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Role of conserved quantities in Fourier's law for diffusive mechanical systems

*Rôle des quantités conservées dans la loi de Fourier pour les systèmes mécaniques diffusifs*

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ABSTRACT

Energy transport can be influenced by the presence of other conserved quantities. We consider here diffusive systems where energy and the other conserved quantities evolve macroscopically on the same diffusive space–time scale. In these situations, the Fourier law depends also on the gradient of the other conserved quantities. The rotor chain is a classical example of such systems, where energy and angular momentum are conserved. We review here some recent mathematical results about the diffusive transport of energy and other conserved quantities, in particular for systems where the bulk Hamiltonian dynamics is perturbed by conservative stochastic terms. The presence of the stochastic dynamics allows us to define the transport coefficients (thermal conductivity) and in some cases to prove the local equilibrium and the linear response argument necessary to obtain the diffusive equations governing the macroscopic evolution of the conserved quantities. Temperature profiles and other conserved quantities profiles in the non-equilibrium stationary states can be then understood from the non-stationary diffusive behavior. We also review some results and open problems on the two step approach (by weak coupling or kinetic limits) to the heat equation, starting from mechanical models with only energy conserved.

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R É S U M É

Le transport d'énergie peut être influencé par la présence d'autres quantités conservées. Nous considérons ici des systèmes diffusifs dans lesquels l'énergie et les autres quantités conservées évoluent macroscopiquement à la même échelle diffusive spatio-temporelle. Dans ces situations, la loi de Fourier dépend aussi du gradient des autres quantités conservées. La chaîne du rotor est un exemple classique de ces systèmes, où l'énergie et le moment angulaire sont conservés. Nous passons en revue ici quelques résultats mathématiques récents sur le transport diffusif de l'énergie et d'autres quantités conservées, en particulier relatifs à des systèmes dans lesquels la dynamique hamiltonienne est perturbée par des termes stochastiques conservateurs. La dynamique stochastique permet de définir les coefficients de transport (conductivité thermique) et, dans certains cas, de prouver l'équilibre local et la réponse linéaire nécessaire pour obtenir les équations diffusives qui

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régissent l'évolution macroscopique des quantités conservées. Les profils de température et les autres profils des quantités conservées dans les états stationnaires hors équilibre peuvent alors être compris à partir du comportement diffusif non stationnaire. Nous passons également en revue certains résultats et problèmes ouverts concernant l'approche en deux étapes (par couplage faible ou limites cinétiques) de l'équation de la chaleur à partir de modèles mécaniques dans lesquels seule l'énergie est conservée.

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1. Introduction

Fourier's law claims that the local energy current is proportional to the local gradient of temperature and the ratio of these quantities, which is a function of the local temperature, is called thermal conductivity. However, in many realistic systems, energy is not the only conserved quantity and the interplay between extra conserved quantities and energy has a deep impact on the thermal properties of the system, for example generating uphill diffusion.

Dynamics that have more conserved quantities, either than energy, often present different time scales for the macroscopic evolution of these. In the present review, we are interested in systems where conserved quantities evolve macroscopically in the same *diffusive* time scale, and their macroscopic evolution is governed by a system of *coupled* diffusive equations. One example is given by the chain of coupled rotors, whose dynamics conserves energy and angular momentum. In Sections 2 and 3, we show that, as a consequence of a linear response argument and certain symmetries in the corresponding Onsager matrix, the macroscopic evolution of these two quantities follows a diffusive system of PDE (14) or equivalently (16). In terms of the evolution of the temperature profile, the usual heat diffusion can be counterbalanced by a local increase of temperature due to the gradient of the momentum profile (see (17)). It seems that there is some universality about equations (17) on the role of the gradients of the other conserved quantities. We give some examples where the deterministic Hamiltonian dynamics is perturbed by a stochastic term conservative of energy and other quantities. In some of these stochastic models, the hydrodynamic limit can be proven mathematically.

This macroscopic coupled evolution generates interesting stationary profiles of temperatures in the non-equilibrium stationary states with thermal and mechanical forces acting on the boundaries of the system, as explained in section 4.

In the last section, we will report on some results concerning the two-step approach for the Fourier law, for dynamics that conserves only energy.

2. Linear response and Onsager matrix

For simplicity, let us consider first a spatially homogeneous dynamics on a lattice \mathbb{Z} such that there are two conserved quantities: *momentum* and *energy*. A typical and commonly studied example is given by the rotor chain, where the configurations are given by $\{q_i(t) \in \mathbb{S}^1, p_i(t) \in \mathbb{R}, i \in \mathbb{Z}\}$, where \mathbb{S}^1 is the unit circle. Nearest-neighbor rotators interact through a periodic potential $V(q_{i+1} - q_i)$. For example $V(r) = 1 - \cos(2\pi r)$, but the considerations below are valid for more general interactions. The Hamiltonian dynamics is given by

$$\dot{q}_i(t) = p_i(t), \quad \dot{p}_i(t) = V'(q_{i+1}(t) - q_i(t)) - V'(q_i(t) - q_{i-1}(t)) \quad (1)$$

In the following, we will denote $r_i = q_i - q_{i-1}$. There are two locally conserved (or balanced) quantities: the momentum p_i and the total energy $e_i = \frac{p_i^2}{2} + V(r_i)$. In fact, we have

$$\begin{aligned} \frac{d}{dt} p_i(t) &= j_{i-1,i}^p(t) - j_{i,i+1}^p(t), & j_{i,i+1}^p(t) &= -V'(r_{i+1}(t)) \\ \frac{d}{dt} e_i(t) &= j_{i-1,i}^e(t) - j_{i,i+1}^e(t), & j_{i,i+1}^e(t) &= -p_i(t)V'(r_{i+1}(t)) \end{aligned} \quad (2)$$

where $j_{i,i+1}^\alpha(t)$, $\alpha = p, e$, are the corresponding instantaneous currents. Notice that r_i is **not** a balanced quantity.

One of the main conditions needed in order to have a macroscopic autonomous diffusive evolution of these conserved quantities is that there are no other *translation invariant* conserved quantities for the dynamics of the *infinite* system. This *ergodic* property is very hard to prove for the deterministic dynamics. We may consider also some stochastic perturbation of the dynamics (1) that have the same conserved quantities. The purpose of such perturbations is in fact to guarantee that there are no other balanced quantities [1]. One example is to add a random flip of the signs of r_i : for each particle i , at exponential times with rate γ , r_i changes to $-r_i$, independently from the other particles $j \neq i$. This operation does not change either the momentum or the energy if V is assumed symmetric.

