Time Evolution of Infinite Particle Systems

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The aim of these notes is to give a concise introduction to the theory of deterministic dynamics of infinite interacting particle systems at equilibrium. We will see how existence and uniqueness for time evolution of an infinite system of particles under Newton's law can be proved for almost every initial data with respect to physically relevant invariant measures. Physical intuition will be essential, so we deem it necessary to begin with a (very short and elementary) introduction to the basic concepts of statistical ensembles and equilibrium states. Such introduction, in the easy case of finite systems presented in Section 1, will take place in Section 2, whereas the generalisation to infinite volume and particles will be treated in Section 3. Section 4 will then concern existence of time evolution of particle systems, Section 5 will collect statements of further results, such as uniqueness and invariance of Gibbs' measure.

1 Finite Particles in Finite Volume

Consider N point particles of unitary mass in $\mathbb{R}^d$ evolving according to Newton's law with force given by a configurational pair potential Φ. Their positions and momenta are denoted by

$$(q_1, p_1), \dots (q_N, p_N) \in \mathbb{R}^{d\times d},$$

and they evolve according to the equations

$$\begin{cases} \dot{q_i} = p_i \\ \dot{p_i} = F(q) = -\sum_{j\neq i} \nabla\Phi(q_j - q_i) \end{cases}.$$

We assume $\Phi: \mathbb{R}^d \to \mathbb{R}$ to be a smooth radial function. The precise form of Φ, that is the assumptions one needs to make in order for the mathematical theory to work, is a crucial point. We might ask for physically meaningful potentials, or aim to the greatest mathematical generality. However, especially in the infinite case, we would encounter hard difficulties and even open problems. We will thus limit ourselves to the simplest nontrivial cases.

Such systems are Hamiltonian, that is, their dynamics can be rewritten as

$$\begin{cases} \dot{q_i} = \partial_{p_i} H(q,p) \\ \dot{p_i} = -\partial_{q_i} H(q,p) \end{cases}, \qquad H(q,p) = \frac{1}{2}\sum_i |p_i|^2 + \frac{1}{2}\sum_{j\neq i} \Phi(q_j - q_i),$$

where the Hamiltonian H is equivalently called the energy of the system. Let us recall two fundamental features of this kind of systems.

Proposition 1. *Let $H: (\mathbb{R}^{d\times d})^N \to \mathbb{R}$ be a smooth Hamiltonian. Global well-posedness holds for Hamilton's equations. If $x_t = (p_t, q_t)$ is a solution, then we have*

- ***(evolution of observables)*** *if $f: (\mathbb{R}^{d\times d})^N \to \mathbb{R}$ is a smooth observable, its value $f(x_t)$ on a trajectory of the system satisfies*

$$\frac{d}{dt} f(x_t) = \{f, H\}(x_t) = \sum_{i=1}^N (\partial_{q_i} f \cdot \partial_{p_i} H - \partial_{p_i} f \cdot \partial_{q_i} H)(x_t);$$

as a consequence the Hamiltonian H is an integral of motion, that is, it is constant along x_t;

- ***(evolution of states)*** *if $\rho\colon (\mathbb{R}^{d\times d})^N \to \mathbb{R}$ is a smooth nonnegative probability density, the measure $d\rho_t = (x_t)_\# \rho dpdq = \rho_t dpdq$ on $(\mathbb{R}^{d\times d})^N$ is absolutely continuous and its density satisfies*

$$\partial_t \rho_t = -\{\rho_t, H\} = \int_{(\mathbb{R}^{d\times d})^N} \sum_{i=1}^N (\partial_{q_i}\rho_t \cdot \partial_{p_i} H - \partial_{p_i}\rho_t \cdot \partial_{q_i} H) dpdq;$$

as a consequence Lebesgue's measure $dpdq$ and every absolutely continuous measure $f(H(q, p))dqdp$ with integrable density $f(H)$ are invariant.

It is natural to consider such finite systems of particles inside a fixed finite volume. In what follows, we will do so treating two different models:

- Periodic boundary conditions: we replace the configuration space with the d-dimensional torus $\mathbb{T}^d = \mathbb{R}^d / \mathbb{Z}^d$, so that the phase space is now its tangent bundle $\mathbb{T}^d \times \mathbb{R}^d$; Hamilton's equations do not change in their form, but they are to be considered as differential equations on the (flat) manifold $\mathbb{T}^d \times \mathbb{R}^d$;

- Elastic boundary conditions: we fix a (smooth) domain $D \subset \mathbb{R}^d$ for the positions q_i and impose that whenever a particle hits the boundary ∂D it is elastically reflected towards the interior of D, that is, the tangential part of its velocity changes sign.

The periodic model is easier, since it deals with an actual Hamiltonian system on a (flat) manifold, and in this case it is quite straightforward to deduce again conservation of energy and Liouville's theorem. Let us devote the remainder of this section to the elastic reflection model.

One way to build the elastic boundary is to modify the Hamiltonian, defining

$$\tilde{H}(q, p) = \frac{1}{2} \sum_i |p_i|^2 + \frac{1}{2} \sum_{j \neq i} \Phi(q_j - q_i) + \sum_i 2\langle p_i, \hat{n}\rangle \chi(q_i \notin D).$$

Formal differentiation promptly gives the desired reflection at the boundary; however, distributional derivatives are needed in order to give a precise meaning to Hamilton's equations, thus we prefer to avoid this strategy (which makes very difficult to obtain, for instance, Liouville's theorem).

A somewhat less drastic modification of H is

$$H_\epsilon(q, p) = \frac{1}{2} \sum_i |p_i|^2 + \frac{1}{2} \sum_{j \neq i} \Phi(q_j - q_i) + \sum_i g_\epsilon(q_i),$$

where g_ϵ is a smooth function converging pointwise to $+\infty \cdot \chi(q_i \notin D)$ as $\epsilon \to 0$. The solution (q_ϵ, p_ϵ) of the (classical) Hamilton's equations will converge to the one with instantaneous elastic reflections. Such limit clearly has discontinuous trajectories (of momenta), so it can not be a limit in the topology of continuous functions, or even in Skorohod's topology of *cadlag* functions (since it is a limit of smooth functions, which are a nowhere dense closed set in such topology). The limit might be taken only pointwise in time, or in some L^p space. Again, we refrain from such complicated considerations[1].

