E}; \frac{1}{n}\sum_{j=1}^{n} r_j - r\right)\prod_j dr_j dp_j\\
&= \frac{e^{-n\beta_0\mathcal{E}}}{(2\pi\beta_0^{-1})^{n/2}Z(0,\beta_0)^n}\Gamma_n(r,\mathcal{E}).
\end{aligned}$$

where $\Gamma_n(r,p,\mathcal{E})$ is the volume of the corresponding $2n-2$-dimensional surface on $\mathbb{R}^{2n}$ and does not depend on β_0. Applying (A.5.8) we obtain

$$\lim_{n\to\infty}\frac{1}{n}\log\Gamma_n(r,\mathcal{E}) = S(r,\mathcal{E})\ . \tag{A.5.11}$$

for any $(r,\mathcal{E}) \in \mathcal{D}_S^o$. A sufficient condition to have $\mathcal{D}_S^0 = \mathbb{R}\times(0,\infty)$ is $V(r) \geq cr^2$ for a positive constant c.

Appendix B

Entropy

B.1 Generalities

Let Ω be a polish space and $\mathcal{P}(\Omega)$ the topological space of probability measures on Ω equipped with the weak topology. For $\mu, \nu \in \mathcal{P}(\Omega)$, the relative entropy $H(\nu|\mu) \in [0, \infty]$ of μ with respect to ν is defined by

$$H(\nu|\mu) = \sup_f \left\{ \int f d\nu - \log \left(\int e^f d\mu \right) \right\} \tag{B.1.1}$$

where the supremum is taken over all bounded continuous functions $f : \Omega \to \mathbb{R}$. The positivity of $H(\nu|\mu)$ follows from the choice $f = 0$ in the variational formula. Observe also that the supremum can be restricted to the set of positive bounded continuous functions.

As a trivial but useful consequence we have the following entropy inequality

Proposition B.1.1 (Entropy inequality) *Let $f : \Omega \to \mathbb{R}$ be a bounded measurable function and $\eta > 0$ a positive number. Then*

$$\int f d\nu \le \eta^{-1} \left\{ \log \left(\int e^{\eta f} d\mu \right) + H(\nu|\mu) \right\} \tag{B.1.2}$$

Proof If f is continuous it is a trivial consequence of the definition. Since the class of f's for which (B.1.2) holds is closed under point-wise convergence, (B.1.2) continues to be true for every bounded measurable function. □

Proposition B.1.2 *Relative entropy is convex and lower semicontinuous.*

Proof It is a simple consequence of the variational formula. □

Proposition B.1.3 *The entropy $H(\nu|\mu)$ is equal to $+\infty$ if ν is not absolutely continuous with respect to μ. Otherwise it is given by*

$$H(\nu|\mu) = \int \phi \log \phi d\mu, \quad \phi(x) = \left(\frac{d\nu}{d\mu}\right)(x) \tag{B.1.3}$$

*P*roof Observe first that for any density function ϕ the integral of $\phi \log \phi$ makes sense in $\mathbb{R} \cup \{+\infty\}$ since $x \in [0, \infty) \to x \log x$ is bounded above so that the negative part of $\phi \log \phi$ is integrable with respect to μ.

If ν is not absolutely continuous with respect to μ then there exists a measurable set A such that $\mu(A) = 0, \nu(A) > 0$. Choosing the function $f = \alpha \mathbf{1}_A, \alpha > 0$ in (B.1.2) we get $H(\nu|\mu) \geq \alpha\nu(A)$. Since α is arbitrary we have $H(\nu|\mu) = +\infty$.

We first show that if $d\nu = \phi d\mu$ is absolutely continuous with respect to μ and if $d\nu_\theta = \theta d\mu + (1-\theta)d\nu = \phi_\theta d\mu$ for $\theta \in [0, 1]$ then

$$\lim_{\theta \to 0} \int \phi_\theta \log \phi_\theta d\mu = \int \phi \log \phi d\mu \tag{B.1.4}$$

Since $x \in [0, \infty) \to x \log x$ is convex, we have

$$I(\theta) = \int \phi_\theta \log \phi_\theta d\mu \leq (1-\theta) \int \phi \log \phi d\mu$$

On the other hand since $x \in (0, \infty) \to \log x$ is concave and non-decreasing, $\log \phi_\theta \geq \sup\{\log \theta, (1-\theta) \log \phi\}$. Therefore

$$I(\theta) = \theta \int \log \phi_\theta d\mu + (1-\theta) \int \phi \log \phi_\theta d\mu \geq \theta \log \theta + (1-\theta)^2 \int \phi \log \phi d\mu$$

It proves (B.1.4).