A precise way to state this ergodic property of the infinite dynamics is the characterization of the stationary and translation invariant probability measures, i.e. the fact that the Gibbs measures

$$d\nu_{\beta,p} = \prod_{i \in \mathbb{Z}} \frac{e^{-\beta e_i + \beta p p_i}}{Z_{\beta,\beta p}} dp_i dr_i, \quad \beta > 0, \quad p \in \mathbb{R}, \quad Z_{\beta,\beta p} = \sqrt{2\pi \beta^{-1}} e^{\beta p^2/2} \int e^{-\beta V(r)} dr, \quad (3)$$

are the only stationary and translation invariant probability measures for the dynamics (within a certain class of *regular* distributions). We will denote by $\langle \cdot \rangle_{\beta,p}$ the expectation with respect to $\nu_{\beta,p}$, as well as the expectation of a function of the path of the dynamics under $\nu_{\beta,p}$. These Gibbs measures are called *equilibrium* and they have the following time-reversible property: if $\{(\mathbf{r}(t), \mathbf{p}(t)) = (r_i(t), p_i(t), i \in \mathbb{Z}), t \in [-t_0, t_0]\}$ are stationary distributed with marginal $\nu_{\beta,p}$, then $\{\tilde{r}_i(t) = r_i(-t), \tilde{p}_i(t) = -p_i(-t)\}$ follow the same dynamics, but with marginal $\nu_{\beta,-p}$, i.e. for any function of the path $F(\mathbf{r}, \mathbf{p})$, we have $\langle F(\tilde{\mathbf{r}}(\cdot), \tilde{\mathbf{p}}(\cdot)) \rangle_{\beta,p} = \langle F(\mathbf{r}(\cdot), \mathbf{p}(\cdot)) \rangle_{\beta,-p}$.

In the specific case of the rotators, there is also a *rotational symmetry* of the equilibrium dynamics, i.e. under the equilibrium (β, p) , the distribution of the path of $\tilde{r}_i(t) = r_i(t), \tilde{p}_i(t) = p_i(t) - p$ is the same as the one at equilibrium $(\beta, 0)$, i.e. with zero average velocity.

One way to define the transport diffusion coefficients is through *linear response*. Notice that for any equilibrium state, we have that $\langle j_{i,i+1}^p \rangle_{\beta,p} = 0 = \langle j_{i,i+1}^e \rangle_{\beta,p}$ for any values of $\beta > 0$ and $p \in \mathbb{R}$; consequently, we do not expect any ballistic evolution in these systems. We have to understand how these expectations behave if we impose a gradient of temperature or of momentum, at the first order for small gradients. Given ϵ_1, ϵ_2 , consider the inhomogeneous Gibbs measure

$$d\mu_{\epsilon_1,\epsilon_2} = \prod_{i \in \mathbb{Z}} \frac{e^{-(\beta+\epsilon_1)e_i + (\beta p + \epsilon_2)p_i}}{Z_{\beta+\epsilon_1, \beta p + \epsilon_2}} dp_i dr_i \quad (4)$$

Starting at time $t = 0$ with this inhomogeneous measure, we expect that, at the first order in (ϵ_1, ϵ_2) ,

$$\begin{aligned} \langle j_{0,1}^p(t) \rangle_{\mu_{\epsilon_1,\epsilon_2}} &= K_t^{p,p} \epsilon_2 + K_t^{p,\beta} \epsilon_1 + o(\epsilon_1, \epsilon_2) \\ \langle j_{0,1}^e(t) \rangle_{\mu_{\epsilon_1,\epsilon_2}} &= K_t^{\beta,p} \epsilon_2 + K_t^{\beta,\beta} \epsilon_1 + o(\epsilon_1, \epsilon_2) \end{aligned} \quad (5)$$

and then we are interested in the limit as $t \rightarrow \infty$ for the coefficients $K_t^{u,v}$. Defining $e = \langle e_i \rangle_{\beta,p}$, a straightforward development at the first order gives

$$\begin{aligned} K_t^{p,p} &= \sum_i i \langle j_{0,1}^p(t)(p_i(0) - p) \rangle_{\beta,p}, \quad K_t^{p,\beta} = - \sum_i i \langle j_{0,1}^p(t)(e_i(0) - e) \rangle_{\beta,p} \\ K_t^{\beta,p} &= \sum_i i \langle j_{0,1}^e(t)(p_i(0) - p) \rangle_{\beta,p}, \quad K_t^{\beta,\beta} = - \sum_i i \langle j_{0,1}^e(t)(e_i(0) - e) \rangle_{\beta,p} \end{aligned} \quad (6)$$

assuming that the sums in (6) converge. By using the symmetries of the dynamics (rotational, time stationarity, time reversibility), and recalling that $\langle j_{0,1}^p(0)p_i(0) \rangle_{\beta,0} = 0$, we have

$$\begin{aligned} K_t^{p,p}(\beta, p) &= \sum_i i \langle j_{0,1}^p(t)p_i(0) \rangle_{\beta,0} = - \sum_i i \langle j_{0,1}^p(0)p_i(t) \rangle_{\beta,0} \\ &= - \int_0^t ds \sum_i i \langle j_{0,1}^p(0) (j_{i-1,i}^p(s) - j_{i,i+1}^p(s)) \rangle_{\beta,0} = - \int_0^t ds \sum_i \langle j_{0,1}^p(0) j_{i,i+1}^p(s) \rangle_{\beta,0} \end{aligned} \quad (7)$$

So, we define the limit as $t \rightarrow \infty$, assuming that it exists, as

$$K^{p,p}(\beta, p) = - \int_0^\infty ds \sum_i \langle j_{0,1}^p(0) j_{i,i+1}^p(s) \rangle_{\beta,0} = K^{p,p}(\beta, 0) := K^{p,p}(\beta) \quad (8)$$

Notice that $K^{p,p}$ is only a function of β and does not depend on p . This is a consequence of the rotational symmetry of the dynamics. We define similarly $K^{p,\beta}(\beta, p), K^{\beta,p}(\beta, p), K^{\beta,\beta}(\beta, p)$.

Similar calculations give, recalling that $\langle j_{0,1}^p(0)e_i(0) \rangle_{\beta,p} = 0$ for any p and β ,

$$\begin{aligned} K_t^{p,\beta} &= - \sum_i i \langle j_{0,1}^p(t)(e_i(0) - e) \rangle_{\beta,p} = - \sum_i i \langle j_{0,1}^p(0)(e_i(t) - e) \rangle_{\beta,-p} = - \int_0^t ds \sum_i \langle j_{0,1}^p(0)j_{i,i+1}^e(s) \rangle_{\beta,-p} \\ &= - \int_0^t ds \sum_i \langle j_{0,1}^p(0)p_i(s)j_{i+1,i+2}^p(s) \rangle_{\beta,-p} = \int_0^t ds \sum_i \langle j_{0,1}^p(s)p_i(0)j_{i+1,i+2}^p(0) \rangle_{\beta,p} \\ &= -pK_t^{pp} + \int_0^t ds \sum_i \langle j_{0,1}^p(s)(p_i(0) - p)j_{i+1,i+2}^p(0) \rangle_{\beta,p} = -pK_t^{pp} + \int_0^t ds \sum_i \langle j_{0,1}^p(s)p_i(0)j_{i+1,i+2}^p(0) \rangle_{\beta,0} \end{aligned} \tag{9}$$

