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ENERGY DIFFUSION AND SUPERDIFFUSION IN OSCILLATORS LATTICE NETWORKS

STEFANO OLLA

ABSTRACT. I review here some recent result on the thermal conductivity of chains of oscillators whose hamiltonian dynamics is perturbed by a noise conserving energy and momentum.

1. INTRODUCTION

Let us consider a 1-dimensional chain of oscillators indexed by $x \in \mathbb{Z}$, whose formal Hamiltonian is given by

$$\mathcal{H}(p, q) = \sum_x \left[\frac{p_x^2}{2} + V(q_{x+1} - q_x) + W(q_x) \right], \quad (1.1)$$

where q_x indicate the displacement of the atom x from its equilibrium position, and p_x its momentum (we fix for the moment all masses equal to 1). The potential V and W are some smooth positive function growing at infinity fast enough. The W potential is often called *pinning*.

We want to understand the *macroscopic* properties of energy transport for the corresponding hamiltonian dynamics

$$\dot{q}_x = p_x, \quad \dot{p}_x = -\partial_{q_x} \mathcal{H}. \quad (1.2)$$

When we say “macroscopic energy transport” we are meaning a certain non-equilibrium evolution that we want to observe in a space–time macroscopic scale that should be specified. This space–time scale can be typical of the model and the same model can have distinct macroscopic scalings under which it will behave very differently. For example in the case that $W = 0$ (unpinned system), total momentum is also conserved and hyperbolic scaling (in which space and time are scaled in the same way) is a natural one. In the hyperbolic scaling energy is carried around by the momentum of the particles and macroscopic evolution equation is given by the Euler equations.

Another important scaling is the diffusive scaling (time scaled as square of space) where transport of energy happens by diffusion. The macroscopic

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equation is usually given by heat equation. For example, when the pinning potential W is present, total momentum is not conserved and nothing moves in the hyperbolic scale. Energy will *move* on the diffusive space-time scale, and macroscopically its evolution should be governed by heat equation. More precisely, defining the empirical distribution of the energy

$$\tilde{\mathcal{E}}^\varepsilon(G, t) = \varepsilon \sum_x G(\varepsilon x) \mathcal{E}_x(\varepsilon^{-2}t) \quad (1.3)$$

where $\mathcal{E}_x = \frac{p_x^2}{2} + V(q_{x+1} - q_x) + W(q_x)$ is the energy of particle x , and G is a smooth test function on \mathbb{R} with compact support. We expect that

$$\lim_{\varepsilon \rightarrow 0} \tilde{\mathcal{E}}^\varepsilon(G, t) = \int G(y) u(y, t) dy \quad (1.4)$$

in *some statistical sense*, with $u(y, t)$ solution of the (non-linear) heat equation

$$\partial_t u = \partial_x (\kappa(u) \partial_x u) . \quad (1.5)$$

The function $\kappa(u)$ is called thermal conductivity and can be expressed in terms of the dynamics in equilibrium:

$$\kappa(u) = \lim_{t \rightarrow \infty} \frac{1}{2tT^2} \sum_x x^2 [\langle \mathcal{E}_x(t) \mathcal{E}(0) \rangle_T - u^2] \quad (1.6)$$

where the temperature $T = T(u)$ correspond thermodynamically to the average energy u , $\langle \cdot \rangle_T$ is the expectation of the dynamics in equilibrium at temperature T .

Proving (1.4)–(1.5) from an hamiltonian microscopic dynamics is one of the major challenge in non-equilibrium statistical mechanics [7]. It is not clear under which conditions on the interaction and initial conditions this result could be valid. Even the proof of the existence of the limit (1.6) defining the thermal conductivity is completely open for any deterministic system. What is clear is that (1.4)–(1.5) are not always valid. For example if V and W are quadratic (harmonic chains), then the energy corresponding to each Fourier mode is conserved and carried ballistically without any interaction with the other modes. It results that thermal conductivity is infinite in this case ([16], and for a macroscopic equation in the hyperbolic scaling see [8], as explained in section 4).

