The mathematical derivation of thermodynamic laws from interacting oscillators

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Abstract

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Contents

1. Hamiltonian chains of oscillators

1.1. The model. We consider a chain of n particles connected by strings. A *configuration* $(\mathbf{q},\mathbf{p}) := (q_1,\dots,q_n,p_1,\dots,p_n)$ is a sequence of *positions* $q_j \in \mathbb{R}$ and *velocities* $p_j \in \mathbb{R}$. Note that the positions q_j can reach negative values, therefore the oscillators are not necessarily ordered in space.

Between each pair of consecutive particles $(j, j+1)$ there is a spring described by its *potential energy* $V(q_{j+1} - q_j)$. Assumptions on V will be given later on. We adopt the boundary conditions

$$\begin{aligned} p_{j+n} &= p_j \\ q_{j+n} &= q_j + nL, \qquad \text{for some } L \in \mathbb{R}. \end{aligned}$$

In this setting $L \in \mathbb{R}$ is the "average algebraic distance".

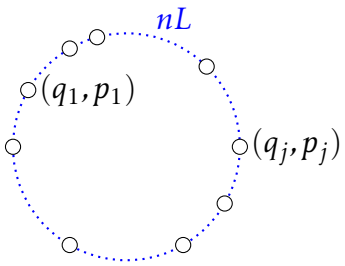

Figure 1: A particle configuration.

Changing $q_j \mapsto q_j - jL$, one can choose $L \equiv 0$ and then the *elongation* variable $r_j := q_j - q_{j-1}$ is periodic ($r_{j+n} = r_j$). In fact it turns out to be convenient to

write the dynamics in terms of the elongation coordinates

$$\mathbf{r} := (r_j)_{j=1,\dots,n} \qquad \text{with } r_j = q_j - q_{j-1}.$$

Therefore from now on we identify $j \in \mathbb{T}_n := \mathbb{Z}/n\mathbb{Z}$ and we call *configuration* the sequence $(\mathbf{r}, \mathbf{p})$ which belongs to the *state space* $\Gamma_n := (\mathbb{R}^{\mathbb{T}_n})^2$.

The *Hamiltonian dynamics* (consistent with Newton's laws) is given, for any $j \in \mathbb{T}_n$ by

$$\begin{aligned} \dot{r}_j(t) &= p_j(t) - p_{j-1}(t) \\ \dot{p}_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)). \end{aligned} \tag{1.1}$$

The *Hamiltonian* associated with this dynamics is

$$\mathcal{H}_n(t) := \sum_{j \in \mathbb{T}_n} e_j(t), \qquad e_j := V(r_j) + \frac{1}{2} p_j^2$$

and is constant in time: $\mathcal{H}_n(t) \equiv \mathcal{H}_n(0)$. The *generator* of this dynamics is the differential operator acting on functions $f(\mathbf{r}, \mathbf{p})$ defined on Γ_n which is given by

$$\mathcal{A}_n = \sum_{j \in \mathbb{T}_n} \Big\{ (p_j - p_{j-1}) \partial_{r_j} + \big(V'(r_{j+1}) - V'(r_j) \big) \partial_{p_j} \Big\}.$$

It satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t} f(\mathbf{r}(t), \mathbf{p}(t)) = (\mathcal{A}_n f)(\mathbf{r}(t), \mathbf{p}(t)),$$

and its domain is given by $\mathcal{D}_n := \mathcal{C}_c^1(\Gamma_n)$, the set of compactly supported and $\mathcal{C}^1$ functions on Γ_n.

1.2. Conserved quantities and stationary measures. This dynamics conserves in particular three important (extensive) quantities, that we assume propor-

tional to n at initial time:

$$\begin{aligned}
\mathcal{H}_n &:= \sum_{j\in\mathbb{T}_n} e_j = nE, \qquad \text{the total energy} \\
\mathcal{P}_n &:= \sum_{j\in\mathbb{T}_n} p_j = nP, \qquad \text{the total momentum} \\
\mathcal{R}_n &:= \sum_{j\in\mathbb{T}_n} r_j = nL, \qquad \text{the total length.}
\end{aligned}$$

Consequently, the trajectories must stay in the *microcanonical surface*, namely

$$\Sigma^{(n)}_{E,P,L} := \big\{(\mathbf{r},\mathbf{p})\in\Gamma_n\ ;\ (\mathcal{H}_n,\mathcal{P}_n,\mathcal{R}_n) = n(E,P,L)\big\}.$$

Remark 1.1 (Harmonic case). If $V(r) = \frac{1}{2}r^2$ (which means that the chain is *harmonic*), then $\Sigma^{(n)}_{E,P,L}$ is the intersection of a sphere with two hyperplanes, and more precisely it is a sphere of dimension $2n-3$ with radius

$$\sqrt{2n(E-\tfrac{1}{2}P^2-\tfrac{1}{2}L^2)}.$$

Therefore $\Sigma^{(n)}_{E,P,L}$ is not empty iff $E \geqslant \frac{1}{2}P^2+\frac{1}{2}L^2$.

Remark 1.2. There may be other conserved quantities, and in this case the motion will happen in some submanifold of $\Sigma^{(n)}_{E,P,L}$. The *ergodic property* (which we will also mention later on) roughly says that, in some sense, as $n\to+\infty$, the other submanifold "fold densely" inside $\Sigma^{(n)}_{E,P,L}$. This does not always happen, and even when it is true, it is a very hard mathematical problem to prove it.