The second term on the right-hand side is equal to 0, since $\int_0^t ds \sum_i j_{0,1}^p(s)$ is symmetric by time reversal $s \rightarrow t - s$ while $p_i(0)j_{i+1,i+2}^p(0)$ is antisymmetric. This implies that $K^{p,\beta} = -pK^{pp}$. A similar argument gives

$$K^{\beta,p}(\beta, p) = K^{p,\beta}(\beta, -p) = pK^{pp}(\beta) \tag{10}$$

Similarly,

$$\begin{aligned} K_t^{\beta,\beta} &= - \sum_i i \langle j_{0,1}^e(t)(e_i(0) - e) \rangle_{\beta,p} = \sum_i i \langle j_{0,1}^e(0)(e_i(t) - e_i(0)) \rangle_{\beta,-p} \\ &= \int_0^t ds \sum_i \langle j_{0,1}^e(0)j_{i,i+1}^e(s) \rangle_{\beta,-p} = \int_0^t ds \sum_i \langle j_{0,1}^e(0)j_{i,i+1}^e(s) \rangle_{\beta,p} \end{aligned} \tag{11}$$

Using again the symmetries and recalling that $j_{i,i+1}^e = p_i j_{i+1,i+2}^p$, we obtain also that

$$K^{\beta,\beta}(\beta, p) = K^{\beta,\beta}(\beta, 0) - p^2 K^{p,p}(\beta) \tag{12}$$

Finally thanks to the symmetries of the system, all the coefficients can be calculated from $K^{p,p}(\beta)$ and $K^{\beta,\beta}(\beta) := K^{\beta,\beta}(\beta, 0)$, computed at zero average velocity. Relations (10) and (12) were already noted in [2].

One of the main mathematical problems in dealing with the deterministic infinite dynamics is in proving that the limits defining $K^{p,p}(\beta)$ and $K^{\beta,\beta}(\beta)$ exist and are finite. If this is an open problem for the deterministic dynamics, where stochastic perturbations can help. In fact, adding random independent flips of the r_i 's, one can prove that $K^{p,p}(\beta)$ and $K^{\beta,\beta}(\beta)$ are well defined and finite, by adapting the argument used in [3].

3. The diffusive macroscopic equations

3.1. Macroscopic diffusive equations for the rotors model

The linear response analysis of the previous section gives a heuristic argument for the macroscopic equations governing the evolution in the diffusive space–time scale. In order to state the macroscopic equations, we need some thermodynamic functions. The *internal energy* (or *thermal energy*) as a function of β is given by $u(\beta) = -\partial_\beta \log Z_{\beta,0}$, where $Z_{\beta,0}$ is the partition function appearing in (3). The temperature is given by $T = \beta^{-1}$, and the heat capacity is defined as $c_v(T) = \frac{du}{dT} = \beta^2 \text{Var}_{\beta,0}(e_i)$. The thermodynamic entropy is $S(u) = \inf_{\beta>0} \{ \beta u + \log Z_{\beta,0} \}$, and $\beta(u) = S'(u)$ provides the inverse function of $u(\beta)$.

The linear response argument (5) suggests the following macroscopic equations for the evolution of the profiles $p(t, x)$, $e(t, x)$ of the conserved quantities:

$$\begin{aligned} \partial_t p &= -\partial_x (K^{p,p}(\beta) \partial_x (\beta p) + K^{p,\beta}(\beta, p) \partial_x \beta) \\ \partial_t e &= -\partial_x (K^{\beta,p}(\beta, p) \partial_x (\beta p) + K^{\beta,\beta}(\beta, p) \partial_x \beta) \end{aligned} \tag{13}$$

with the profiles $\beta(t, x) := \beta(u(t, x))$, and $u(t, x) = e(t, x) - \frac{1}{2} p^2(t, x)$. By using the relations (10) and (12), the only coefficient involved are $K^{p,p}(\beta)$ and $K^{\beta,\beta}(\beta) = K^{\beta,\beta}(\beta, 0)$. Expressing the equations in terms of the temperature profile $T(t, x) = \beta^{-1}(t, y)$, (13) are equivalent to

$$\begin{aligned} \partial_t p &= \partial_x (D^p(T) \partial_x p) \\ \partial_t e &= \partial_x \left(D^p(T) \partial_x \left(\frac{p^2}{2} \right) + \kappa(T) \partial_x T \right) \end{aligned} \tag{14}$$

where

$$\begin{aligned} D^p(T) &:= -T^{-1}K^{p,p}(T^{-1}) && \text{momentum diffusivity,} \\ \kappa(T) &:= T^{-2}K^{\beta,\beta}(T^{-1}) && \text{thermal conductivity.} \end{aligned} \quad (15)$$

Alternatively, rewriting (14) as closed equations in $p(t, x)$ and $e(t, x)$:

$$\begin{aligned} \partial_t p &= \partial_x (D^p \partial_x p) \\ \partial_t e &= \partial_x \left((D^p - D^e) \partial_x \left(\frac{p^2}{2} \right) + D^e \partial_x e \right) \end{aligned} \quad (16)$$

with the energy diffusivity defined by $D^e = \frac{\kappa(T)}{c_v(T)}$.

It is more interesting to close the equations in the temperature profile $T(t, x)$ obtaining

$$\begin{aligned} \partial_t p &= \partial_x (D^p(T) \partial_x p) \\ c_v(T) \partial_t T &= \partial_x (\kappa(T) \partial_x T) + D^p(T) (\partial_x p)^2 \end{aligned} \quad (17)$$

There are two remarkable consequences from the equations (17):

- the gradient in the temperature does not contribute to the diffusion of the momentum, but the momentum diffusivity depends only on the temperature;
- the gradient of the momentum **increases** locally the temperature. The time evolution of the temperature is composed by the usual heat diffusion term $\partial_x (\kappa(T) \partial_x T)$ plus an increase due to inhomogeneities in the momentum distribution.

The total energy $e(t, x)$ is the sum of the mechanical energy $p^2(t, x)/2$ and an *internal* energy $u(t, x)$. Notice that $\partial_t u = c_v(T) \partial_t T$, i.e. the momentum diffusion decreases the mechanical energy, which dissipates into internal energy, and the term $D^p(T) (\partial_x p)^2$ is the rate of dissipation of the mechanical energy in internal energy. We can also read this in the increase of the total entropy of the system:

$$\frac{d}{dt} \int S(u(t, x)) dx = \int \left[\frac{D^p(T)}{T} (\partial_x p)^2 + \frac{\kappa(T)}{T^2} (\partial_x T)^2 \right] dx \quad (18)$$

3.2. Mathematical problems

We have obtained the equations (17) heuristically from the linear response argument and some symmetries of the dynamics. In fact, they are quite general, the details of the microscopic dynamics are contained in the macroscopic transport coefficients $D^p(T)$ and $\kappa(T)$. A rigorous mathematical statement would be given by a *hydrodynamic limit*: consider the empirical profile distributions

$$\hat{p}_\epsilon(t, x) = \epsilon \sum_i p_i(\epsilon^{-2}t) \delta_{\epsilon i}(x), \quad \hat{e}_\epsilon(t, x) = \epsilon \sum_i e_i(\epsilon^{-2}t) \delta_{\epsilon i}(x) \quad (19)$$

These are random variables valued on distributions on \mathbb{R} . We would like to prove that, as $\epsilon \rightarrow 0$, they converge in probability to the solution $p(t, x)$, $e(t, x)$ of (16). We have already mentioned that, for the deterministic dynamics, even the existence of $D^p(T)$ and $\kappa(T)$ is an open problem. Adding stochastic conservative terms to the dynamics can help to prove the existence of the transport coefficient [3], but still the proof of the hydrodynamic limit is a difficult task. The main problem is the following. In the hydrodynamic limit, on the microscopic scale, gradients have order ϵ , but one has to look at a time scale ϵ^{-2} . In the linear response argument, we have first made an expansion in the first order of the gradients (cf. (5)) because of a large space scale, and subsequently we took the large time limit. In the hydrodynamic limit, we have to take the limit in space and time together, with the diffusive scaling.