What we will do is to consider the quotient phase space

$$\Omega = (D \times \mathbb{R}^d)/\sim, \qquad (q, p) \sim (q', p') \Leftrightarrow q = q' \in \partial D, \quad \langle p, \hat{n}\rangle = -\langle p', \hat{n}\rangle,$$

1. The two outlined approaches are often referred to by physicists modifying the Hamiltonian by adding the potential term $V(q) = +\infty \cdot \chi(q_i \notin D)$.

where $\hat{n}$ is the outward normal versor on ∂D. Indeed, Ω is a flat manifold just as in the periodic case, so we get, as above, conservation of energy and Liouville's theorem with no additional effort, at least for the Hamiltonian dynamics on Ω. Let us observe, though, that continuous trajectories on Ω can be lifted uniquely to *cadlag*[2] trajectories on $D \times \mathbb{R}^d$, and we thus recover the desired model. Conservation of energy is now trivially preserved by the lifting, and so is Liouville's theorem, since the measures we consider give 0 mass to the boundary $\partial D \times \mathbb{R}^d$.

2 Gibbs Measures for Finite Particle Systems

The topics we are going to treat are very classical, and we thus refer to any basic text on Statistical Mechanics for a proper introduction to the subject. Our presentation aims to be motivational, so it will be tailored on a particular model, the Newtonian particles on the torus $\mathbb{T}$. As in the last section, we restrict to the case of smooth, compactly supported pair potential U.

The point of view of statistical mechanics is the following: when the number of particles N is large, on one hand the precise configuration (*microstate*) of the physical system is very difficult to determine, on the other it is somewhat irrelevant if we aim to give a good description of the system as a whole. Such a description will in fact depend on a small number of macroscopic observable quantities, such as total energy, temperature, entropy and so on. The mathematical interpretation of this idea is to associate to each choice of those relevant quantities a (probability) measure on the phase space: such measures are called *states* of the system, and they are meant to "collect" configurations with the specified macroscopic quantities.

A prominent role is played by *equilibrium states*. It beyond our scope to give a correct physical definition of equilibrium here: what we will do in the remainder of the section is to derive mathematically the invariant measures corresponding to equilibrium states from physical principles that we take as granted. An equilibrium state describes the long-time behaviour of a system. As time passes and the physical system evolves, the *free energy*

$$A = \langle E \rangle - TS$$

will decrease towards its minimum, so an equilibrium state should be a measure minimising the free energy.

Let us make this vague consideration more precise: we fix three macroscopic observables of the system, namely the number of particles N, the volume allowed for the particles' positions V and the temperature T, or rather its inverse $\beta = \frac{1}{T}$. Temperature should be interpreted as an "average energy": in fact it is a quantity only defined at equilibrium.

In the definition of A above, E is the *internal energy* of the system, and in our case it coincides with the Hamiltonian H, the bracket denote average with respect the considered state and S is the entropy with respect a reference measure, which we assume to be Lebesgue's. In other terms,

$$\forall \rho dp dq \in \mathrm{Pr}(\Omega) \qquad A(\rho) = \int_{\Omega_N} H(p,q)\rho(p,q)dpdq + \beta \int_{\Omega_N} \rho(p,q)\log\rho(p,q)dpdq,$$

where we denoted the phase space with $\Omega_N = (\mathbb{T}^d \times \mathbb{R}^d)^N$.

Proposition 2. (Variational Principle) *Let $N \in \mathbb{N}$ and $\beta > 0$ be fixed. There exists a unique minimum $m_{N,\beta}$ for the functional $A(\rho)$ among all the nonnegative probability densities ρ with respect to Lebesgue's measure: such measure is called the* Gibbs' measure *relative to the* Canonical Ensemble*, it is characterised by*

$$A(m_{N,\beta}) = \min_{\rho} A(\rho) = \log Z_{N,\beta},$$

2. The choice of right-continuous paths is arbitrary: what really matters is to choose uniquely the momentum at boundary hitting times of the trajectory.

and it has the explicit form

$$dm_{N,\beta}(p,q) = \frac{1}{Z_{N,\beta}} e^{-\beta H(p,q)} dp dq, \qquad Z_{N,\beta} = \int_{\Omega} e^{-\beta H(p,q)} dp dq.$$

The proof of the latter statement is a simple application of Jensen's inequality. The name *Canonical Ensemble* refers to the fact that we fixed N, V, T, while the name *Gibbs's measure* to the specific expression we found. Let us remark that such a characterisation of equilibrium measures is in general difficult to obtain for more complex systems.

Remark 3. (Maxwellian distribution of momenta) Let us observe that, whatever the interaction potential U might be, under Gibbs' measure the momenta p_i of particles are independent Gaussian variables with mean 0 and variance $\beta^{-1/2}$.

The reader might wonder why we did not consider, and fix, the observable H (energy) instead of the temperature (we would have obtained the so called *Microcanonical Ensemble*). The reason is technical: even if less intuitive, the Canonical ensemble is easier to treat in terms of mathematics. In fact, we are going to replace in an analogous fashion the observable N (number of particles) with the *chemical potential* μ or the *activity* z, taking the role of "average number of particles", thus defining the *Grand Canonical Ensemble*. This is going to be an important step towards a good understanding of Gibbs' measure for infinite particles.