Note that, if $(\mathbf{r},\mathbf{p})\in\Sigma^{(n)}_{E,P,L}$, then

$$nE = \sum_{j\in\mathbb{T}_n}\frac{1}{2}p_j^2+V(r_j) = \underbrace{\frac{nP^2}{2}}_{\substack{\text{energy of}\\ \text{center of mass}}} + \underbrace{\sum_{j\in\mathbb{T}_n}\frac{1}{2}(p_j-P)^2+V(r_j)}_{\text{internal energy}}.$$

Namely, the quantity $nU := n(E-\frac{1}{2}P^2)$ is the *internal energy*, and it is in fact the relevant *thermodynamic quantity*. Changing p_j to p_j-P only corresponds to a change of reference framework (if $P\neq 0$ then the system as a whole moves

with a kinetic energy of $nP^2/2$), and does not contribute to other thermodynamic quantities (like the entropy, see below). Without loss of generality, in this section we assume:

$$P = 0, \qquad \text{and we simply denote } \Sigma_{E,L}^{(n)} \equiv \Sigma_{E,0,L}^{(n)}.$$

Finally, we give our assumptions on the interaction potential: assume that V is smooth, non-negative, and it satisfies $V(r) \to +\infty$ as $|r| \to +\infty$ and besides, for any $\beta > 0$ et $\tau \in \mathbb{R}$,

$$\int_{\mathbb{R}} e^{-\beta(V(r)-\tau r)}\,\mathrm{d}r < +\infty.$$

One of the first goals is to find *stationary measures* for the microscopic dynamics, namely we look for probability distributions μ on Γ_n such that, for any observable $f \in \mathcal{D}_n$,

$$\int_{\Gamma_n} \mathcal{A}_n f \,\mathrm{d}\mu = 0.$$

Next proposition provides the existence of such a measure:

Proposition 1.3. *Given the values of E, L, there exists a stationary measure for the dynamics given by the projection of the Lebesgue measure on $\Sigma_{E,L}^{(n)}$.*

Namely, we define the measure $\mathrm{d}\sigma_{E,L}^{(n)}$ with support on $\Sigma_{E,L}^{(n)}$, as follows: for all test functions $F : \Gamma_n \to \mathbb{R}$ and $G : \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$,

$$\int_{\Gamma_n} F(\mathbf{r},\mathbf{p}) G\big(\tfrac{1}{n}\mathcal{H}_n, \tfrac{1}{n}\mathcal{R}_n\big)\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{p} = \int_{\mathbb{R}_+\times\mathbb{R}} \mathrm{d}E\ \mathrm{d}L\ G(E,L) \int_{\Sigma_{E,L}^{(n)}} F(\mathbf{r},\mathbf{p})\,\mathrm{d}\sigma_{E,L}^{(n)}.$$

Moreover $\Sigma_{E,L}^{(n)}$ has finite 'volume'[1], hence $\mathrm{d}\sigma_{E,L}^{(n)}$ can be normalized to a probability measure called the microcanonical Gibbs measure *and denoted by $\mathrm{d}\mu_{E,L}^{(n)}$.*

This result is a consequence of the well-known *Liouville's Theorem* for Hamiltonian systems, which states that the elementary volume in the phase space is

[1] In the harmonic case, one can compute explicitely the area of the $(2n-3)$-dimensional sphere, which equals

$$\frac{2\pi^{n-1}}{\Gamma(n-1)}\big(2n(E-\tfrac{1}{2}L^2)\big)^{n-\frac{3}{2}}.$$

time invariant. The first important result is the behavior of the microcanonical measure as $n \to +\infty$, called the *equivalence of ensembles Theorem*.

Theorem 1.4 (Equivalence of ensembles)**.** *For any $\beta > 0$ and $\tau \in \mathbb{R}$, let $\mathrm{d}\nu_{\beta,\tau}$ be the (infinite-dimensional)* canonical Gibbs measure *given by*

$$\mathrm{d}\nu_{\beta,\tau} := \prod_{j\in\mathbb{Z}} e^{-\beta(e_j+\tau r_j)-\mathcal{G}(\beta,\tau)}\, \mathrm{d}r_j\, \mathrm{d}p_j, \tag{1.2}$$

which is a probability measure on $(\mathbb{R}\times\mathbb{R})^{\mathbb{Z}}$. Then the microcanonical Gibbs measure $\mathrm{d}\mu^{(n)}_{E,L}$ converges as $n \to +\infty$ to the canonical Gibbs measure $\mathrm{d}\nu_{\beta,\tau}$ (in the sense of the convergence of the finite dimensional distributions[2]) where (β,τ) are defined as functions of (E,L) from the following (invertible – see below) thermodynamic relations

$$L(\beta,\tau) = \frac{1}{\beta}\frac{\partial\mathcal{G}}{\partial\tau}(\beta,\tau) \qquad E(\beta,\tau) = -\frac{\partial\mathcal{G}}{\partial\beta}(\beta,\tau) + \tau L,$$

The function $\mathcal{G}(\beta,\tau)$ is called the Gibbs potential.

Its proof is based on some general theorem about large deviations for the sum of independent variables and is valid for very general systems, see [CO17].