Since $\phi_\theta \geq \theta > 0$, Jensen's inequality shows

$$\exp\left[\int \psi d\nu_\theta - I(\theta)\right] \leq \int \frac{e^\psi}{\phi_\theta} d\nu_\theta = \int \exp(\psi) d\mu$$

Hence we have

$$\int \psi d\nu_\theta \leq I(\theta) + \log\left(\int e^\psi d\mu\right)$$

It implies $H(\nu_\theta|\mu) \leq I(\theta)$. Recall that relative entropy is lower semi-continuous. In view (B.1.4) we have

$$H(\nu|\mu) \leq \int \phi \log \phi d\mu$$

To obtain the reversed inequality we observe that if ϕ is uniformly positive and uniformly bounded, it is trivial, by the variational formula defining $H(\nu|\mu)$, that

$$\int \phi \log \phi d\mu \leq H(\nu|\mu)$$

If ϕ is uniformly strictly positive but not bounded we define $\phi_n = \phi \wedge n$ and by Fatou's lemma we have

$$\begin{aligned}
&\int \phi \log \phi d\mu = \int \log \phi d\nu \\
&\leq \liminf_{n\to\infty} \int \log \phi_n d\nu \\
&\leq H(\nu|\mu) + \liminf_{n\to\infty} \log\left(\int (f \wedge n) d\mu\right) = H(\nu|\mu)
\end{aligned}$$

Finally to treat the general case we assume ϕ is uniformly bounded and use ϕ_θ defined above. We proved that $\int \phi_\theta \log \phi_\theta d\mu \leq H(\nu_\theta|\mu)$. Since $\theta \in [0,1] \to H(\nu_\theta|\mu)$ is bounded, lower semi-continuous and convex, it is continuous. Using also (B.1.4) the result follows. □

We now consider the case $\Omega = (\mathbb{R}^2)^{\mathbb{Z}}$ equipped with the product topology. The closed set of translation invariant probability measures on Ω is noted $\mathcal{T}$. Let Λ be a subset of $\mathbb{Z}$ and $\mu, \nu \in \mathcal{P}(\Omega)$. The relative entropy $H_\Lambda(\nu|\mu)$ of ν with respect to ν in Λ is defined by

$$H_\Lambda(\nu|\mu) = H(\mu_\Lambda|\nu_\Lambda) \tag{B.1.5}$$

where μ_Λ, ν_Λ are the marginals of μ and ν with respect to Λ.

Proposition B.1.4 (Superadditivity) *Assume $\mu \in \mathcal{T}$ is product. We have the following superadditivity property of the entropy:*

$$H_{\Lambda\cup\Lambda'}(\nu|\mu) \geq H_\Lambda(\nu|\mu) + H_{\Lambda'}(\nu|\mu) \tag{B.1.6}$$

if $\Lambda \cap \Lambda' = \emptyset$.

Proof Let f_Λ (resp. $f_{\Lambda'}$) be an arbitrary continuous bounded function depending only on ω through sites in Λ (resp. Λ'). We have

$$\int f_\Lambda d\nu_\Lambda - \log\left(\int e^{f_\Lambda} d\mu_\Lambda\right) = \int f_\Lambda d\nu_{\Lambda\cup\Lambda'} - \log\left(\int e^{f_\Lambda} d\mu_{\Lambda\cup\Lambda'}\right)$$

and similarly with Λ replaced by Λ'. Summing the two equalities obtained and using independence of f_Λ and $f_{\Lambda'}$ under $\mu_{\Lambda\cup\Lambda'}$, we get

$$\begin{aligned} H_{\Lambda\cup\Lambda'}(\nu|\mu) &\geq \int (f_\Lambda + f_{\Lambda'}) d\nu_{\Lambda\cup\Lambda'} - \log\left(\int e^{[f_\Lambda + f_{\Lambda'}]} d\mu_{\Lambda\cup\Lambda'}\right) \\ &= \left\{\int f_\Lambda d\nu_\Lambda - \log\left(\int e^{f_\Lambda} d\mu_\Lambda\right)\right\} + \left\{\int f'_\Lambda d\nu'_\Lambda - \log\left(\int e^{f'_\Lambda} d\mu'_\Lambda\right)\right\} \end{aligned}$$