In nonlinear unpinned cases ($W = 0$) one expects, generically in dimension 1, that $\kappa = +\infty$, and correspondingly a superdiffusion of energy. This fact seems confirmed by all numerical simulation of molecular dynamics [11], even though there is not a general agreement about the order of this superdiffusivity. Most interesting would be to understand what kind of stochastic process would govern this superdiffusion.

Adding a stochastic perturbation to the hamiltonian dynamics certainly helps to obtain some mathematical result in these problems. Of course adding noise to the microscopic dynamics may change the macroscopic behavior. The ideal is to add noise terms that change as little as possible the

macroscopic behaviour, at least qualitatively. For example it is important that this noise conserves energy, and eventually momentum, since these are the quantities we expect being *conserved* in the infinite system.

2. CONSERVATIVE STOCHASTIC DYNAMICS

We consider the Hamiltonian dynamics weakly perturbed by a stochastic noise acting only on momenta and locally preserving momentum and kinetic energy. The generator of the dynamics is

$$L = A + \gamma S \quad (2.1)$$

with $\gamma > 0$, where A is the usual Hamiltonian vector field

$$A = \sum_{y \in \mathbb{Z}} \{p_x \partial_{q_x} - (\partial_{q_x} \mathcal{H}) \partial_{p_x}\}, \quad (2.2)$$

while S is the generator of the stochastic perturbation. The operator S acts only on the momenta $\{p_y\}$ and generates a diffusion on the surface of constant kinetic energy and constant momentum. S is defined as

$$S = \frac{1}{6} \sum_{z \in \mathbb{Z}} (Y_z)^2, \quad (2.3)$$

where

$$Y_z = (p_z - p_{z+1}) \partial_{p_{z-1}} + (p_{z+1} - p_{z-1}) \partial_{p_z} + (p_{z-1} - p_z) \partial_{p_{z+1}}$$

which is a vector field tangent to the surface of constant kinetic energy and of constant momentum for three neighbouring particles. As a consequence energy and momentum are locally conserved which, of course, implies also the conservation of total momentum and total energy of the system, i.e. formally

$$S \sum_{x \in \mathbb{Z}} p_x = 0, \quad S \mathcal{H} = 0.$$

Since also the hamiltonian dynamics conserves energy, we also have $L \mathcal{H} = 0$. Furthermore in the unpinned case ($W = 0$), $L \sum_x p_x = 0$.

The evolution of $\{p(t), q(t)\}$ is given by the following stochastic differential equations

$$\begin{aligned} dq_x &= p_x dt, \\ dp_x &= -\partial_x \mathcal{H} dt + \frac{\gamma}{6} \Delta (4p_x + p_{x-1} + p_{x+1}) dt \\ &\quad + \sqrt{\frac{\gamma}{3}} \sum_{k=-1,0,1} (Y_{x+k} p_x) dw_{x+k}(t). \end{aligned} \quad (2.4)$$

Here $\{w_y(t)\}_{y \in \mathbb{Z}}$ are independent standard Wiener processes and Δ is the discrete laplacian on \mathbb{Z} : $\Delta f(z) = f(z+1) + f(z-1) - 2f(z)$.

In the unpinned 1-dimensional case, the equilibrium measures are particularly simple. In fact the right coordinates are $r_x = q_{x+1} - q_x$, and the family of product measures

$$\mu_{\lambda,\pi,\beta}(dp, dr) = \prod_{x \in \mathbb{Z}} \frac{e^{-\beta(p_x - \pi)^2/2}}{\sqrt{2\pi}} \frac{e^{-\beta V(r_x) + \lambda r_x}}{Z(\lambda, \beta)} \quad (2.5)$$

are stationary for the dynamics. The three parameters λ, π, β correspond to the 3 conserved quantities of the dynamics (energy, momentum and $\sum_x r_x$, the *stretch* of the chain), while $Z(\lambda, \beta)$ is the normalization constant. It can be proven that these are the only translation invariant stationary measures of the dynamics ([13], we call this property “ergodicity of the infinite dynamics”). In more dimensions the unpinned case is much more complex and even the definition of these equilibrium measures are problematic (cf. [9]).