Remark 1.5 (Harmonic case). If $V(r) = \frac{1}{2}r^2$ all these relations can be exactly computed, since p_j and $r_j - \tau$ are independent centered Gaussian variables under $\mathrm{d}\nu_{\beta,\tau}$. We have

$$\mathcal{G}(\beta,\tau) = \log(2\pi) - \log(\beta) + \frac{\beta\tau^2}{2}, \qquad L = \tau, \qquad E = \beta^{-1} + \frac{\tau^2}{2}.$$

1.3. Thermodynamic entropy. Let us now define the *microcanonical volume* $W_n(E,L)$ of the set of all admissible microscopic configurations of total length nL and total energy nE, as follows: it satisfies, for any test function G defined

[2]Namely, for any $k \in \mathbb{N}$ and any bounded continuous function F defined on $\mathbb{R}^{2k}$,

$$\lim_{n\to+\infty} \int_{\Sigma^{(n)}_{E,L}} F(r_1,\dots,r_k,p_1,\dots,p_k)\, \mathrm{d}\mu^{(n)}_{E,L} = \int_{\mathbb{R}^{2k}} F\, \mathrm{d}\nu^{\#k}_{\beta,\tau},$$

where $\nu^{\#k}_{\beta,\tau}$ is the projection of the first $2k$ coordinates of the canonical measure.

on $\mathbb{R}_+ \times \mathbb{R}$,

$$\int_{\mathbb{R}^{2n}} G\big(\tfrac{1}{n}\mathcal{H}_n, \tfrac{1}{n}\mathcal{R}_n\big) \prod_{i=1}^{n} \mathrm{d}r_i \, \mathrm{d}p_i = \int_{\mathbb{R}_+ \times \mathbb{R}} G(E,L) W_n(E,L) \, \mathrm{d}E \, \mathrm{d}L.$$

It is also equivalently given by

$$W_n(E,L) = \frac{1}{n!} \mathrm{Vol}(\Sigma_{E,L}^{(n)})$$

where the $n!$ comes from the fact that particles are indistinguishable, therefore all the configurations that differ only by particle permutations belong to the same microstate.

Since $\Sigma_{E,L}^{(n)} \times \Sigma_{E,L}^{(m)} \subset \Sigma_{E,L}^{(n+m)}$, we have

$$\log W_n(E,L) + \log W_m(E,L) \leqslant \log W_{n+m}(E,L)$$

and this gives the existence of the limit

$$S(E,L) := \lim_{n \to +\infty} \frac{1}{n} \log W_n(E,L) \in \mathbb{R} \cup \{\pm\infty\}, \tag{1.3}$$

called *thermodynamic entropy*.

Lemma 1.6 (Thermodynamic entropy)**.** *For all $L \in \mathbb{R}$ and $E \geqslant 0$, the thermodynamic entropy $S(E,L)$ given by (1.3) satisfies*

$$S(E,L) = \inf_{\substack{\tau \in \mathbb{R} \\ \beta > 0}} \big\{ \beta E - \beta \tau L + \mathcal{G}(\beta, \tau) \big\}. \tag{1.4}$$

The identity (1.4) is one of the fundamental relations that connect the microscopic system to its thermodynamic macroscopic description. It implies that S is concave, and moreover we can deduce the inverse thermodynamic relations:

$$\tau(E,L) = -\frac{1}{\beta(E,L)} \frac{\partial S}{\partial L}(E,L) \qquad \beta(E,L) = \frac{\partial S}{\partial E}(E,L). \tag{1.5}$$

Remark 1.7 (Harmonic case). If $V(r) = \frac{1}{2}r^2$ then

$$S(E,L) = 1 + \log\pi + \log\left(E - \tfrac{1}{2}L^2\right).$$

1.4. Local equilibrium and ergodicity assumption. Proving *local thermal equilibrium* consists in defining a local temperature $\beta^{-1}(x,t)$, for a macroscopically small but microscopically large volume, at every point x for every time t. The existence of local thermal equilibrium is strongly related to the notion of *ergodicity* for infinite systems, even if a consensual definition of that notion is still missing. Roughly speaking, in the finite-dimensional case, one wonder whether the system, after a long time evolution, passes close to almost all the dynamical states compatible with energy conservation. For finite systems, this is equivalent to prove that the microcanonical measure is the only time-invariant law of the dynamics. If the system is ergodic, the microcanonical distribution can then be used to calculate equilibrium values: suppose that f is some macroscopic observable and that the system is started at time zero from some dynamical state $\omega \in \Gamma_n$, for which $f(\omega)$ has a value that may be very far from its equilibrium value. As time evolves, we expect the current value to approach and stay very close to an equilibrium value, which is equal to its time average. Ergodicity tells us that this equilibrium value is almost always equal to the average of f with respect to the microcanonical Gibbs measure.

Proving ergodicity for generic finite dimensional Hamiltonian systems is an unsolved problem. More precisely, since the work of Kolmogorov, Arnold and Moser (KAM) in the 60's, we cannot expect ergodicity for generic sufficiently regular (and finite dimensional) Hamiltonians. The so far strongest method used to derive macroscopic hydrodynamic equations has been initiated by the seminal work from Olla, Varadhan and Yau [SOY93]. A sufficient condition for their method to work (in some cases) is the following *ergodicity assumption*:

> *Every regular*[3] *infinite state, invariant with respect to both translations in the space and the dynamics, is a mixture of canonical (infinite di-*

[3] Regularity means that the state has finite relative entropy (per unit volume) with respect to the Gibbs measure.

mensional) Gibbs measures.