Taking now the supremum over f_Λ and $f_{\Lambda'}$ we obtain the desired inequality. □

So if ν, μ are translation invariant and μ is product, denoting $\Lambda_n = \{-n, \dots, n\}$, we have that $H_{\Lambda_n}(\nu|\mu)$ is a superadditive function of n, and consequently it exists the limit

$$\bar{H}(\nu|\mu) = \lim_{n\to\infty} \frac{1}{2n+1} H_{\Lambda_n}(\nu|\mu) = \sup_n \frac{H_{\Lambda_n}(\nu|\mu)}{2n+1} \tag{B.1.7}$$

Moreover it is easy to show that $\nu \in \mathcal{T} \to \bar{H}(\nu|\mu)$ inherits properties of relative entropy. Hence it is convex and lower semicontinuous.

For any bounded continuous function ϕ with support in $\{-n_0, \dots, n_0\}$ define the limit

$$\bar{F}(\phi) = \lim_{n\to\infty} \frac{1}{2n+1} \bar{F}_n(\phi), \quad \bar{F}_n(\phi) = \log \int e^{\sum_{i=-n}^{n} \tau_i \phi}\, d\mu \tag{B.1.8}$$

where τ_i is the shift operator on functions on $(\mathbb{R}^2)^{\mathbb{Z}}$. Existence of the limit is proved in the following proposition.

Proposition B.1.5 *Let ν a translation invariant probability on Ω, then*

$$\bar{H}(\nu|\mu) = \sup_\phi \left\{\int \phi\, d\nu - \bar{F}(\phi)\right\} \tag{B.1.9}$$

where the supremum is taken over all bounded continuous functions ϕ.

Proof We claim it is sufficient to prove that

$$\liminf_{n\to\infty} (2n+1)^{-1} \bar{F}_n(\phi) \geq \sup_{\nu\in\mathcal{T}} \left\{\int \phi d\nu - \bar{H}(\nu|\mu)\right\} \tag{B.1.10}$$

and

$$\limsup_{n\to\infty} (2n+1)^{-1} \bar{F}_n(\phi) \leq \sup_{\nu\in\mathcal{T}} \left\{\int \phi d\nu - \bar{H}(\nu|\mu)\right\} \tag{B.1.11}$$

Assume we proved (B.1.10) and (B.1.11). Let $\mathcal{M}(\Omega)$ the vector space of finite signed measures on Ω equipped with the weak topology. We extend $\bar{H}$ to $\mathcal{M}(\Omega)$ by

$\bar{H}(\nu|\mu) = +\infty$ if $\mu \notin \mathcal{T}$. Since $\mathcal{T}$ is a closed convex set the function $\bar{H}$ extended in this way remains convex and lower semi-continuous. Let $(\mathcal{M}(\Omega))'$ be the topological dual of $\mathcal{M}(\Omega)$ and consider the application $\Phi \in (\mathcal{M}(\Omega))' \to f_\Phi \in C_b(\Omega)$ defined by $f_\Phi(x) = \Phi(\delta_x)$. Remark that f_Φ is continuous and that $\int f_\Phi d\nu = \Phi(\nu)$. Moreover it is injective since the finite support signed measures are dense (for the weak topology) into $\mathcal{M}(\Omega)$ (see [?], appendix III, theorem 4) and surjective since for any $f \in C_b(\Omega)$ the linear form $\Phi : \nu \in \mathcal{M}(\Omega) \to \int_\Omega f d\nu \in \mathbb{R}$ is such that $f_\Phi = f$. Hence $\Phi \to f_\Phi$ is an isomorphism between $(\mathcal{M}(\Omega))'$ and $C_b(\Omega)$. Then Fenchel-Moreau's theorem implies

$$\bar{H}(\nu|\mu) = \sup_\phi \left\{ \int \phi \, d\nu - \bar{F}(\phi) \right\} \tag{B.1.12}$$

for any $\nu \in \mathcal{M}(\omega)$ and in particular for $\nu \in \mathcal{T}$.