In the unpinned one-dimensional case, since momentum is conserved, there is a non trivial macroscopic evolution on the conserved quantities in the hyperbolic scaling (space and time scaled in the same way). Let us define the energy of particle x as

$$\mathcal{E}_x = \frac{p_x^2}{2} + \frac{1}{2} (V(r_{x-1}) + V(r_x))$$

Locally the conservation of energy can be written as

$$L\mathcal{E}_x = j_{x-1,x}^{\mathcal{E}} - j_{x,x+1}^{\mathcal{E}} \quad (2.6)$$

where the instantaneous current of energy $j_{x,x+1}^{\mathcal{E}}$ is the sum of the current due to the hamiltonian mechanism plus the current due to the stochastic term of the dynamics:

$$\begin{aligned} j_{x,x+1}^{\mathcal{E}} &= j_{x,x+1}^{\mathcal{E},a} + j_{x,x+1}^{\mathcal{E},s} \\ j_{x,x+1}^{\mathcal{E},a} &= -\frac{1}{2} (p_x + p_{x+1}) V'(r_x), \quad j_{x,x+1}^{\mathcal{E},s} = -\gamma \nabla \varphi_x \end{aligned} \quad (2.7)$$

with $\varphi_x = (p_{x+1}^2 + 4p_x^2 + p_{x-1}^2 + p_{x+1}p_{x-1} - 2p_{x+1}p_x - 2p_xp_{x-1})$. Similarly conservation of momentum reads as

$$\begin{aligned} Lp_x &= j_{x-1,x}^p - j_{x,x+1}^p \\ j_{x,x+1}^p &= V'(r_x) + \frac{\gamma}{6} \nabla (4p_x + p_{x-1} + p_x) \end{aligned} \quad (2.8)$$

while mass conservation is simply given by

$$Lr_x = p_{x+1} - p_x. \quad (2.9)$$

Let $G(y)$ a test function continuous with compact support. We expect that

$$\epsilon \sum_x G(\epsilon x) \begin{pmatrix} r_x(\epsilon^{-1}t) \\ p_x(\epsilon^{-1}t) \\ \mathcal{E}_x(\epsilon^{-1}t) \end{pmatrix} \xrightarrow[\epsilon \rightarrow 0]{\text{probability}} \int G(y) \begin{pmatrix} \mathbf{r}(t, y) \\ \mathbf{p}(t, y) \\ \mathbf{e}(t, y) \end{pmatrix} dy \quad (2.10)$$

where $\mathbf{r}(t, y)$, $\mathbf{p}(t, y)$, $\mathbf{e}(t, y)$ are given by the solution of the Euler hyperbolic system of equations

$$\begin{aligned}\partial_t \mathbf{r} &= \partial_y \mathbf{p} \\ \partial_t \mathbf{p} &= \partial_y P(\mathbf{r}, \mathbf{e} - \mathbf{p}^2/2) \\ \partial_t \mathbf{e} &= \partial_y (\mathbf{p}P(\mathbf{r}, \mathbf{e} - \mathbf{p}^2/2))\end{aligned}\tag{2.11}$$

Here $P(r, u)$ is the thermodynamic pressure, which is related to the thermodynamic entropy $S(r, u)$ by the relation

$$P(r, u) = -\frac{\partial_r S(r, u)}{\partial_u S(r, u)}\tag{2.12}$$

and S is defined from $Z(\lambda, \beta)$ with a Legendre transform:

$$S(r, u) = \sup_{\lambda, \beta} \left\{ \lambda r - \beta u - \log \left(Z(\lambda, \beta) \sqrt{\beta/2\pi} \right) \right\}\tag{2.13}$$

Pressure $P(r, u)$ is also give by the expectation of $V'(r_x)$ with respect to $\mu_{\lambda, \pi, \beta}$, for the corresponding values of the parameters λ and β .