Since we want to let N vary, we need to fix some additional notation. In the remainder of this section, we consider the phase space

$$\tilde{\Omega} = \bigsqcup_{N=0}^{\infty} (\mathbb{T}^d \times \mathbb{R}^d)^N / \sim,$$

where $\sim$ denotes equivalence by permutations of the variables in the N-fold product. We take such quotients to ensure that the particles are *indistinguishable*. This was not a problem when their number was fixed, but in this new setting overcounting would cause a problem known as *Gibbs' paradox*, namely entropy would not be an *extensive* quantity. We refer the reader to the literature about such problems. The Lebesgue's measure on $\tilde{\Omega}$ is defined as

$$d\tilde{x} = \bigoplus_{N=0}^{\infty} d\tilde{p}^N d\tilde{q}^N = \bigoplus_{N=0}^{\infty} \frac{1}{N!} dp_1 \ldots dp_N dq_1 \ldots dq_N.$$

Remark 4. The latter expression should remind the reader that any function $f \in L^1(X^N/\sim)$ is in fact a symmetric function on X^N, and it holds

$$\int_{X^N/\sim} f dx = \int_{X^N} f d\tilde{x} = \frac{1}{N!} \int_{X^N} f dx.$$

For fixed $\beta, \mu \geq 0$, we define the Gibbs' measure relative to the *Grand Canonical Ensemble* as

$$dm_{\mu,\beta}(\tilde{x}) = \frac{1}{Z_{\mu,\beta}} e^{-\beta(H(\tilde{x}) - \mu N(\tilde{x}))} d\tilde{x}, \qquad Z_{\mu,\beta} = \int_{\tilde{\Omega}} e^{-\beta(H(\tilde{x}) - \mu N(\tilde{x}))} d\tilde{x},$$

where $N(\tilde{x}) = \chi_{(\mathbb{T}^d \times \mathbb{R}^d)^N/\sim}(\tilde{x})$ and $H(\tilde{x})$ is the Hamiltonian on $(\mathbb{T}^d \times \mathbb{R}^d)^N/\sim$ if $N(\tilde{x}) = N$. The same variational principle of the Canonical Ensemble is satisfied, with the only difference that μN should be subtracted to the internal energy.

Everything can be more conveniently expressed in terms of non-symmetrised variables and substituting $z = e^{\mu\beta} \geq 1$,

$$dm_{z,\beta}(x) = \frac{1}{Z_{\mu,\beta}} \bigoplus_{N=0}^{\infty} \frac{z^N}{N!} e^{-\beta H(p,q)} dp^N dq^N, \qquad Z_{z,\beta} = \sum_{N=0}^{\infty} \frac{z^N}{N!} \int_{(\mathbb{T}^d \times \mathbb{R}^d)^N} e^{-\beta H(p,q)} dp^N dq^N.$$

Remark 5. (Poisson distribution of N) In the limit case $\beta = 0$, it is easily observed that under $m_{z,\beta}$ the number of particles N is a Poisson random variable of mean 1. The general case is more complicated, let us only observe that in the free interaction case $U = 0$ we have

$$Z_{z,\beta} = \sum_{N=0}^{\infty} \frac{z^N}{N!} \left(\frac{2\pi}{\beta}\right)^{\frac{dN}{2}} = \sum_{N=0}^{\infty} \frac{\lambda(z,\beta)^N}{N!},$$

and, as a consequence,

$$dm_{z,\beta}(x) = \bigoplus_{N=0}^{\infty} \frac{\lambda(z,\beta)^N e^{\lambda(z,\beta)}}{N!} \left(\frac{2\pi}{\beta}\right)^{\frac{dN}{2}} e^{-\frac{\beta p_1^2}{2}} dp_1 \ldots e^{-\frac{\beta p_N^2}{2}} dp_N,$$

thus N is Poisson with mean $\lambda(z,\beta)$ and momenta are centred Gaussian variables of variance β^{-1}.

Exercise 1. (Gibbs' measures for Gradient Diffusions) Consider, for suitably smooth and integrable potential $U: \mathbb{R}^d \to \mathbb{R}$, the following SDE:

$$dX_t = -\nabla U(X) dt + \sqrt{\frac{2}{\beta}} dB_t,$$

where B is a d-dimensional Brownian motion. Prove, by studying the associated Fokker-Planck equation, that such diffusion process has a unique invariant measure $m_\beta = \frac{1}{Z_\beta} e^{-\beta U(x)} dx$, that such measure satisfies a variational principle analogous to the one we stated above, and that the corresponding free energy functional is a Lyapunov function for the Fokker-Planck equation, that is, it decreases along solutions of the equation.

3 Configuration Space for Infinite Particles

In order to study infinite particle systems, the first step is to clarify what is the phase space in which we set the problem. Motivated by the above discussion, we expect momenta of particles to have Maxwellian distributions, that is, to be independent Gaussian variables. We thus ignore momenta in this section, and discuss only the configurational part of phase space. Overall, the aim of this section is to provide the correct generalisation of Gibbs' measures on the configuration space for infinite particles; however we will not discuss whether our definitions can be motivated by physical principles, such as the variational principles of Section 2 (which, by the way, is the case).

Let us begin by introducing the following set:

$$\begin{aligned} \Omega &= \{\text{locally finite sequences } (q_i) \subset \mathbb{R}^d\} \\ &\subset \Omega' = \{\text{discrete positive Radon measures on } \mathbb{R}^d\} \\ &\subset \mathcal{M}^+(\mathbb{R}^d) = \{\text{positive Radon measures on } \mathbb{R}^d\}. \end{aligned}$$

We endow $\mathcal{M}^+(\mathbb{R}^d)$ with the vague topology (induced by the duality with $C_c^\infty(\mathbb{R}^d)$), and its subsets Ω, Ω' with the subspace topology. Let us emphasise that while Ω' is a closed set in this topology, Ω is not. However, it can be shown that Ω with this topology is in fact a Polish space, that is, its topology is induced by a distance which makes it complete (and it is separable). In what follows we will sistematically identify configurations $q \in \Omega$ with measures on $\mathbb{R}^d$ made of the (countable) sums of Dirac's deltas on the points q_i.