It should be mentioned here that this possible *mathematical* statement about the diffusive limit does not explain the superdiffusive behavior that the rotor chain may have at low temperatures in certain space–time scales. This is due to a kind of *metastable* low-temperature states, where rotors have mostly an oscillatory behavior, like an FPU chain of anharmonic springs, and the r_i behave like an *almost conserved quantity* (see discussion and simulations in [4,5] and for a related model in [6]).

A technique to approach this hydrodynamic limit problem in stochastic dynamics was developed by Varadhan [7] (see also chapter 7 in [8]). It consists in decomposing, by approximations, the microscopic currents in a gradient term (dissipation) plus a term in the range of the generator L of the dynamics (fluctuation). In the present context, this would mean

$$j_{0,1}^p \sim -D^p(T)(p_1 - p_0) + LF^p, \quad j_{0,1}^e \sim -D^e(T)(e_1 - e_0) - p(D^p(T) - D^e(T))(p_1 - p_0) + LF^e \quad (20)$$

where the approximation symbol means that there exist sequences of local functions F^p, F^e in the domain of the generator L such that the space–time variance of the difference, calculated for the dynamics in the equilibrium with average momentum p and temperature T , vanishes. Such fluctuation–dissipation decompositions allow us to substitute, locally, currents with gradients and eventually close the equations after the hydrodynamic limit. In [7] Varadhan used first this approach to prove the hydrodynamic limit for a non-gradient reversible stochastic Ginzburg–Landau dynamics (one conserved quantity). Reversibility here is intended for a dynamics that has a self-adjoint generator with respect to the stationary Gibbs measures. Then Quastel, in his PhD thesis [9], proved by this technique the diffusion of colors in the symmetric simple exclusion process (still reversible but with two conserved quantities). There have been many other results extending this method to non-reversible dynamics. In the context of a chain of anharmonic oscillators with a stochastic perturbation conserving only the energy, the fluctuation–dissipation decomposition has been proved in [10]. One of the limitations of this non-gradient approach is that it requires that the generator of the dynamics L has a very ‘large’ symmetric part S , whose finite-dimensional version has a spectral gap uniformly bounded with respect to the dimension; furthermore L should satisfy a spectral sector condition with respect to S . This requires to consider only stochastic perturbations that act on both positions and velocities (S locally elliptic).

3.3. Macroscopic diffusive equations for the harmonic chain with bulk noise

In the case when κ and D^e are constant independent of the temperature T , there are examples of dynamics where the hydrodynamic limit can be proven rigorously. This is the case of a chain of harmonic oscillators whose Hamiltonian dynamics is perturbed by a random sign change of the interparticle distance. The dynamics is defined as in (1), but now $r_i \in \mathbb{R}$ and $V(r) = \frac{r^2}{2}$. Furthermore, any particle i has an independent Poisson process with intensity γ , when it rings r_i changes sign. Momentum and energy are conserved and it can be proven that the empirical distribution defined by (19) converges to the solution to (16), with explicit κ and D^e depending only on γ . Of course, these coefficients diverge for $\gamma \rightarrow 0$ as the deterministic harmonic chain does not have a diffusive behavior.

A rigorous mathematical proof of such hydrodynamic limit for a different dynamics of springs, with random perturbations that do not conserve momentum but conserve r_i can be found in [11,12]. In [12] is considered a harmonic chain, but with a random flip of the velocities sign. In this case, the two conserved quantities are the volume stretch r_i (with currents $J_{i,i+1}^r = -p_i$) and the energy. In [12], it is proven that the empirical distributions

$$\hat{r}_\epsilon(t, x) = \epsilon \sum_i r_i(\epsilon^{-2}t)\delta_{\epsilon i}(x), \quad \hat{T}_\epsilon(t, x) = \epsilon \sum_i \frac{1}{2}p_i^2(\epsilon^{-2}t)\delta_{\epsilon i}(x) \tag{21}$$

converge to the solution $r(t, x), T(t, x)$ to

$$\begin{aligned} \partial_t r &= \frac{1}{2\gamma} \partial_x^2 r \\ \partial_t T &= \frac{1}{2\gamma} (\partial_x r)^2 + \frac{1}{4\gamma} \partial_x^2 T \end{aligned} \tag{22}$$

that have the same structure as (17). Similar results with a different stochastic perturbation are contained in [11]. In these models, where the transport coefficients are constant, the fluctuation–dissipation relations (20) are exact for explicit local functions F . Still, the equations (22) are non linear and the proof in [12] demands the application of Wigner distributions techniques in order to control the separate evolution of the thermal and mechanical energy.

For the anharmonic chain with velocity flip, the corresponding macroscopic equations are given by [13,14]

$$\begin{aligned} \partial_t r &= \frac{1}{2\gamma} \partial_x^2 \tau(r, T) \\ c_v(r, T) \partial_t T &= \partial_x (\kappa(r, T) \partial_x T) + \frac{1}{2\gamma} (\partial_x \tau(r, T))^2 \end{aligned} \tag{23}$$

where $\tau(r, T)$ is the thermodynamic tension at temperature T and volume r , $c_v(r, T)$ being the corresponding heat capacity. The thermal conductivity $\kappa(r, T)$ may depend on r in a non-explicit way, as we do not have the same symmetries as in the rotor model. Notice that in this case, thanks to the noise in the dynamics, the current of the volume strain is $J_{0,1}^r = -p_1$ and it has an explicit fluctuation–dissipation decomposition of the type (20):

$$J_{0,1}^r = -p_1 = \frac{1}{2\gamma} Lp_1 - \frac{1}{2\gamma} (V'(r_1) - V'(r_0)) \tag{24}$$

that explains the first of the equations (23).

3.4. Dynamics with three conserved quantities

There are dynamics with three conserved quantities that evolve macroscopically in the diffusive space–time scaling. In [15], we study a harmonic chain where the potential energy does not depend on the volume strain or the tension of the system, but on its bending or *curvature*. This implies that we add springs between next nearest neighbor particles with negative potential, such that the total potential energy is given by

$$\frac{1}{2} \sum_i (q_{i+1} - q_{i-1} - 2q_i)^2 \tag{25}$$

To the Hamiltonian dynamics, we add a random exchange, with intensity γ , of velocities between nearest neighbor particles. It results that there are three conserved quantities:

$$k_i = q_{i+1} - q_{i-1} - 2q_i, \quad p_i, \quad e_i = \frac{p_i^2}{2} + \frac{k_i^2}{2} \tag{26}$$

We call k_i the *curvature or bending*. In [15], we prove that the corresponding empirical distributions converge to $k(t, x)$, $p(t, x)$, $e(t, x)$ solutions to the diffusive system

$$\begin{aligned} \partial_t k &= -\partial_x^2 p \\ \partial_t p &= \partial_x^2 k + \gamma \partial_x^2 p \\ \partial_t T &= \frac{1}{\gamma} \partial_x^2 T + \gamma (\partial_x p)^2 \end{aligned} \tag{27}$$

where the temperature profile is defined as $T(t, x) = e(t, x) - \frac{p^2(t, x)}{2}$. We can see this as a diffusive perturbation of Bernoulli’s beam wave equation $\partial_t^2 k = -\partial_x^4 k$. Notice the similar structure as in equations (17) and (22), with a *heating* term $\gamma (\partial_x p)^2$.