In particular, ergodicity for finite dimensional systems is not really needed, and only the infinite system has to be ergodic in the sense above. Thus, KAM results do not really impede the derivation of hydrodynamic limits. Nevertheless, Fritz et al. [FFL94] remark that such an ergodicity condition is still very challenging for deterministic Hamiltonian systems.

2. Random perturbations and harmonic potential

2.1. The momentum-exchange noise. The ergodicity assumption remains the main problem, but adding a random perturbation of the dynamics permits to ensure this property. The random part of the dynamics must be *local* and conserves the total energy $\mathcal{H}_n$. The most simple one is an exchange of momenta between nearest neighbor atoms (similar to ellastic collisions) at random Poissonian times. With that noise, both $\mathcal{P}_n$ and $\mathcal{R}_n$ are also conserved.

More precisely, the generator of this *momentum-exchange nosie* is given by $\mathcal{S}_n^{\mathrm{ex}}$, acting on functions $f(\mathbf{r},\mathbf{p})$ defined on Γ_n as

$$\mathcal{S}_n^{\mathrm{ex}} f(\mathbf{r},\mathbf{p}) = \sum_{j\in\mathbb{T}_n} \Big\{ f(\mathbf{r},\mathbf{p}^{j,j+1}) - f(\mathbf{r},\mathbf{p}) \Big\}, \tag{2.1}$$

where $\mathbf{p}^{j,j+1}$ is equal to the configuration $\mathbf{p}$ after the exchange $p_j \leftrightarrow p_{j+1}$. This means that there are independent Poisson processes $\{N_{j,j+1}(t)\}_{j\in\mathbb{T}_n}$ at which the exchanges $p_j \leftrightarrow p_{j+1}$ happen.

We regulate this noise by adding an intensity $\gamma > 0$. Therefore the final stochastic dynamics is a Markov process on Γ_n with generator $\mathcal{A}_n + \gamma\mathcal{S}_n^{\mathrm{ex}}$ and the evolution equations (1.1) then become stochastic differential equations written as

$$\begin{aligned} \dot r_j(t) &= p_j(t) - p_{j-1}(t) \\ \mathrm{d}p_j(t) &= \big(V'(r_{j+1}(t)) - V'(r_j(t))\big)\,\mathrm{d}t + (p_{j+1}(t^-) - p_j(t^-))\,\mathrm{d}N_{j,j+1}(\gamma t) \\ &\qquad + (p_{j-1}(t^-) - p_j(t^-))\,\mathrm{d}N_{j-1,j}(\gamma t). \end{aligned} \tag{2.2}$$

This stochastic noise ensures that every stationary measure for $\mathcal{A}_n + \gamma \mathcal{S}_n^{\mathrm{ex}}$ has to be *exchangeable* in the variables p_j's. This is enough, when $n \to +\infty$, for ensuring that the only regular stationary translation invariant measure are the canonical Gibbs measures, see [FFL94]. This happens for any interaction potential V, even those for which the ergodicity assumption does not hold for the deterministic dynamics (like the harmonic case for instance).

2.2. The momentum-flip noise. Another stochastic noise which ensures the ergodicity assumption is the perturbation which flips the momenta at random Poissonian times. The generator of this *momentum-flip noise* is given by $\mathcal{S}_n^{\mathrm{flip}}$, acting on functions $f(\mathbf{r}, \mathbf{p})$ defined on Γ_n as

$$\mathcal{S}_n^{\mathrm{flip}} f(\mathbf{r}, \mathbf{p}) = \sum_{j \in \mathbb{T}_n} \Big\{ f(\mathbf{r}, \mathbf{p}^j) - f(\mathbf{r}, \mathbf{p}) \Big\}, \tag{2.3}$$

where $\mathbf{p}^j$ is equal to the configuration $\mathbf{p}$ after the flip $p_j \mapsto -p_j$. As before we regulate this noise by adding an intensity $\gamma > 0$. The final stochastic dynamics is a Markov process on Γ_n with generator $\mathcal{A}_n + \gamma \mathcal{S}_n^{\mathrm{flip}}$ and the evolution equations become

$$\begin{aligned} \dot{r}_j(t) &= p_j(t) - p_{j-1}(t) \\ \dot{p}_j(t) &= V'(r_{j+1}(t)) - V'(r_j(t)) - 2p_j(t^-)\, \mathrm{d}N_j(\gamma t), \end{aligned} \tag{2.4}$$

where $\{N_j(t)\}_{j \in \mathbb{T}_n}$ are independent Poisson processes.

2.3. The harmonic potential. As we mentioned earlier, the harmonic potential $V(r) = \frac{1}{2} r^2$ is very peculiar, since (1.1) becomes linear and the system is completely integrable. The linearity makes really convenient to work with Fourier transforms.