Remark 6. The distance on Ω we just mentioned can be chosen as the following L^2-Wasserstein-like distance: for $q, q' \in \Omega$, we set

$$d(q, q') = \inf \sqrt{\int \int |x - y|^2 \pi_{q, q'}(dx, dy)},$$

where the infimum is taken over all the locally finite sequences $(q_i, q_i') \subset \mathbb{R}^d \times \mathbb{R}^d$ (identified as measures $\pi_{q, q'}$ on the product $\mathbb{R}^d \times \mathbb{R}^d$) with marginals q and q'.

The reader can check that a base for the topology on Ω is given by

$$B_{m, \Lambda, K} = \{q \in \Omega: q(K) = q(\Lambda) = m\}, \qquad m \in \mathbb{N}, K \subset_{\text{compact}} \Lambda \subset_{\text{open}} \mathbb{R}^d,$$

while the associated Borel σ-algebra is generated by

$$B_{m, \Lambda} = \{q \in \Omega: q(\Lambda) = m\}, \qquad m \in \mathbb{N}, \Lambda \subset \mathbb{R}^d \,\text{bounded Borel set}.$$

Let us set up some notation: for a fixed Borel subset $\Lambda \subset \Omega$,

$$\Omega_\Lambda = \{q \in \Omega: q(\Lambda^c) = 0\} \simeq \bigsqcup_{N=0}^{\infty} \Lambda^N / \sim,$$

where we denote by $\sim$ the equivalence under permutation of variables,

$$\begin{aligned} \pi_\Lambda: \Omega \to \Omega_\Lambda, &\quad \pi_\Lambda q(A) = q_\Lambda(A) = q(A \cap \Lambda), \\ f_\Lambda(q) = f(\pi_\Lambda q), &\quad \text{for } f: \Omega \to \mathbb{R} \text{ measurable}, \\ \mu_\Lambda = (\pi_\Lambda)_\sharp \mu &\quad \text{for } \mu \text{ Borel measure on } \Omega. \end{aligned}$$

To describe measures on Ω, which is a matter of paramount importance for us, we need to resort to conditional distribution on bounded regions of $\mathbb{R}^d$. Making our treatment precise will require some facts about conditional probabilities which we recall in the forthcoming Remark.

Remark 7. Let $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space, $(T, \mathcal{T})$ and $(S, \mathcal{S})$ measurable spaces. A probability kernel from T to S is a map $p: T \times \mathcal{S} \to \mathbb{R}^+$ which is $\mathcal{T}$-measurable in T and a probability measure on $(S, \mathcal{S})$ for each $t \in T$. If $\xi: \Omega \to S$ and $\eta: \Omega \to T$ are random variables, ξ has a *regular conditional distribution* with respect to η if there exists a probability kernel p from T to S such that

$$p(\eta, B) = \mathbb{P}(\xi \in B | \eta) = \mathbb{E}[\chi_B(\xi) | \sigma(\eta)].$$

If S, T are regular enough (say Polish spaces), conditional distributions always have regular versions.

The following proposition will allow us to build measures on Ω starting from systems of conditional distributions on bounded regions, provided they are consistent in the sense we are going to specify.

Proposition 8. *Given m a probability measure (a nonnegative Borel measure of total mass 1) on Ω, there exists regular conditional distributions*

$$\Pi_\Lambda(q_{\Lambda^c}, \Delta) = m(q \in \Delta | q_{\Lambda^c}),$$

where Λ is any bounded Borel set of $\mathbb{R}^d$, Δ a Borel set of Ω, and q, q_{Λ^c} are to be understood as random variables under m. Moreover, Π_Λ satisfy the compatibility relations

- $\Pi_\Lambda(\cdot, \Delta \cap \Delta') = \chi_{\Delta'}(\cdot) \Pi_\Lambda(\cdot, \Delta)$ *for all $\Delta \in \mathcal{B}(\Omega)$ and $\Delta' \in \mathcal{B}(\Omega_{\Lambda^c})$,*

- $\Pi_{\Lambda'}(q,\Delta) = \int \Pi_\Lambda(q',\Delta)\Pi_{\Lambda'}(q,dq')$ *for all* $\Lambda \subset \Lambda' \subset \mathbb{R}^d$ *bounded Borel sets.*

Conversely, given a system of probability kernels Π_Λ *from* Ω_{Λ^c} *to* Ω *satisfying the relations above, there exists a (possibly non unique) measure* m *which has them as conditional distributions on bounded regions.*

Remark 9. The first part of the statement is a simple consequence of the facts we recalled above on conditional probabilities, thanks to the fact that $q\colon \Omega \to \Omega$ (the identity) and $q_{\Lambda^c}\colon \Omega \to \Omega_{\Lambda^c}$ are random variables on Polish spaces. As for the second part, we want to point out that uniqueness of the measure built from a system of conditional distribution is quite a subtle matter. In particular, non-uniqueness might occur in the case of equilibrium (Gibbs) measures, a fact which is related to the physical phenomenon of phase transitions.

Remark 10. As a consequence of the first compatibility relation,

$$\Pi_\Lambda(q_{\Lambda^c},\Delta) = \Pi_\Lambda(q_{\Lambda^c},\Delta_\Lambda \cap \Delta_{\Lambda^c}) = \chi_{\Delta_{\Lambda^c}}(q_{\Lambda^c})\Pi_\Lambda(q_{\Lambda^c},\Delta_\Lambda),$$

where we used the notation (valid only inside this remark)

$$\Delta_\Lambda = \{q \in \Omega \mid \exists q' \in \Delta\colon \pi_\Lambda q = \pi_\Lambda q'\},$$

the analogous holding for Δ_{Λ^c}. In particular without loss of generality we can consider Π_Λ as a measure on $\Omega_\Lambda \simeq \bigsqcup_{N=0}^\infty \Lambda^N / \sim$. Indeed, the intuitive understanding of Π_Λ as the law of $\pi_\Lambda q$ conditioned to a given $\pi_{\Lambda^c} q$ is now a formal statement.