It is an open question if similar macroscopic equations will hold for a non-linear dynamics with potential $V(k_i)$, without any stochastic term. Numerical dynamical simulations have been inconclusive about this possible diffusive behavior.

4. Non-equilibrium stationary states

4.1. Stationary temperature profiles and up-hill diffusion in rotor model

In this section we review some results concerning the non-equilibrium stationary states for the rotors model contained in [16], more details can be found there. Let us consider the finite dynamics on $N + 1$ -rotors as in (1), where we add boundary forces or heath baths such that gradients are imposed on the conserved quantities in the corresponding stationary state. In order to establish a gradient in the temperature profile, we apply at the boundaries two Langevin heat baths at different temperatures T_L, T_R , while constant forces τ_L, τ_R act respectively on the first rotor on the LHS and last rotor on the RHS. The equations of motion read as:

$$\begin{aligned} \dot{r}_i(t) &= p_i(t) - p_{i-1}(t), \quad 1, \dots, N \\ \dot{p}_i(t) &= V'(r_{i+1}(t)) - V'(r_i(t)), \quad i = 2, \dots, N - 1 \\ dp_0(t) &= (\tau_L + V'(r_1(t)) - \gamma p_0(t)) dt + \sqrt{2\gamma T_L} dw_L(t) \\ dp_N(t) &= (\tau_R - V'(r_N(t)) - \gamma p_N(t)) dt + \sqrt{2\gamma T_R} dw_R(t) \end{aligned} \tag{28}$$

where $w_L(t), w_R(t)$ are two independent Wiener processes.

We expect here that an hydrodynamic limit holds for the empirical profile distribution (20) scaling with $\epsilon = N^{-1}$, with the equation (17) in $x \in [0, 1]$ provided with the boundary conditions

$$p(t, 0) = \frac{\tau_L}{\gamma}, \quad T(t, 0) = T_L, \quad p(t, 1) = \frac{\tau_R}{\gamma}, \quad T(t, 1) = T_R.$$

As $t \rightarrow \infty$, the system, at fixed size N , should approach a stationary state μ_{ss}^N depending in principle on T_L, T_R, τ_L, τ_R and γ . This probability distribution is called non-equilibrium stationary state (NESS) and only in the case $T_L = T_R = \beta^{-1}$ and $\tau_L = \tau_R = \tau$ it coincides with the equilibrium measure $\nu_{\beta, p}$ with $p = \gamma^{-1}\tau$.

From the mathematical side, the study of the NESS and its asymptotic properties as $N \rightarrow \infty$ is harder than the non-stationary behavior. This is because in the NESS the time scales are hidden. For the rotors model, even the existence of the NESS is an open problem, and only recently there have been some progress for $N = 2$ and 3 [17,18].

Assuming the existence of the NESS, by stationarity the expectation of the currents of the conserved quantities have to be homogeneous along the chain, i.e. denoting with $\langle \cdot \rangle_{ss}$ the expectation with respect to μ_{ss}^N , we have

$$J_N^p := \langle j_{i,i+1}^p \rangle_{ss}, \quad J_N^e := \langle j_{i,i+1}^e \rangle_{ss}, \quad i = 1, \dots, N - 1 \tag{29}$$

are constant in i . Taking into account also the boundary currents, we have

$$\begin{aligned} J_N^p &= -\tau_R + \gamma \langle p_N \rangle_{ss} = \tau_L - \gamma \langle p_0 \rangle_{ss} \\ J_N^e &= \gamma \left(T_L - \langle p_0^2 \rangle_{ss} \right) - \tau_L \langle p_0 \rangle_{ss} = \gamma \left(\langle p_N^2 \rangle_{ss} - T_R \right) + \tau_R \langle p_N \rangle_{ss} \end{aligned} \tag{30}$$

The diffusive behavior implies that $J_N^p, J_N^e \sim O\left(\frac{1}{N}\right)$, and we expect that

$$\begin{aligned} \lim_{N \rightarrow \infty} N J_N^p &= J^p = -D^p(T_{ss}(x)) \partial_x p_{ss}(x) \\ \lim_{N \rightarrow \infty} N J_N^e &= J^e = -D^p(T_{ss}(x)) \partial_x \left(\frac{p_{ss}(x)^2}{2} \right) - \kappa(T_{ss}(x)) \partial_x T_{ss}(x) \end{aligned} \tag{31}$$

where $p_{ss}(x), T_{ss}(x)$ are the stationary solutions to equations (14) with boundary conditions

$$p_{ss}(0) = \frac{\tau_L}{\gamma}, \quad T_{ss}(0) = T_L, \quad p_{ss}(1) = \frac{\tau_R}{\gamma}, \quad T_{ss}(1) = T_R$$

Notice that the energy current is the sum of the *heat current* $J^Q(x) = -\kappa(T_{ss}(x)) \partial_x T_{ss}(x)$, and the *mechanical energy current* $-D^p(T_{ss}) \partial_x \left(\frac{p_{ss}^2}{2} \right)$. They can be of opposite signs, giving rise to the phenomenon of *uphill diffusion* (J^e of the same sign as the gradient of temperature, cf. [19]).

Some other relations can be obtained from (31). By multiplying the first equation by $p_{ss}(x)$ and subtracting the second, we have

$$p_{ss}(x) J^p - J^e = \kappa(T_{ss}(x)) \partial_x T_{ss}(x) = -J^Q(x) \tag{32}$$

while the second derivative of $T_{ss}(x)$ must satisfy

$$J^p \partial_x p_{ss}(x) = \kappa(T_{ss}(x)) \partial_{xx} T_{ss}(x) + \kappa'(T_{ss}(x)) (\partial_x T_{ss}(x))^2 \tag{33}$$

Equations (31) predict a maximum for the temperature profile $T_{ss}(x)$ inside the interval $(0, 1)$ higher than the boundary temperatures T_L, T_R . In fact, without losing generality, assume $\tau_R = \tau > 0$ and $\tau_L = 0$, then $p_{ss}(x) \geq 0, J^p < 0$ and $p_{ss}(x)$ is strictly increasing from $p_{ss}(0) = 0$ to $p_{ss}(1) = \tau/\gamma$. Consequently, from (32), we can have only one stationary point for T_{ss} , and by (33) it must be a maximum, which we denote by x_{\max} , that must satisfy $p_{ss}(x_{\max}) J^p = J^e$. This implies that J^p and J^e are of the same sign and, if $J^e \neq 0$, the strict increase property of p_{ss} implies that x_{\max} must be inside the interval $(0, 1)$. Since there are no other stationary points, the maximal temperature $T_{ss}(x_{\max})$ must be higher than the temperatures at the boundaries.