We start by proving (B.1.10). Let $\nu \in \mathcal{T}$ such that $\bar{H}(\nu|\mu) < \infty$. By the variational formula defining $H_{\Lambda_n}(\nu|\mu)$ applied with $\sum_{i=-n}^{n} \tau_i \phi$ and the translation invariance of ν we have

$$\begin{aligned} \frac{\bar{F}_n(\phi)}{2n+1} &\geq \int \frac{1}{2n+1} \left(\sum_{i=-n}^{n} \tau_i \phi \right) d\nu - \frac{H_{\Lambda_n}(\nu|\mu)}{|\Lambda_n|} \\ &\geq \int \phi \, d\nu - \bar{H}(\nu|\mu) \end{aligned}$$

Taking the liminf in n and the supremum over $\nu \in \mathcal{T}$ we get (B.1.10).

Observe that for any $n \geq 1$, we have

$$\log \left(\int e^{\sum_{i=-n}^{n} \tau_i \phi} d\mu \right) = \sup_\alpha \left\{ \int \left(\sum_{i=-n}^{n} \tau_i \phi \right) d\alpha - H_{\Lambda_{n+n_0}}(\alpha|\mu) \right\} \tag{B.1.13}$$

where the supremum is carried over all probability measures α on $(\mathbb{R}^2)^{\Lambda_{n+n_0}}$. One sense of the inequality is trivial by the variational formula defining $H_{\Lambda_{n+n_0}}(\alpha|\mu)$ and the other sense is obtained by taking the optimal α which maximizes the supremum in (B.1.13). This α is such that $H_{\Lambda_{n+n_0}}(\alpha|\mu) < +\infty$.

For such α we define $\bar{\alpha} \in \mathcal{T}$ in two steps. First α^* is obtained by taking independent copies of α on all translated disjoint cubes $(C_k)_{k \in \mathbb{Z}}$ of Λ_{n+n_0}:

$$\alpha^* = \otimes_{k \in \mathbb{Z}} \tau_{2k(n+n_0)+1} \alpha, \quad C_k = \tau_{2k(n+n_0)+1} \Lambda_{n+n_0}$$

The family of probability measures $(\alpha^p)_{p \geq 1}$ defined by

$$\alpha^p = \frac{1}{2p+1} \sum_{\ell=-p}^{p} \tau_\ell \alpha^*$$

is tight and we denote by $\bar{\alpha}$ a fixed limit point of the family. To simplify notations we denote the subsequence along which the limit is achieved by the same letter p. It is trivial that $\bar{\alpha}$ is translation invariant.

Let $B_j = \cup_{k=-j}^{j} C_k$. Since entropy is lower semicontinuous we have

$$\bar{H}(\bar{\alpha}|\mu) \le \lim_{j\to\infty} \liminf_{p\to\infty} |B_j|^{-1} H_{B_j}(\alpha^p|\mu) \tag{B.1.14}$$

By convexity of entropy and translation invariance of μ we have

$$\begin{aligned} |B_j|^{-1} H_{B_j}(\alpha^p|\mu) &\le \frac{1}{\Lambda_{n+n_0}} \frac{1}{(2p+1)(2j+1)} \sum_{\ell=-p}^{p} H_{B_j}(\tau_\ell \alpha^*|\mu) \\ &= \frac{1}{\Lambda_{n+n_0}} \frac{1}{(2p+1)(2j+1)} \sum_{\ell=-p}^{p} H_{\tau_{-\ell} B_j}(\alpha^*|\mu) \end{aligned}$$

Observe that $\tau_{-\ell} B_j$ can be written as the disjoint union $I \cup \cup_{k=j_\ell}^{j_\ell+2j-2} C_k \cup F$ where $j_\ell \in \mathbb{Z}$, $I \subset C_{j_\ell - 1}$ and $F \subset C_{j_\ell+2j-1}$.