The *discrete Fourier transform* $\widehat{f}$ of a complex sequence $\{f_j\}_{j \in \mathbb{T}_n}$ is defined as

$$\widehat{f}(k) := \sum_{k \in \mathbb{T}_n} f_j e^{-2\pi i j k}, \qquad k \in \widehat{\mathbb{T}}_n := \Big\{0, \tfrac{1}{n}, \dots, \tfrac{n-1}{n}\Big\}.$$

The *inverse Fourier transform* $\check{g}$ of $g : \widehat{\mathbb{T}}_n \to \mathbb{C}$ is then given by

$$\check{g}_j := \frac{1}{n} \sum_{k \in \widehat{\mathbb{T}}_n} g(k) e^{2\pi i j k}, \qquad j \in \mathbb{T}_n$$

and the Parseval identity reads

$$\sum_{j \in \mathbb{T}_n} f_j g_j^\star = \frac{1}{n} \sum_{k \in \widehat{\mathbb{T}}_n} \widehat{f}(k) \widehat{g}^\star(k).$$

The deterministic dynamics (1.1) can be diagonalized using Fourier transforms. This is also called the *normal mode representation*. If we denote by $\widehat{\mathbf{r}}(t,\cdot)$ and $\widehat{\mathbf{p}}(t,\cdot)$ the respective Fourier transforms of $\mathbf{r}(t)$ and $\mathbf{p}(t)$, then the deterministic harmonic evolution is equivalent to

$$\begin{aligned} \partial_t \widehat{\mathbf{r}}(t,k) &= (1 - e^{-2\pi i k}) \mathbf{p}(t,k), \\ \partial_t \widehat{\mathbf{p}}(t,k) &= (e^{2\pi i k} - 1) \mathbf{r}(t,k). \end{aligned}$$

Therefore we can see that each *mode* k evolves autonomously, without interacting with the other modes. We note that since $\mathbf{r}$ and $\mathbf{p}$ are real valued, we have

$$\widehat{\mathbf{r}}^\star(t,k) = \widehat{\mathbf{r}}(t,-k), \qquad \widehat{\mathbf{p}}^\star(t,k) = \widehat{p}(t,-k).$$

It is quite convenient to introduce the *wave function*

$$\widehat{\varphi}(t,k) = \widehat{\mathbf{r}}(t,k) + i\widehat{\mathbf{p}}(t,k), \qquad t \geqslant 0, k \in \widehat{\mathbb{T}}_n. \tag{2.5}$$

First, it follows an autonomous evolution, and second, the Hamiltonian $\mathcal{H}_n$ can be rewritten thanks to Parseval identity as

$$\mathcal{H}_n(t) = \frac{1}{2} \sum_{j \in \mathbb{T}_n} |p_j + i r_j|^2(t) = \frac{1}{2n} \sum_{k \in \widehat{\mathbb{T}}_n} \left|\widehat{\varphi}(t,k)\right|^2.$$

This motivates us to define the *energy of the mode* $k \in \widehat{\mathbb{T}}_n$ by

$$\mathcal{E}(t,k) := \frac{1}{2} \left|\widehat{\varphi}(t,k)\right|^2.$$

Finally, in the harmonic case, the (infinite volume) canonical Gibbs measures are given by the following product of independent Gaussians:

$$\nu^{\mathrm{har}}_{\beta,\tau,P} = \bigotimes_{j\in\mathbb{Z}} \big(\underbrace{\mathcal{N}(\tau,\beta^{-1})}_{\text{law of } r_j} \otimes \underbrace{\mathcal{N}(P,\beta^{-1})}_{\text{law of } p_j} \big), \qquad \tau, P \in \mathbb{R}, \beta > 0. \tag{2.6}$$

Note that we work in full generality here and authorize the case $P \neq 0$. An important remark is the following: for any $j \in \mathbb{Z}$,

$$T = \beta^{-1} = \int (p_j - P)^2 \, \mathrm{d}\nu^{\mathrm{har}}_{\beta,\tau,P}, \qquad \tau = \int r_j \, \mathrm{d}\nu^{\mathrm{har}}_{\beta,\tau,P}.$$

3. Macroscopic limits in the harmonic case

From now on we focus on the case $V(r) = \frac{1}{2}r^2$ and therefore the Hamiltonian generator equals

$$\mathcal{A}_n = \sum_{j\in\mathbb{T}_n} \Big\{ (p_j - p_{j-1})\partial_{r_j} + (r_{j+1} - r_j)\partial_{p_j} \Big\}. \tag{3.1}$$

3.1. Purely deterministic chain: mechanical non-equilibrium. We assume that at time $t = 0$, the variables r_j and p_j are independent Gaussians with same variance β^{-1} but with different averages, which vary slowly according to some continuous profiles $\overline{p}_{\mathrm{ini}}, \overline{r}_{\mathrm{ini}}$ defined on $\mathbb{T}$, where $\mathbb{T} = [0,1)$ is the continuous torus of size 1.

Namely, let the microscopic dynamics start from the *local Gibbs measure*

$$\mathrm{d}\nu^n_{\mathrm{ini}} := \prod_{j\in\mathbb{T}_n} \frac{\beta}{2\pi} e^{-\frac{1}{2}\beta\left[(p_j - \overline{p}_{\mathrm{ini}}(\frac{j}{n}))^2 + (r_j - \overline{r}_{\mathrm{ini}}(\frac{j}{n}))^2\right]} \mathrm{d}r_j \, \mathrm{d}p_j \tag{3.2}$$

Physically speaking, this means that the system is *thermalized* at homogeneous temperature $T = \beta^{-1}$, but in mechanical non-equilibrium with given *macroscopic profiles* $\overline{p}_{\mathrm{ini}}, \overline{r}_{\mathrm{ini}}$ of momentum and volume stretch.

Let us denote by ν^n_t the probability distribution of the configuration at time

$t > 0$, namely the law of $(\mathbf{r}, \mathbf{p})(t)$. We are now ready to give the first result concerning the limiting behavior of the periodic chain in the *hyperbolic space-time scaling*.