From (33), a flex point x_{flex} of $T_{ss}(x)$ must satisfy the relation

$$-D^p(T_{ss}(x_{\text{flex}})) (\partial_x p_{ss}(x_{\text{flex}}))^2 = J^p \partial_x p_{ss}(x_{\text{flex}}) = \kappa'(T_{ss}(x_{\text{flex}})) (\partial_x T_{ss}(x_{\text{flex}}))^2$$

It follows that such flex points can exist only around values where $\kappa(T)$ is a strictly decreasing function of T .

Another qualitative property of the solution can be seen from the first equation of (31), i.e. we have that $\partial_x p_{ss}(x) = \frac{-J^p}{D^p(T_{ss}(x))}$. There is a numerical evidence that $D^p(T)$ is a decreasing function of T , so we have that $\partial_x p_{ss}(x)$ is proportional to $T_{ss}(x)^\alpha$ for some α . It follows that

$$\partial_x^2 p_{ss}(x) = \frac{J^p (D^p)'(T_{ss}(x))}{D^p(T_{ss}(x))^2} \partial_x T_{ss}(x) \tag{34}$$

that implies a flex point for $p_{ss}(x)$ at the point of maximum temperature.

The energy current J^e can present a negative linear response with respect to $T_R - T_L$, due to the decrease of $D^p(T)$ as a function of the temperature. In fact, in the case $\tau_R > 0, \tau_L = 0$ and $T_R \geq T_L$, we have that $\partial_x \left(\frac{p_{ss}^2(x)}{2} \right) > 0$, increasing T_R will increase the whole profile $T_{ss}(x)$. This may create a positive increase to $-D^p(T_{ss}(x)) \partial_x \left(\frac{p_{ss}^2(x)}{2} \right)$ larger than the negative increase of $J^Q = -\kappa(T_{ss}(x)) \partial_x T_{ss}(x)$.

From the stationary equation, we can compute the entropy production of the stationary state, that we can define as

$$\Sigma = \left(T_R^{-1} - T_L^{-1} \right) J^e - \gamma^{-1} \left(T_R^{-1} \tau_R - T_L^{-1} \tau_L \right) J^p \tag{35}$$

It turns out that $\Sigma > 0$ and that it is equal to

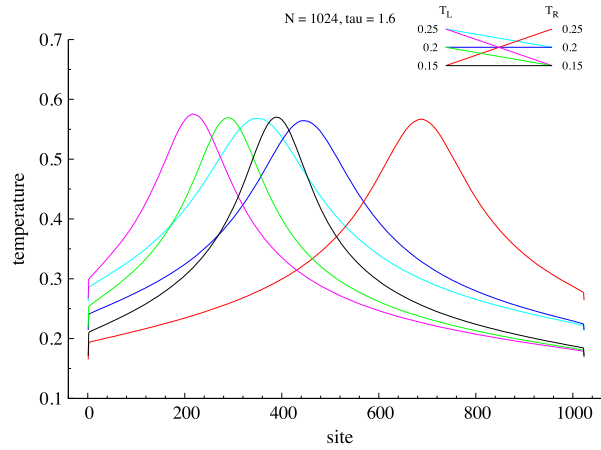


Fig. 1. Stationary temperature profiles in rotors dynamics, with $\tau_R = \tau$, $\tau_L = 0$ and different values of temperatures for the Langevin heat bath. Reprinted from [20].

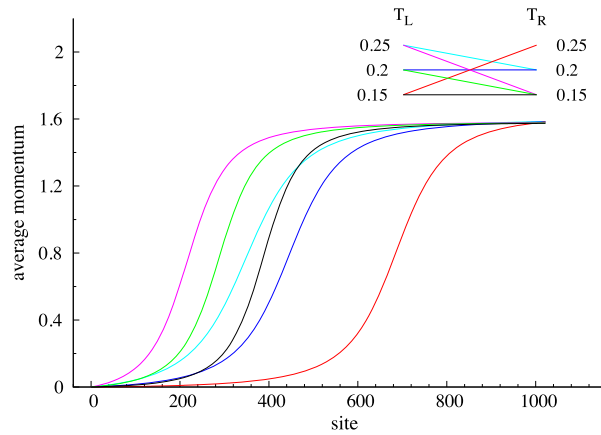


Fig. 2. Stationary momentum profiles in rotors dynamics, with $\tau_R = \tau$, $\tau_L = 0$ and different values of temperatures for the Langevin heat bath. Reprinted from [20].

$$\Sigma = \int_{-1}^1 \left[\frac{\kappa(T_{ss}(x))}{T_{ss}^2(x)} (\partial_x T_{ss}(x))^2 + \frac{D^p(T_{ss}(x))}{T_{ss}(x)} (\partial_x p_{ss}(x))^2 \right] dx \quad (36)$$

Notice that this expression coincide with the time derivative of Clausius's entropy S given in (18).

Dynamical simulations of the rotors chain in the stationary state under an exterior torque τ were first performed in [20]. The resulting stationary profiles of $T_{ss}(\cdot)$ and $p_{ss}(\cdot)$ are reported in Figs. 1 and 2, respectively, for different choices of boundary temperatures, and $\tau_L = 0$ and $\tau_R = \tau$.

The profiles of temperatures in Fig. 1 present a maximum inside the interval with temperatures much higher than at the boundaries. Two flex points are present, which get closer as the temperature at the border decreases.

In Fig. 2 are displayed the corresponding profiles of $p_{ss}(x)$. The maximum of the temperature corresponds to the flex point of p_{ss} , in agreement with (34). Fig. 3 shows the energy current J^e as function of $\tau_R = \tau$ (with $\tau_L = 0$) for different sizes of the system N . In black is the case of same temperature, while in red the curve when T_R is risen. Notice in Fig. 3 that for τ large enough the curves cross, which implies a negative response to the temperature gradient. This is in agreement with the remark made above, as consequence of the decrease of $D^p(T)$ with T .

The plots in Figs. 1, 2, and 3 are obtained by direct dynamical simulations of the NESS. In [16], we attempt to solve numerically equations (31) after having estimated $D^p(T)$ and $\kappa(T)$ with dynamical simulations of the system in equilibrium. Agreement of the corresponding plots will confirm the correctness of the heuristic coming from the linear response theory.

For a general review about up-hill diffusion, see [19]. This phenomenon can also appear in models with phase transitions, even if there is only one conserved quantity [21].

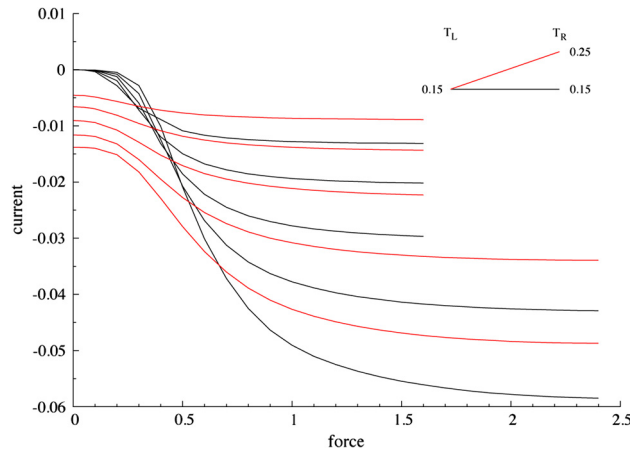


Fig. 3. Energy current J^e as function of $\tau_R = \tau$, for $\tau_L = 0$. Reprinted from [20].