As a first example (and in order to provide a "uniform" reference measure on Ω), we define the Poisson-Lebesgue measure, which is in a sense the simplest possible measure on Ω. In the light of the latter remark, we directly write Π_Λ as a measure on Ω_Λ, in fact Lebesgue's measure, and we take it independent of q_{Λ^c}:

$$\Pi_\Lambda(q_{\Lambda^c}, dq_\Lambda) = \sum_{N=0}^\infty \frac{e^{-|\Lambda|}|\Lambda|^N}{N!} dq_1^\Lambda \ldots dq_N^\Lambda,$$

(where we denoted by dq_i^Λ the Lebesgue's measure on Λ normalised to be a probability measure). We will denote with m the Poisson-Lebesgue measure on Ω, and with m_z the measure built in the same way but starting from Lebesgue's measure on Λ multiplied by $z \geq 0$.

In the terms of the remark above, the conditional distribution Π_Λ gives to $\pi_\Lambda q$ the following law: independently of the distribution of $\pi_{\Lambda^c} q$, the number of particles is chosen with a Poisson random variable of mean $|\Lambda|$, then the positions of the N particles are chosen independently (of $\pi_{\Lambda^c} q$, N and of each other) with law dq^Λ. When considering m_z, the only change is in the Poisson variables mean, which becomes $z|\Lambda|$.

The following important facts on the Poisson-Lebesgue measures are left to the reader as exercises: indeed, they are just facts about sequences of independent Poisson variables.

Exercise 2. (Moment Generating Function) For any $f \in C_c^\infty(\mathbb{R}^d)$, it holds

$$\mathbb{E}^m\left[\exp \int_{\mathbb{R}^d} f(x) dq(x)\right] = \exp \int_{\mathbb{R}^d} (e^{f(x)} - 1) dx.$$

Exercise 3. In dimension $d = 1$, it holds

$$m\left(\limsup_{n\to\infty} \frac{q([n,n+1])}{\log n / \log \log n} = 0\right) = 1,$$

which gives an upper bound (which is unfortunately not sharp) on the growth of local densities. (Hint: use Stirling's formula).

Exercise 4. Let $\lambda = |\Lambda|$, then for $N > \lambda$, uniformly in the $\Lambda' s$ with same measure,

$$m(q(\Lambda) > N) \leq \frac{e^{-\lambda}(e\lambda)^N}{N^N},$$

which, for instance, gives a uniform bound on the mean number of particles in unitary cubes. (Hint: use the exponential Chebichev's inequality).

We can now define Gibbs' measures on Ω using the Poisson-Lebesgue measure as a reference. Let us fix parameters $\beta > 0$ and $z > 1$, and consider the *local energy* on a bounded borel set $\Lambda \subset \mathbb{R}^d$,

$$E_\Lambda: \Omega \to \mathbb{R}, \qquad E_\Lambda(q) = \frac{1}{2} \sum_{q_i, q_j \in \Lambda} U(q_i, q_j) + \sum_{q_i \in \Lambda, q_j \notin \Lambda} U(q_i, q_j),$$

where U is a pair potential on which we need to make (as in the finite case) some assumptions. We will consider $U(x, y) = U(|x - y|)$ given by a smooth, compactly supported, radial function. We then define conditional distributions as

$$\Pi_\Lambda(q_{\Lambda^c}, \Delta) = \chi_{Z_\beta^\Lambda < \infty}(q_{\Lambda^c}) \frac{1}{Z_\beta^\Lambda(q_{\Lambda^c})} \int_\Omega \chi_\Delta(q_{\Lambda^c} + \pi_\Lambda q') e^{-\beta E_\Lambda(q_{\Lambda^c} + \pi_\Lambda q')} m_z(dq'),$$

where the partition function is given by

$$Z_\beta^\Lambda(q_{\Lambda^c}) = \int_\Omega e^{-\beta E_\Lambda(q_{\Lambda^c} + \pi_\Lambda q')} m_z(dq').$$

Exercise 5. Check that the Π_Λ thus defined satisfy the compatibility relations.

A measure having these conditional distributions, which we denote by $m_{z,\beta}$, is called a Grand Canonical Gibbs' measure. As we have already said, it might not be unique. It is possible, but very difficult, to prove uniqueness for z small (that is, smaller than a constant depending on β and the particular U we chose).

Remark 11. If we choose $U = 0$, we get again (independently of β) the Poisson-Lebesgue measure, so our notation m for both measures but with different subscripts is in this sense coherent.

Proposition 12. (Ruelle's probability bounds) *Let U be a pair potential satisfying:*

- Superstability: *the potential can be written as a sum $U = U' + U''$, where U' is such that there exists $B > 0$ such that for any finite configuration $q_1 \dots q_m$ it holds*

$$\frac{1}{2} \sum_{i,j=0}^{m} U'(q_i - q_j) \geq -mB,$$

(U' is stable*) and U'' is a positive continuous function such that $U''(0) > 0$;*

- Lower regularity: *there exists a positive decreasing function $u: [0, \infty) \to \mathbb{R}^+$ such that*

$$U(x) \geq -u(|x|) \, \forall x \in \mathbb{R}^d \quad \text{and} \quad \int_0^\infty t^{d-1} u(t) dt < \infty.$$

Let $\{Q_k\}_{k \in \mathbb{Z}^d}$ is the partition of unitary lattice cubes of $\mathbb{R}^d$ indexed by their bottom-left vertex, then

$$\exists g > 0, d \geq 0 \quad \forall k \in \mathbb{Z}^d \quad m_{z,\beta}(q(Q_k) > n) \leq \exp(-g n^2 + d n).$$

Note that such estimate is quite stronger than the one we got for the Poisson-Lebesgue measure in the exercise above.

Remark 13. We observe that the zero potential $U=0$ is stable but not superstable, and it is thus ruled out by our hypothesis. We refer to the original work of Ruelle for a thorough derivation of the result and deeper analysis of the hypothesis above. For the sake of simplicity, our reader should think of a potential shaped like $\chi_{\{r\leq 1\}} e^{(1-r^2)^{-1}}$, even if this is far from the most general assumptions we might make.