Proposition 3.1 (Euler equations for the purely harmonic chain)**.** *Assume the initial condition* (3.2)*, and assume that the evolution of* $(\mathbf{r}, \mathbf{p})(t)$ *is governed by the Hamiltonian generator* (3.1)*.*

Then, for any continuous test function G*, and any* $t > 0$*,*

$$\frac{1}{n} \sum_{j \in \mathrm{T}_n} G\big(\tfrac{j}{n}\big) \begin{pmatrix} r_j(tn) \\ p_j(tn) \\ e_j(tn) \end{pmatrix} \xrightarrow[n \to +\infty]{\textit{in prob.}} \int_{\mathrm{T}} G(y) \begin{pmatrix} \overline{r}(t,y) \\ \overline{p}(t,y) \\ \overline{e}(t,y) \end{pmatrix} \mathrm{d}y$$

where $\overline{r}(0,\cdot) = \overline{r}_{\mathrm{ini}}, \overline{p}(0,\cdot) = \overline{p}_{\mathrm{ini}}$ *and*

$$\partial_t \overline{r} = \partial_y \overline{p}, \qquad \partial_t \overline{p} = \partial_y \overline{r} \tag{3.3}$$

and for any $t \geqslant 0, y \in \mathbb{T}$*, we have* $\overline{e}(t,y) = \beta^{-1} + \frac{1}{2}(\overline{r}^2 + \overline{p}^2)(t,y)$*, meaning*

$$\partial_t \overline{e} = \partial_y (\overline{rp}). \tag{3.4}$$

The proof is based on linearity (recall that (1.1) becomes a linear system), and the use of Fourier transforms (in particular the wave function defined in (2.5)). It also crucially uses the following fact. The total energy $\overline{e}$ has two distinct contributions: it can be written as

$$\overline{e}(t,y) = e^{\mathrm{th}}(t,y) + e^{\mathrm{mech}}(t,y), \qquad \begin{cases} e^{\mathrm{th}}(t,y) = \beta^{-1} \\ e^{\mathrm{mech}}(t,y) = \frac{1}{2}(\overline{r}^2 + \overline{p}^2)(t,y) \end{cases}. \tag{3.5}$$

This decomposition corresponds at the microscopic level to the following:

$$\mathbb{E}[e_j(t)] = \int \tfrac{1}{2}(p_j^2 + r_j^2) \, \mathrm{d}\nu_t^n = \mathcal{E}_j^{\mathrm{th}}(t) + \mathcal{E}_j^{\mathrm{mech}}(t) \tag{3.6}$$

where

$$\begin{cases} \mathcal{E}_j^{\text{mech}} := \frac{1}{2}\big(\mathbb{E}[r_j]\big)^2 + \frac{1}{2}\big(\mathbb{E}[p_j]\big)^2 \\ \mathcal{E}_j^{\text{th}} := \mathbb{E}\Big[\frac{1}{2}(r_j - \mathbb{E}[r_j])^2 + \frac{1}{2}(p_j - \mathbb{E}[p_j])^2\Big]. \end{cases} \tag{3.7}$$

These two microscopic values can be investigated separately, and this is quite crucial in the argument (this will also be quite important for the next results). In particular, one can see that the mechanical energy corresponds to the evolution of the *low modes*, and the thermal energy corresponds to the other ones, which in this case are already in thermal equilibrium at temperature $T = \beta^{-1}$ and therefore there is no evolution for them. In fact, since we start from the local Gibbs measure (3.2), then one can easily see that at any time $t > 0$, $r_j(t) - \mathbb{E}[r_j](t)$ and $p_j(t) - \mathbb{E}[p_j](t)$ are centered Gaussians with variance T.

Remark 3.2. The three equations (3.3) and (3.4) are called the *Euler equations*. In fact, they have been rigorously obtained also for *anharmonic systems* under the ergodicity assumption, see for instance [EO14], and for more general initial conditions (even out of thermal equilibrium). In the anharmonic case (for general potentials V), they become

$$\partial_t \overline{r} = \partial_y \overline{p}, \qquad \partial_t \overline{p} = \partial_y \tau(\overline{u}, \overline{r}), \qquad \partial_t \overline{e} = \partial_y (\overline{p}\tau(\overline{u}, \overline{r})),$$

where $\overline{u} = \overline{e} - \frac{1}{2}\overline{p}^2$ is the internal energy and τ is the tension given by the thermodynamic relation (1.5). This is a non-linear hyperbolic system of equations, and it is expected that any nontrivial solution will develop shocks. After appearance of shocks, the equations should be considered in a weak sense and a criterion of choice of the weak solution should be a positive production of entropy, however a mathematical theorem that guarantee uniqueness of this entropy solution is still lacking. Eventually shocks will create dissipations and the entropy solution should converge as $t \to +\infty$ to a solution with a constant profile of tension τ_∞, *i.e.* a mechanical equilibrium. Still the system could be in *thermal* non-equilibrium, therefore one needs to look for another evolution of the energy, see Section 3.2 below.