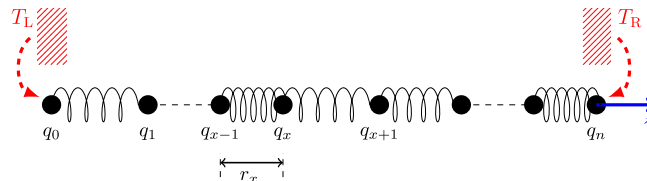


Fig. 4. Chain of harmonic oscillators with random flip of velocities sign, heat bath, and tension applied on the right-hand side. Reprinted from [22].

4.2. Stationary states for harmonic chains with random dynamics

Mathematical rigorous results can be obtained for the NESS of the harmonic oscillators dynamics with random flip of velocities, such that kinetic energy is conserved. The conserved quantities are the volume and the total energy, and the non-stationary evolution is governed in the diffusive scaling by (22). In [22], we study this dynamics when the system has N harmonic oscillators connecting $N + 1$ particles, with Langevin heat baths attached to the first left particle and the last right particle, and a constant force τ is attached to the last right particle (see Fig. 4). The system is driven out of equilibrium by the presence of the external force τ , and the stochastic part of the dynamics has only equilibrium states with 0 average velocities. Thanks to the stochastic dynamics in the bulk, the NESS exists. For $\tau = 0$ this NESS was studied in [31].

In [22], we prove the hydrodynamic limit in the NESS, and the stationary profiles of volume stretch $r_{ss}(x)$ and temperature $T_{ss}(x)$ satisfy the equations

$$\partial_x^2 r_{ss}(x) = 0, \quad \partial_x^2 T_{ss}(x) = -2(\partial_x r_{ss}(x))^2, \quad r_{ss}(0) = 0, \quad T_{ss}(0) = T_L, \quad r_{ss}(1) = \tau, \quad T_{ss}(1) = T_R \tag{37}$$

These can be explicitly solved obtaining $r_{ss}(x) = \tau x$ and

$$T_{ss}(x) = \tau^2 x(1 - x) + (T_R - T_L)x + T_L, \quad x \in [0, 1]$$

that shows again an heating phenomena at the center of the system. The stationary energy current can also be calculated and gives

$$J^e = -\frac{1}{4\gamma} (T_R - T_L) - \frac{\tau^2}{2\gamma} \tag{38}$$

So if uphill diffusion is possible, no negative response to temperature gradient can happen in this system, as these were due to the non-linearities in the temperature of the diffusivities in the rotor chain. Also there are no flex points in these profiles of temperature, as also these were due to the temperature dependence of thermal conductivity.

5. The two-step approach: weak coupling limits, kinetic limits, and hydrodynamic limits

As we mentioned in Section 3, one of the major difficulties in order to obtain the diffusive equations in the hydrodynamic limit is that it involves a simultaneous scaling of space and time. One way to simplify the problem is to introduce a small parameter in the dynamics that makes the interaction weak (*weak coupling*) or the collisions rarefied (*kinetic limit*), in order to break the procedure in two steps:

- a weak coupling or kinetic limit where it is obtained an autonomous *mesoscopic* stochastic dynamics,
- a subsequent hydrodynamic limit for these stochastic dynamics.

5.1. Weak coupling limit

In the case of dynamics that conserve macroscopically only energy, some progress have been obtained in the past years in the weak coupling limit, even though the full program is not yet complete.

Consider the generic Hamiltonian dynamics

$$\dot{q}_i(t) = p_i(t), \quad \dot{p}_i(t) = \delta V'(q_{i+1}(t) - q_i(t)) - \delta V'(q_i(t) - q_{i-1}(t)) + U'(q_i(t)) \tag{39}$$

where $\delta > 0$ is a small parameter, $q_i \in M$ where M is some d -dimensional manifold, and U is a potential defined on M . With $q_{i+1} - q_i$ is intended some distance defined on M . When $\delta = 0$, there will be no interaction between the particles and no exchange of energy. When $\delta > 0$, there will be an instantaneous energy current between the particles given by

$$\delta j_{i,i+1}^e(t) = -\delta p_i(t) \cdot V'(q_{i+1}(t) - q_i(t)) \tag{40}$$

Notice that in any equilibrium the average of j^e is null. In order to see a energy diffusion in the limit as $\delta \rightarrow 0$, we have to look at a time scale $\delta^{-2}t$. In fact,

$$e_i(\delta^{-2}t) = \delta \int_0^{\delta^{-2}t} (j_{i-1,i}^e(s) - j_{i,i+1}^e(s)) ds \tag{41}$$

Let us assume that a central limit theorem is valid for the uncoupled dynamics ($\delta = 0$), and *somehow stable* for small $\delta > 0$. The first step consists in proving that $e_i(\delta^{-2}t)$ converges in law to an autonomous stochastic dynamics of energies:

$$e_i(\delta^{-2}t) \xrightarrow[\delta \rightarrow 0]{} \mathcal{E}_i(t) \tag{42}$$

where the $\mathcal{E}_i(t)$ satisfy the stochastic differential equations

$$\begin{aligned} d\mathcal{E}_i(t) &= dJ_{i-1,i}(t) - dJ_{i,i+1}(t) \\ dJ_{i,i+1}(t) &= \alpha(\mathcal{E}_i(t), \mathcal{E}_{i+1}(t)) dt + \sqrt{2}\sigma^2(\mathcal{E}_i(t), \mathcal{E}_{i+1}(t)) dB_i(t) \end{aligned} \tag{43}$$

where $B_i(t)$ are independent standard Wiener processes, and σ^2 are the variances of the energy currents $j_{i,i+1}^e(t)$ in the CLT of the uncoupled dynamics:

$$\sigma^2(\mathcal{E}_1, \mathcal{E}_2) = \int_0^\infty \langle j_{1,2}^e(t) j_{1,2}^e(0) \rangle_{\mathcal{E}_1, \mathcal{E}_2} dt \tag{44}$$

Here $\langle \cdot \rangle_{\mathcal{E}_1, \mathcal{E}_2}$ denotes the expectation with respect to the uncoupled dynamics of two particles in the microcanonical equilibrium at fixed energies \mathcal{E}_1 and \mathcal{E}_2 . The functions $\alpha(\mathcal{E}_1, \mathcal{E}_2)$ are antisymmetric and are defined by

$$\alpha(\mathcal{E}_1, \mathcal{E}_2) = (\partial_{\mathcal{E}_1} - \partial_{\mathcal{E}_2}) \sigma^2(\mathcal{E}_1, \mathcal{E}_2) + \sigma^2(\mathcal{E}_1, \mathcal{E}_2) \left(\frac{Z'(\mathcal{E}_1)}{Z(\mathcal{E}_1)} - \frac{Z'(\mathcal{E}_2)}{Z(\mathcal{E}_2)} \right) \tag{45}$$

where $Z(\mathcal{E})$ is the volume on the microcanonical manifold of energy \mathcal{E} of the single uncoupled particle. The equations (44) define a stochastic dynamics reversible with respect to the stationary measures:

$$d\tilde{\nu}_\beta = \prod_i \frac{Z(\mathcal{E}_i) e^{-\beta \mathcal{E}_i}}{\tilde{Z}_\beta} d\mathcal{E}_i, \quad \beta > 0. \tag{46}$$

A proof of this first step, i.e. the limit (42), would require that the uncoupled dynamics be *chaotic* enough for the CLT theorem to be valid and *stable* for small perturbations.