Since the relative entropy of a product of measures $\beta \otimes \gamma$ is the sum of the relative entropies of β and γ, we have

$$\begin{aligned} H_{\tau_{-\ell} B_j}(\alpha^*|\mu) &= H_I(\alpha^*|\mu) + \sum_{k=j_\ell}^{j_\ell+2j-2} H_{C_k}(\alpha^*|\mu) + H_F(\alpha^*|\mu) \\ &= H_I(\alpha^*|\mu) + (2j-1) H_{\Lambda_{n+n_0}}(\alpha^*|\mu) + H_F(\alpha^*|\mu) \end{aligned}$$

Since $H_I(\alpha^*|\mu) \le H_{\Lambda_{n+n_0}}(\alpha|\mu)$ and $H_F(\alpha^*|\mu) \le H_{\Lambda_{n+n_0}}(\alpha|\mu)$, taking first the limit in p and then the limit in j we get

$$\bar{H}(\bar{\alpha}|\mu) \le \frac{H_{\Lambda_{n+n_0}}(\alpha|\mu)}{|\Lambda_{n+n_0}} \tag{B.1.15}$$

Moreover it is clear that

$$\lim_{n\to\infty} \left| \frac{1}{2n+1} \sum_{i=-n}^{n} \int (\tau_i \phi)\, d\alpha - \int \phi d\bar{\alpha} \right| = 0$$

and we get (B.1.11). □

B.2 Entropy Production

Let $(\omega_t)_{t\geq 0}$ be a Markov process on $\Omega_\Lambda = (\mathbb{R}^2)^\Lambda$, $\Lambda \subset \mathbb{Z}$, with generator L_Λ and invariant probability measure μ. We denote by A_Λ (resp. S_Λ) the antisymmetric (resp. symmetric) part of L_Λ in $\mathbb{L}^2(\Omega_\Lambda, \mu)$. We assume the space of smooth bounded functions on Ω_Λ is a common core of A_Λ and S_Λ and that $L_\Lambda = A_\Lambda + S_\Lambda$ and $L_\Lambda^* = -A_\Lambda + S_\Lambda$ are generators of Feller semigroups $(P_\Lambda^t)_{t\geq 0}$ and $(P_\Lambda^{*t})_{t\geq 0}$. We suppose that L_Λ (resp. S_Λ) can be extended to strong Feller semigroups on $\mathbb{L}^2(\Omega_\Lambda, \mu)$. The semigroup generated by L_Λ (resp. L_Λ^* on $\mathbb{L}^2(\Omega_\Lambda, \mu)$) is also denoted P_Λ^t (resp. P_Λ^{*t}).

The first proposition below shows that entropy w.r.t. invariant probability measures can only decrease

Proposition B.2.1 *For any probability measure ν on Ω_Λ we have*

$$H(\nu P_\Lambda^t|\mu) \leq H(\nu|\mu) \tag{B.2.1}$$

Proof By definition we have

$$H(\nu P_\Lambda^t|\mu) = \sup_\phi \left\{ \int P_\Lambda^t \phi d\nu - \log\left(\int e^\phi d\mu \right) \right\}$$

and by Jensen's inequality and stationarity of μ we have

$$\int e^{P_\Lambda^t \phi} d\mu = \int d\mu(\omega) \exp\left(\mathbb{E}_\omega(\phi(\omega_t))\right) \leq \int \mathbb{E}_\omega(e^{\phi(\omega_t)}) d\mu(\omega) = \int e^\phi d\mu$$

and then the result follows since $P_\Lambda^t \phi$ is a bounded continuous function. □

In particular this shows that if we start from a probability measure ν with finite entropy then at any time the probability measure νP_Λ^t has finite entropy and hence is absolutely continuous with respect to μ. Let $g_\Lambda(t)$ be the density of νP_Λ^t w.r.t. μ.

We are now interested in the entropy production rate. The Dirichlet form of ν w.r.t. μ is defined by

$$D_\Lambda(\nu|\mu) = \sup\left\{ -\int \frac{S_\Lambda \psi}{\psi} d\nu \ : \ \psi \in \mathrm{Dom}(S_\Lambda), \inf \psi > 0 \right\} \tag{B.2.2}$$

Proposition B.2.2 *Let ν be a probability measure on Ω_Λ with finite entropy $H(\nu|\mu) = H_\Lambda(\nu|\mu) < \infty$. For every $t, h \geq 0$, we have that*

$$H(\nu P_\Lambda^{t+h}|\mu) - H(\nu P_\Lambda^t|\mu) \leq 2 \int_t^{t+h} ds D_\Lambda(\nu P_\Lambda^s|\mu) \tag{B.2.3}$$

Proof Let α and β two probability measures on Ω_Λ. Jensen's inequality shows that

$$H(\alpha P_\Lambda^t|\beta P_\Lambda^t) \leq H(\alpha|\beta) \tag{B.2.4}$$

It is sufficient to show the proposition for $t = 0$. Let ψ be a smooth bounded positive function with mean one with respect to μ. Fix a positive time τ. We define the probability measure β by $d\beta = \psi d\mu$. Then we have βP_Λ^τ is absolutely continuous with respect to μ with density $P_\Lambda^{*\tau}\psi$.