In fact, the above estimate is the only thing we will use in dealing with Gibbs' measures on Ω, so one might as well try and restrict the discussion of Newton's equations to a certain set of initial data satisfying an upper bound on particle densities at infinity derived by Ruelle's bound, ultimately ignoring all the complications of there measures. However, aside from the motivational purpose, we have decided to introduce Gibbs' measures, even if in a way which is all but lacking of formal completeness, because they will play an important role in at least two different ways. The first, as we just mentioned, is to determine a full measure subset of Ω of "good" initial data for the dynamics. The second is the fact that they will be left invariant by the dynamics, thus providing the estimates needed for a global (in time) well-posedness result. All of this will be the content of the next Section.

Exercise 6. Let m_β be a Gibbs' measure (with intensity $z=1$) associated to a potential satisfying Ruelle's hypothesis. Then, independently of β,

$$m_\beta\left(\sup_{k\in\mathbb{Z}^d} \frac{q(Q_k)}{\sqrt{\log|k|\vee 1}} < \infty\right) = 1.$$

Exercise 7. Include in the definition of Gibbs' measures Maxwellian momenta for the particles. More precisely: define the phase space for infinite particles in $\mathbb{R}^d$ (still called Ω) including both the configurational part discussed above, that is the sequences (q_i), and coordinates for momenta, that is a sequence $(p_i)\subset\mathbb{R}^d$. A Gibbs' measure with parameters z,β on the new space should give to the configuration q the same law of the ones we just built, and make the momenta p_i centred independent Gaussian variables of variance β^{-1} (independent also of q).

From now on, we will denote by Ω the phase space for positions *and* momenta described in the latter exercise, and by m_β a Gibbs' measure on such space. We will set $z=1$ to lighten notation.

4 Existence of Infinite Particles Dynamics

The aim of this section is the following: given an initial datum (p_0,q_0) belonging to a full-measure subset of Ω with respect to a Gibbs measure m_β, we will prove the existence of solutions to the infinite set of differential equations

$$\begin{cases} \dot{q}_i = p_i \\ \dot{p}_i = -\sum_{j\neq i} \nabla U(q_j - q_i) \\ q_i(0) = q_{0,i}, \quad p_i(0) = p_{0,i}, \end{cases} \tag{1}$$

(the indices i denoting an arbitrary enumeration of the particles in the initial datum). Such solutions will define a measure preserving flow on (Ω, m_β).

In order to carry out our program, we need a good set of approximate solutions, in the sense that they should be easy to treat mathematically, and some good *a priori* estimates, in the sense that they should provide compactness of our approximants.

We will use as approximated solutions the following well-posed dynamics. Let $R>0$, and denote by B_R the ball of $\mathbb{R}^d$ centred in the origin with radius R. We will denote by (p_t^R, q_t^R) the evolution of (p_0,q_0) given by:

1. particles outside B_R (that is, particles with $q_i\notin B_R$) remain still: $\dot{q}_i=\dot{p}_i=0$;

2. particles inside B_R evolve according to our system of equations but are elastically reflected by the boundary (as in the first section).

Proposition 14. *The expression $T_t^R(p_0, q_0) = (p_t^R, q_t^R)$ defines a semigroup of measurable mappings $T_t^R: \Omega \to \Omega$ which preserve any Gibbs' measure m_β (independently of β).*

Proof. Thanks to the results of the first section, it is readily checked that for any fixed R, T_t^R does preserve the conditional probabilities Π_Λ. Indeed, since it acts as identity on the Π_Λ with Λ disjoint from B_R, by the compatibility relations one reduces himself to check that Π_{B_R} is preserved. However, Π_{B_R} is the grand canonical Gibbs' measures on B_R with elastic boundary, up to adding to the Hamiltonian the interaction with the fixed part of the configuration outside B_R, which is not touched by T_t^R. Thus, the evolution is in fact the Newtonian evolution of particles inside B_R with reflecting boundary under a given (constant in time) external force, so Liouville's theorem applies and the proof is concluded. □

Remark 15. To be precise, checking only the conditional distributions, we are implicitly assuming uniqueness of the Gibbs' measure. Since this might not be true, either one assumes it, or instead he says that T_t^R maps a Gibbs' measure to another with same potential and temperature. To fix ideas, our reader should assume uniqueness.

Let us turn to the estimates. The key quantity to estimate is the desplacement of positions q_i in a finite interval of time, since increments of momenta depend only on such displacement because of the Newtonian nature of our problem. We begin with a small but significative computation: from now on we denote

$$\log_+ x = \log|x| \vee 1 \qquad \forall x \in \mathbb{R}^d.$$

Lemma 16. *For any $b > 0$ there exists a constant $M(b) > 0$ such that any $f \in C^1([0, T], \mathbb{R}^d)$ satisfying*

$$\int_0^T \frac{|f'(t)|}{\log_+ f(t)} dt \le b$$

also satisfies

$$|f(T) - f(0)| \le M(b) \log_+ |f(0)|.$$

Proof. It is clear that for any such f it holds

$$|f(T) - f(0)| \le b \cdot \log_+ \| f \|_\infty,$$

so we only need to control $\log_+ \| f \|_\infty$ in terms of $\log_+ |f(0)|$. By triangular inequality the line above implies that

$$\| f \|_\infty - b \cdot \log_+ \| f \|_\infty \le |f(0)|,$$

hence, setting $c(b) = \min_{r \ge 0} \frac{\log_+ r}{\log_+ (r - b \log_+ r)}$ (which is always a positive number as the reader can check), we get

$$\frac{\log_+ \| f \|_\infty}{\log_+ |f(0)|} \le c(b),$$

and this, together with the above inequality, concludes the proof with $M(b) = b \cdot c(b)$. □