What happens if we know start the microscopic dynamics is not in thermal equibrium, but starts from the local Gibbs measure with non-homogeneous

temperature profile? Namely, we assume that $(\mathbf{r},\mathbf{p})(0)$ are such that, independently for any j,

$$r_j(0) \sim \mathcal{N}\Big(\overline{r}_{\rm ini}\big(\tfrac{j}{n}\big), \overline{T}_{\rm ini}\big(\tfrac{j}{n}\big)\Big) \qquad p_j(0) \sim \mathcal{N}\Big(\overline{p}_{\rm ini}\big(\tfrac{j}{n}\big), \overline{T}_{\rm ini}\big(\tfrac{j}{n}\big)\Big), \tag{3.8}$$

for continuous profiles $\overline{r}_{\rm ini}, \overline{p}_{\rm ini}, \overline{T}_{\rm ini}$. In this case, the first two equations (3.3) remain valid, but the equation for the energy will not have a closed form, because the thermal modes will now have a macroscopic evolution. In fact the presence of more conservation laws prevents from diffusion of thermal energy.

This is why we now add to the deterministic dynamics the stochastic noises introduced in Section 2.

3.2. Harmonic chain with exchange of momenta: from Euler to superdiffusion of thermal energy. In this section, we consider, for any $\gamma > 0$, the generator $\mathcal{L}_n = \mathcal{A}_n + \gamma \mathcal{S}_n^{\rm ex}$ where $\mathcal{A}_n$ is given in (3.1) and $\mathcal{S}_n^{\rm ex}$ is defined in (2.1). Thanks to the stochastic noise, the "only" conserved quantities are $\mathcal{H}_n$, $\mathcal{P}_n$ and $\mathcal{R}_n$, and the ergodicity assumption holds, namely: the only stationary and translation invariant probability measures for the infinite dynamics, which are also regular, are mixtures of the canonical Gibbs measures $\mathrm{d}\nu^{\rm har}_{\beta,\tau,P}$ given in (2.6), parametrized by temperature β^{-1}, momentum P and tension τ.

In this case, there are two different time scales which govern the macroscopic evolution of the system. First, we have:

Theorem 3.3 (Euler equations in the hyperbolic time scale, [EO14])**.** *Assume that the evolution of $(\mathbf{r},\mathbf{p})(t)$ is governed by the generator $\mathcal{L}_n^{\rm ex}$, starting from the initial condition* (3.8)*, namely the local Gibbs measure*

$$\mathrm{d}\nu^n_{\rm ini} = \prod_{j\in\mathbb{T}_n} \frac{\beta_j}{2\pi} e^{-\frac{1}{2}\beta_j\left[(p_j-\overline{p}_{\rm ini}(\frac{j}{n}))^2+(r_j-\overline{r}_{\rm ini}(\frac{j}{n}))^2\right]}\,\mathrm{d}r_j\,\mathrm{d}p_j, \qquad \textit{with } \beta_j^{-1} := \overline{T}_{\rm ini}(\tfrac{j}{n})$$

for some continuous profiles $\overline{T}_{\rm ini} : \mathbb{T} \to (0,+\infty)$, and $\overline{p}_{\rm ini}, \overline{r}_{\rm ini} : \mathbb{T} \to \mathbb{R}$.

Then, for any continuous test function G, and any $t > 0$,

$$\frac{1}{n}\sum_{j\in \mathrm{T}_n} G\big(\tfrac{j}{n}\big)\begin{pmatrix} r_j(tn)\\ p_j(tn)\\ e_j(tn)\end{pmatrix} \xrightarrow[n\to+\infty]{\text{in prob.}} \int_{\mathrm{T}} G(y)\begin{pmatrix} \overline{r}(t,y)\\ \overline{p}(t,y)\\ \overline{e}(t,y)\end{pmatrix}\mathrm{d}y$$

where $\overline{r}(0,\cdot)=\overline{r}_{\mathrm{ini}}$, $\overline{p}(0,\cdot)=\overline{p}_{\mathrm{ini}}$, $\overline{e}(0,\cdot)=\overline{T}_{\mathrm{ini}}+\frac{1}{2}(\overline{r}^2_{\mathrm{ini}}+\overline{p}^2_{\mathrm{ini}})$, *and*

$$\partial_t\overline{r}=\partial_y\overline{p}, \qquad \partial_t\overline{p}=\partial_y\overline{r}, \qquad \partial_t\overline{e}=\partial_y(\overline{rp}). \tag{3.9}$$

This convergence result can be proven using relative entropy methods, in the smooth regime of the Euler equations.

Note that, remarkably, the macroscopic Euler equations do not depend on the value of $\gamma > 0$ (the noise intensity). Moreover, following decomposition (3.5) we can write

$$\overline{e}=e^{\mathrm{th}}+e^{\mathrm{mech}}, \qquad e^{\mathrm{mech}}=\tfrac{1}{2}(\overline{r}^2+\overline{p}^2),$$

and from (3.9) one can easily see that $\partial_t e^{\mathrm{th}}=0$, which means that the *thermal energy does not evolve in the hyperbolic time scale*. Therefore we need to look at larger time scales in order to understand the macroscopic behavior of the thermal energy. This is done in:

Theorem 3.4 (Fractional diffusion for the thermal energy, [JKO15])**.** *Assume that the evolution of $(\mathbf{r},\mathbf{p})(t)$ is governed by the generator $\mathcal{L}_n^{\mathrm{ex}}$, starting from the initial condition*

$$\mathrm{d}\nu^n_{\mathrm{ini}}=\prod_{j\in\mathbb{T}_n}\frac{\beta_j}{2\pi}e^{-\frac{1}{2}\beta_j(p_j^2+r_j^2)}\,\mathrm{d}r_j\,\mathrm{d}p_j, \qquad \text{with } \beta_j^{-1}:=\overline{T}_{\mathrm{ini}}\big(\tfrac{j}{n}\big)$$

for some smooth profile $\overline{T}_{\mathrm{ini}}:\mathbb{T}\to(0,+\infty)$. Then, for any suitable test function G on $\mathbb{R}_+\times\mathbb{T}$, and any $t>0$,

$$\frac{1}{n}\sum_{j\in\mathbb{T}_n}\int_0^{+\infty} G\big(t,\tfrac{j}{n}\big)\mathbb{E}[e_j(tn^{3/2})]\,\mathrm{d}t \xrightarrow[n\to+\infty]{} \int_0^{+\infty}\int_{\mathbb{T}} G(y)\,T(t,y)\,\mathrm{d}y\,\mathrm{d}t$$

where $T(0,\cdot) = \overline{T}_{\mathrm{ini}}$, *and there is a constant* $\kappa > 0$ *(explicit) such that*

$$\partial_t T(t,y) = -\frac{\kappa}{\sqrt{\gamma}} |\partial_y|^{3/4} T(t,y).$$

The nature of this convergence result (namely convergence in means and weakly in time) comes from the tools which are used in the proof. Indeed, the *Wigner distribution* (which has been originally introduced in quantum mechanics) is a powerful tool to localize in space energy modes, separating microscopic from macroscopic scale. Its explicit resolution goes through Laplace transforms, hence coming with integration in time.

3.3. Harmonic chain with flip of momenta: diffusion of thermal energy. Finally, for any $\gamma > 0$, we consider the generator $\mathcal{L}_n^{\mathrm{flip}} := \mathcal{A}_n + \gamma \mathcal{S}_n^{\mathrm{flip}}$, where $\mathcal{A}_n$ is given in (3.1) and $\mathcal{S}_n^{\mathrm{flip}}$ is defined in (2.3). Because of the random flips, the total momentum is not preserved anymore, and in fact the "only" conserved quantities for this dynamics are the total energy and volume stretch. As before the ergodicity assumption holds in the following way: the "unique" invariant measures are the canonical Gibbs measure $\nu^{\mathrm{har}}_{\beta,\tau,0}$ defined in (2.6) parametrized by the temperature $\beta^{-1} > 0$ and tension $\tau \in \mathbb{R}$.

On the contrary to the previous case, here both conserved quantities evolve in the *same* time scale, namely the diffusive one, as shown in:

Theorem 3.5 (Diffusive system for the flipped harmonic chain, [KOS18])**.** *Assume that the evolution of* $(\mathbf{r},\mathbf{p})(t)$ *is governed by the generator* $\mathcal{L}_n^{\mathrm{flip}}$, *starting from the local Gibbs measure*

$$\mathrm{d}\nu^n_{\mathrm{ini}} = \prod_{j\in\mathbb{T}_n} \frac{\beta_j}{2\pi} e^{-\frac{1}{2}\beta_j\left[p_j^2 + (r_j - \overline{r}_{\mathrm{ini}}(\frac{j}{n}))^2\right]} \mathrm{d}r_j\,\mathrm{d}p_j, \qquad \text{with } \beta_j^{-1} := \overline{T}_{\mathrm{ini}}(\tfrac{j}{n})$$

for some continuous profiles $\overline{T}_{\mathrm{ini}} : \mathbb{T} \to (0,+\infty)$ *and* $\overline{r}_{\mathrm{ini}} : \mathbb{T} \to \mathbb{R}$.

Then, for any continuous test function G, and any $t > 0$,

$$\frac{1}{n}\sum_{j\in \mathrm{T}_n} G\left(\tfrac{j}{n}\right)\begin{pmatrix}\mathbb{E}[r_j(tn^2)]\\ \mathbb{E}[e_j(tn^2)]\end{pmatrix} \xrightarrow[n\to+\infty]{} \int_{\mathrm{T}} G(y)\begin{pmatrix}\overline{r}(t,y)\\ \overline{e}(t,y)\end{pmatrix}\mathrm{d}y$$

where, first, $\overline{r}(0,\cdot) = \overline{r}_{\mathrm{ini}}$ and $\overline{r}$ satisfies the autonomous diffusive equation

$$\partial_t \overline{r} = \frac{1}{2\gamma}\partial_{yy}\overline{r}(t,y) \tag{3.10}$$

and moreover, the total energy $\overline{e}$ reads as $\overline{e} = e^{\mathrm{th}} + e^{\mathrm{mech}}$ with

- *for any $t \geqslant 0, y \in \mathbb{T}$, $e^{\mathrm{mech}}(t,y) = \frac{1}{2}\overline{r}^2(t,y)$*
- *the thermal energy e^{th} is the solution to*

$$\begin{cases} \partial_t e^{\mathrm{th}}(t,y) = \dfrac{1}{4\gamma}\partial_{yy}e^{\mathrm{th}}(t,y) + \dfrac{1}{2\gamma}\left(\partial_y\overline{r}\right)^2(t,y) \\ e^{\mathrm{th}}(0,y) = \overline{T}_{\mathrm{ini}}(y) \end{cases} \tag{3.11}$$

From (3.11) we can see that the mechanical energy is transformed, in the bulk, into the thermal one at the rate $\frac{1}{2\gamma}\left(\partial_y\overline{r}\right)^2$. Here the convergence still holds in means, however there is no integration in time.

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