It is an elementary fact that

$$H(\alpha|\beta) = H(\alpha|\mu) - \int \log\psi \, d\alpha \tag{B.2.5}$$

It follows that

$$H(\alpha P_\Lambda^t|\beta P_\Lambda^t) = H(\alpha P_\Lambda^\tau \mu) - \int \log(P_\lambda^{*\tau}\psi \, d(\alpha P_\Lambda^\tau) \tag{B.2.6}$$

Hence, with (B.2.4), we get

$$\begin{aligned}
H(\alpha|\mu) - H(\alpha P_\Lambda^\tau|\mu) &\geq \int \log\psi \, d\alpha - \int P_\Lambda^\tau \log\left(P_\Lambda^{*\tau}\psi\right) \, d\alpha \\
&\geq \int \log\psi \, d\alpha - \int \log\left(P_\Lambda^\tau P_\Lambda^{*\tau}\psi\right) \, d\alpha \\
&\geq - \int \log\left(\frac{P_\Lambda^\tau P_\Lambda^{*\tau}\psi}{\psi}\right) \, d\alpha \\
&\geq \int \left(\frac{\psi - P_\Lambda^\tau P_\Lambda^{*\tau}\psi}{\psi}\right) \, d\alpha
\end{aligned}$$

where we used Jensen's inequality and $\log(1+\eta) \leq \eta$.

Since $(P_\Lambda^t)_{t\geq 0}$ and $(P_\Lambda^{*t})_{t\geq 0}$ are Feller semigroups we have

$$\psi - P_\Lambda^\tau P_\Lambda^{*\tau}\psi = \psi - P_\Lambda^\tau\psi - \psi - P_\Lambda^\tau(P_\Lambda^{*\tau}\psi - \psi) = -2\tau S_\Lambda\psi + \tau\varepsilon(\psi,\tau)$$

where $\|\varepsilon(\psi,\tau)\|_\infty \to 0$ as $\tau \to 0$.

Let be $t > 0$ and divide the time interval $[0,t]$ in m small intervals of length

$\tau = t/m$ and let m goes to infinity. We have

$$\begin{aligned} H(\alpha|\mu) - H(\alpha P_\Lambda^t|\mu) &= \sum_{i=0}^{m-1} \left[H(\alpha P_\Lambda^{\frac{i}{m}t}|\mu) - H(\alpha P_\Lambda^{\frac{i+1}{m}t}|\mu) \right] \\ &\geq \limsup_{m\to\infty} \sum_{i=0}^{m-1} \left[H(\alpha P_\Lambda^{\frac{i}{m}t}|\mu) - H(\alpha P_\Lambda^{\frac{i+1}{m}t}|\mu) \right] \\ &\geq \limsup_{m\to\infty} \left[-\frac{2t}{m} \sum_{i=0}^{m-1} \int \left(P_\Lambda^{\frac{it}{m}} \left(\frac{S_\Lambda \psi}{\psi} \right) \right) d\alpha + t\varepsilon(\psi, t/m)) \right] \\ &= -2 \int_0^t ds \int P_\Lambda^s \left(\frac{S_\Lambda \psi}{\psi} \right) d\alpha \end{aligned}$$

By taking the supremum over all ψ considered we conclude the proof. □

Proposition B.2.3 (Donsker-Varadhan) *Let Λ be a finite set. Assume that $D_\Lambda(\nu|\mu)$ is finite and that ν is abolutely continuous with respect to μ with a density denoted by g. Then $\sqrt{g}$ belongs to the domain of $(-S_\Lambda)^{1/2}$ and*

$$D_\Lambda(\nu|\mu) = \sum_{x\in\Lambda} \int d\mu((-S_\Lambda)^{1/2}\sqrt{g})^2 \tag{B.2.7}$$

Proof See theorem 5 in [?]. □

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