In [23], this is proven for particles moving (deterministically) as geodesic flow in a manifold M with strictly negative curvature, with dynamical system techniques. For anharmonic oscillators with a stochastic noise acting on the velocities and conserving energy, the first step has been proven in [24], using hypocoercive estimates. One particular case of [24] is the harmonic case (V and U quadratic), where $\sigma^2(\mathcal{E}_1, \mathcal{E}_2) = \gamma^{-2} \mathcal{E}_1 \mathcal{E}_2$, and $\alpha(\mathcal{E}_1, \mathcal{E}_2) = \gamma^{-2} (\mathcal{E}_1 - \mathcal{E}_2)$, where γ is the intensity of the noise in the dynamics.

The second step consists in obtaining the hydrodynamic limit for the energy evolution of the stochastic dynamics given by (43), i.e. the convergence of the empirical distributions

$$\epsilon \sum_i \delta_{\epsilon i}(\mathbf{d}\mathbf{x}) \mathcal{E}_i(\epsilon^{-2}t) \xrightarrow{\epsilon \rightarrow 0} \mathcal{E}(t, \mathbf{x}) \, \mathbf{d}\mathbf{x} \tag{47}$$

where

$$\partial_t \mathcal{E} = \partial_x \left(\tilde{D}(\mathcal{E}) \partial_x \mathcal{E} \right) \tag{48}$$

with the energy diffusivity of the stochastic dynamics given by $\tilde{D} = \tilde{C}_v^{-1} \tilde{\kappa}$, where \tilde{C}_v is the variance of the energies \mathcal{E}_i under $d\tilde{\nu}_\beta$ and the conductivity $\tilde{\kappa}$ is given by the corresponding Green–Kubo formula

$$\tilde{\kappa}(\beta^{-1}) = \beta^2 \sum_i \int_0^\infty \langle \alpha(\mathcal{E}_i(t), \mathcal{E}_{i+1}(t)), \alpha(\mathcal{E}_0(0), \mathcal{E}_1(0)) \rangle_\beta \, dt \tag{49}$$

The relation between $\tilde{\kappa}(T)$ and the thermal conductivity of the original dynamics with $\delta > 0$, i.e. $\kappa_\delta(T)$ defined as in (15), is studied in [25], and it turns out that

$$\kappa_\delta(T) = \tilde{\kappa}(T)\delta + o(\delta) \tag{50}$$

The reversible stochastic dynamics (43) is a version of the conservative Ginzburg–Landau dynamics considered by Varadhan in [7]. With respect to [7], this dynamics is restricted on $\mathbb{R}_+^{\mathbb{Z}}$, and we call the *energy Ginzburg–Landau dynamics*. In order to apply the method of [7], we need a lower bound on the spectral gap for the generator on the corresponding finite dimensional dynamics, i.e. it should be bounded below by CN^{-2} , where N is the dimension of the system, for some constant C that may depend on the energy but not on the dimension. When this spectral gap bound can be proven, the second step can be performed [26]. This is the case for the (43) arising from the weak coupling limit in the anharmonic chain with noise (cf. [24]) with some conditions on the pinning potential U . In fact, if $\text{Hess } U(0) > 0$, it follows that $\sigma^2(\mathcal{E}_1, \mathcal{E}_2) = \mathcal{E}_1 \mathcal{E}_2 G(\mathcal{E}_1, \mathcal{E}_2)$, with $G \geq c > 0$. This implies that the generator of (43) has a spectral gap bound (this can be proven following the argument in [10]). For the energy Ginzburg–Landau dynamics emerging from the deterministic dynamics of the geodesic flows [23], we have that

$$\sigma^2(\mathcal{E}_1, \mathcal{E}_2) \sim \frac{\mathcal{E}_1 \mathcal{E}_2}{\mathcal{E}_1^{3/2} + \mathcal{E}_2^{3/2}} \tag{51}$$

Unfortunately, in the case of a behavior like (51), it is not clear whether a spectral gap bound will hold, it certainly depends on the energy. At this time step 2 remains an open problem when starting from a purely Hamiltonian deterministic dynamics.

5.2. Kinetic limit

A different two-step approach consists in studying models where energy is exchanged between particles through collisions that are rarefied because of constraints in the geometry of the system. Time is scaled in such a way that on a unit time there is, in average, a finite number of collisions per unit time. In this sense, the first step is similar to the Boltzmann–Grad limit.

A typical model considered in this approach (cf. [27] [28]) is given by a chain of Sinai’s billiards, where each particle is confined in one billiard, but it can collide with a particle in a neighbor billiard through a small window. The size δ of this window is the small parameter of the limit. The energy is the only conserved quantity, and it is exchanged through these collision. Because of the chaoticity of the billiard, after time rescaling as $\delta \rightarrow 0$, the differences in the collision times, conditioned on the energy of each billiard, become independent. Consequently, it is expected that the energies per particle $e_i(\delta^{-1}t)$ converge to a Markov jump process $\mathcal{E}_i(t)$ whose generator is given by

$$LF(\{\mathcal{E}_j\}) = \sum_i \int_0^1 d\alpha \Lambda(\mathcal{E}_i, \mathcal{E}_{i+1}, \alpha) [F(T_{i,i+1,\alpha}\{\mathcal{E}_j\}) - F(\{\mathcal{E}_j\})] \tag{52}$$

$$(T_{i,i+1,\alpha}\{\mathcal{E}_j\})_k = \alpha(\mathcal{E}_i + \mathcal{E}_{i+1})\delta_{(k=i)} + (1 - \alpha)(\mathcal{E}_i + \mathcal{E}_{i+1})\delta_{(k=i+1)} + \mathcal{E}_k\delta_{(k \neq i, i+1)}$$

This means that at random times, exponentially distributed with intensity $\Lambda(\mathcal{E}_i, \mathcal{E}_{i+1}, \alpha)$, the total energy of the sites i and $i + 1$ is redistributed in the two sites with proportions α and $1 - \alpha$. The precise form of the rate function Λ can be found in [28] and [29], but what matters is that $\Lambda(\mathcal{E}_i, \mathcal{E}_{i+1}, \alpha) \sim (\mathcal{E}_i + \mathcal{E}_{i+1})^{1/2}$.

Unlike the weak coupling limit, no rigorous results about this first step exist at the moment starting from the deterministic dynamics. Some partial attempts and a detailed discussion of the problem can be found in [30].

The second step will be the hydrodynamic limit on the stochastic dynamics generated by (52) in order to obtain the diffusive equation for energy. This is a *non-gradient* dynamics where in principle could be applied Varadhan’s approach [7].

With respect to the stochastic dynamics emerging in the weak coupling case from a purely mechanical model, there exists a proof of the spectral gap bound (cf. [29]), necessary in order to apply Varadhan's method. Still there are other intrinsic difficulties that do not allow yet to prove the hydrodynamic limit.

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