Before we state and prove the announced *a priori* estimates, let us introduce some useful quantities, the mere definition of which should motivate the computation we just carried out. We set, for $(p,q)=\{(p_i,q_i)_{i\in I}\}\in\Omega$,

$$
\begin{aligned}
B(p,q) &= \sup_{i\in I}\frac{|p_i|}{\log_+ q_i},\\
\tilde{B}(p,q) &= \sup_{k\in\mathbb{Z}^d}\frac{\tilde{B}_k(p,q)}{\log_+ k}, \qquad \tilde{B}_k(p,q)=\max_{q_i\in Q_k}|p_i|,\\
\bar{B}(p_0,q_0) &= \frac{1}{\pi}\int_{-\infty}^{\infty} B(T_t(p_0,q_0))\frac{dt}{1+t^2},
\end{aligned}
$$

where the Q_k's are the usual partition in lattice cubes of $\mathbb{R}^d$ and T_t is a measurable mapping of Ω into itself (which will be specified case by case). We might have defined $\bar{B}$ simply integrating on a bounded interval of time, avoiding the necessity of the weight $(1+t^2)^{-1}$ (the constant π^{-1} is there to normalise the integral). We choose this definition in order to easily treat global (in time) existence.

Proposition 17. (*A priori* estimates) *Let $T_t:\Omega\to\Omega$ be a semigroup of measurable mappings preserving m_β defined by a time evolution $t\mapsto\{(p_{i,t},q_{i,t})_{i\in I}\}$ such that*

$$
\left|\frac{d}{dt}q_{i,t}\right|\le|p_{i,t}| \qquad \forall i\in I, t\in\mathbb{R}.
$$

It holds $\mathbb{E}^{m_\beta}[B]=\mathbb{E}^{m_\beta}[\bar{B}]<\infty$, the value of the integral being independent of the particular evolution T_t we chose. Moreover, on the full-measure set $\bar{\Omega}=\{\bar{B}<\infty\}$ (with respect to m_β), which is also independent of T_t,

$$
|q_{i,t}-q_{i,0}|\le M(\pi(1+\tau^2)\bar{B}(p_0,q_0))\log_+ q_{i,0} \qquad \forall i\in I, |t|\le\tau,
$$

where $M(\cdot)$ is the constant of the lemma above.

Remark 18. We can not stress enough that the constants in the estimate we provide are

- uniform in T_t, so that they can be applied to the whole set of approximations in order to obtain compactness;
- depending on the initial data (p_0,q_0), thus we will not be able to treat *simultaneously* the set of good initial data, or in fact any set of initial data of positive measure. We will come back later on this.

Proof. Note that, up to a universal constant, $0\le B(p,q)\le\tilde{B}(p,q)$, so we can check the integrability of $\tilde{B}$ to obtain the one of B. In other words, we reduce ourselves to control particles inside the cubes Q_k, and thanks to Ruelle's estimates we are exceedingly efficient at it. By conditioning, and since momenta have Gaussian distributions, we first bound

$$
\begin{aligned}
m_\beta\big(\tilde{B}_k(p,q)\ge A\big) &= \sum_{n=0}^{\infty} m_\beta(q(Q_k)=n)\,m_\beta\big(\tilde{B}_k(p,q)\ge A\big|q(Q_k)=n\big)\\
&\le \sum_{n=0}^{\infty} m_\beta(q(Q_k)=n)\cdot nCe^{-C'A^2}=Ce^{-C'A^2}\,\mathbb{E}^{m_\beta}[q(Q_k)]\\
&\le Ce^{-C'A^2},
\end{aligned}
$$

where C and C' are positive constants (depending on β), and the last passage is due to the fact that by Ruelle's bounds $\mathbb{E}^{m_\beta}[q(Q_k)]$ is bounded uniformly in k (we renamed the constant C in the last step). Hence,

$$
m_\beta(\tilde{B}(p,q)\ge A)=\sum_{k\in\mathbb{Z}^d} m_\beta\big(\tilde{B}_k(p,q)\ge A\log_+ k\big)\le C\sum_{k\in\mathbb{Z}^d} e^{-C'A^2(\log_+ k)^2},
$$

which is actually more than we need. Once we have established integrability of B, since by assumption T_t preserves m_β,

$$\mathbb{E}^{m_\beta}[\bar{B}] = \mathbb{E}^{m_\beta}\left[\frac{1}{\pi}\int_{-\infty}^{\infty} B\circ T_t \frac{dt}{1+t^2}\right] = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{dt}{1+t^2}\cdot \mathbb{E}^{m_\beta}[B] = \mathbb{E}^{m_\beta}[B],$$

thus concluding the proof. □

Exercise 8. Explicit the missing detail of the integrability of $\tilde{B}$ integrating in A the estimate we got above.

The reader will notice that the approximants we described above fit the hypothesis of our estimates. Indeed, we are ready to pass to the limit and obtain the promised existence result. In what follows, analogously to $\bar{B}$ above,

$$\begin{aligned} \bar{B}_R(p_0, q_0) &= \frac{1}{\pi}\int_{-\infty}^{\infty} B(T_t^R(p_0, q_0))\frac{dt}{1+t^2}, \\ \bar{B}_\infty(p_0, q_0) &= \liminf_{R\to\infty} \bar{B}_R(p_0, q_0). \end{aligned}$$

By Fatou's lemma (and integrability of $\bar{B}_R$) we have that $\bar{B}_\infty$ is integrable, in particular the set $\bar{\Omega}_\infty = \{\bar{B}_\infty < \infty\} \subset \Omega$ is of full measure.

Proposition 19. *Let $(p_0, q_0) \in \bar{\Omega}_\infty$, then there exists a solution, global in time, of*

$$\begin{cases} \dot{q}_i = p_i \\ \dot{p}_i = -\sum_{j\neq i} \nabla U(q_j - q_i) \\ q_i(0) = q_{0,i}, \quad p_i(0) = p_{0,i}. \end{cases}$$

Proof. By assumption, there exists a constant $b > 0$ and a sequence $R_N \uparrow \infty$ such that $\bar{B}_{R_N}(p_0, q_0) \leq b$, and thus by the *a priori* estimates,

$$|q_{i,t}^{R_N} - q_{i,0}| \leq M(\pi(1+\tau^2)\bar{B}_{R_N}(p_0, q_0))\log_+ q_{i,0} \qquad \forall i \in I, |t| \leq \tau.$$

Let us now fix $i \in I$ and $\tau > 0$, and denote $M = M(\pi(1+\tau^2)\bar{B}_{R_N}(p_0, q_0))$. We can choose N (depending on i, τ) such that the i-th particle does not hit the boundary of B_{R_N} in the time interval $[-\tau, \tau]$, imposing

$$R_N > |q_{i,0}| + M\log_+ q_{i,0}$$

(this is a direct consequence of the estimate above). Moreover, if L is the diameter of the support of U, the *a priori* estimate also gives us that the j-th particle interacts with the i-th one at some moment in the time interval $[-\tau, \tau]$ if and only if

$$|q_{j,0}| - M\log_+ q_{j,0} \leq |q_{i,0}| + M\log_+ q_{i,0} + L.$$

As a consequence, there can be only a finite number of particles which interact with the i-th in the time interval $[-\tau, \tau]$, say n, and this number *does not* depend on N. We thus bound

$$|\dot{p}_{i,t}^{R_N}| \leq n\,\|\nabla U\|_\infty$$

(using in an essential way the smoothness hypothesis on U). Let us stress that this last estimate holds for any $i \in N$, $\tau > 0$ fixed, uniformly in N (big enough) and $|t| \leq \tau$.

Ascoli-Arzela Theorem now ensures (up to subsequences) the uniform convergence of $p_{i,t}^{R_N}$ on $[-\tau, \tau]$, but in fact a diagonal argument provides convergence on compact subsets of $\mathbb{R}$. Since $\dot{q}_{i,t}^{R_N} = p_{i,t}^{R_N}$, the same convergence takes place also for $q_{i,t}^{R_N}$.

Identification of the limit is now a simple exercise: for a given time t there exists N big enough such that

$$\begin{cases} q_{i,t}^{R_N} = q_{i,0} + \int_0^t p_{i,s}^{R_N} ds \\ p_{i,t}^{R_N} = p_{i,0} - \int_0^t \sum_{j \neq i} \nabla U(q_{j,s}^{R_N} - q_{i,s}^{R_N}) ds, \end{cases}$$

that is, the i-th particle satisfies Newton's equations without reflections. Since in $[0, t]$ the i-th particle interacts with finitely many other particles (whose number does not depend on N as noted above), and thus as $N \to \infty$ not only $q_{i,t}$ but also all the $q_{j,t}$ interacting with it converge uniformly, then the above equations pass to the limit (smoothness of U has to be used again here). This argument can be repeated for all particles and all bounded time integrals. □

5 Remarks on Uniqueness and Stationarity

The final result of the previous section leaves of course many questions open. Let us list some of them: we will answer below with a few precise statements that, however, we will not prove here.

- In the existence theorem there is no measure theory, and the construction is adapted to a single phase space point (p_0, q_0). Is there a way to work simultaneously with (almost all) points, or even with a positive measure set of them?

- The latter question is clearly related to this one: can we pass to the limit the invariance result for Gibbs' measures we proved for T_t^R?

- Is it possible to remove some of the hypothesis on U, especially the ones which are not needed for Ruelle's bounds to hold? (Non compact support and presence of singularities are ubiquitous phenomena in physically relevant potentials).

- Does uniqueness of the solution hold for the initial data we chose? Does uniqueness hold for any initial data at all? Does this question require even more hypothesis on U to be answered?

The theory developed since the works of Lanford by Dobrushin, Fritz *et cetera*, answers to many of these questions. Here are some facts already known to Lanford.

Proposition 20. (Uniqueness) *Under the above hypothesis on U, there exists at most one solution of Newton's equations on* $[0, \tau]$ *for initial data satisfying*

$$\sup_{k \in \mathbb{Z}^d} \frac{q(Q_k)}{\sqrt{\log_+ k}} < \infty,$$

among those solutions for which

$$\sup_{t \in [0,\tau]} \sup_{i \in I} \frac{|q_{i,t} - q_{i,0}|}{\log_+ q_{i,0}} < \infty.$$

The hypothesis on the initial data does not really concerns us, since we have proved it to hold for almost every configuration with respect to Gibbs' measure. The second, however, does, since there might be "singular" solutions of the equations (with particles moving quite far from their starting position) not covered by our hypothesis. In fact, we have a sort of "conditional" uniqueness result. We will be reassured about this below, but first let us turn to the issue of "non-uniformity" of the passage to the limit in the existence result.

Proposition 21. *Fix $\epsilon, r, \tau > 0$. There exists $\bar{R}$ such that for $R > \bar{R}$,*

$$|q_{i,t}^R - q_{i,t}| \leq \epsilon \qquad \forall i\colon \quad |q_{i,0}| \leq r, \quad |t| \leq \tau,$$

the latter holding for all (p_0, q_0) of m_β measure at least $1-\epsilon$ (where $q_{i,t}$ without superscripts denotes the limiting solution).

Corollary 22. *The approximant flows T_t^R converge in measure (both in space with respect to Gibbs' measure and on compact time intervals) to a limit T_t which is thus jointly measurable in time and space, a semigroup of mappings and preserves Gibbs' measure for each fixed t.*

Turning back to uniqueness, what happens is that even if there exist multiple anomalous solutions which are not covered by our uniqueness result, they can not be pieced together to form a measure preserving flow.

Proposition 23. *Let S_t be a flow of Newton's equations*[3] *preserving a Gibbs' measure m_β, then (for any fixed t) S_t and T_t, the latter being defined by the solution we built in the existence result, must coincide almost surely with respect to m_β.*

3. That is, a semigroup of measurable mappings of Ω into itself preserving m_β induced by a solution of the usual infinite system of equations.