The hydrodynamic limit (2.10) can be proven rigorously in the smooth regime of equation (2.11), by using the relative entropy method ([14], see also [1] and [13] for the application to this specific model). Note that (2.10) does not depend on the strength of the microscopic noise γ . Noise here is used only to prove some ergodic properties for the dynamics, necessary to obtain the result. In fact without noise this limit may not be true, as for example in the linear case (V quadratic, see below). Note also that for smooth solutions the macroscopic evolution (2.11) is locally isentropic, i.e.

$$\frac{d}{dt} S \left(\mathbf{r}(t, y), \mathbf{e}(t, y) - \frac{\mathbf{p}(t, y)^2}{2} \right) = 0\tag{2.14}$$

A challenging open problem is to extend this result to solutions that present shocks, where the above derivative is (presumably) strictly positive.

3. DIFFUSIVE EVOLUTION: GREEN-KUBO FORMULA

In the pinned model ($W > 0$) momentum is not conserved, energy is the only relevant conserved quantity for the infinite system and the equilibrium measure are the Gibbs measures at given temperature, corresponding to the hamiltonian \mathcal{H} . These probability measures are defined by the usual DLR equations. Consequently the hyperbolic scaling is trivial (nothing moves at that time scale). In order to see energy moving at a macroscopic scale, one has to look at larger time scale. The natural scaling is the diffusive one: we expect, for a given test function G as above,

$$\epsilon \sum_x G(\epsilon x) \mathcal{E}_x(\epsilon^{-2}t) \xrightarrow[\epsilon \rightarrow 0]{\text{probability}} \int G(y) \mathfrak{T}(t, y) dy\tag{3.1}$$

where $\mathfrak{T}(t, y)$ is the solution of the (non-linear) heat equation

$$\partial_t \mathfrak{T} = \partial_x (\kappa(\mathfrak{T}) \partial_x \mathfrak{T}),\tag{3.2}$$

where $\kappa(T)$ is the thermal conductivity at temperature T . This is given by the Green-Kubo formula

$$\kappa(T) = \frac{1}{2\chi(T)} \left[\int_0^\infty \sum_{x=-\infty}^{+\infty} \left\langle j_{x,x+1}^{\mathcal{E},a}(t) j_{0,1}^{\mathcal{E},a}(0) \right\rangle_T dt + \gamma T^2 \right] \quad (3.3)$$

where $\left\langle j_{x,x+1}^{\mathcal{E},a}(t) j_{0,1}^{\mathcal{E},a}(0) \right\rangle_T$ denote the expectation with respect to the dynamics in equilibrium at temperature $T = \beta^{-1}$. The explicit $\gamma T^2/2\chi(T)$ term is the contribution of the stochastic part of the dynamics. Formula (3.3) can be obtained from (1.6) using the conservation of energy (see [4] for a proof). We believe that such statement is always true for non-linear pinned dynamics, also in the deterministic case ($\gamma = 0$). But even for $\gamma > 0$, this is hard to prove and still an open problem. Even the convergence of the integrals defining (3.3) is not known if non-linearities are present (some bounds are proven in [4]). The only case with non-linear interaction in which (3.3) is proven convergent is when the noise is generated by Langevin heat bath attached at each particle of the system [6], a non conservative stochastic perturbation.

In unpinned systems the situation is more complex because of the momentum conservation. To avoid complicate re-centering along characteristics of (2.11), we can consider initial random configurations with momentum of (locally) zero average and constant density profile, only gradients of temperature admitted. Then conductivity κ is also a function of the density of particles and in formula (3.3) the expectation should be taken with respect to the equilibrium dynamics with $\pi = 0$ (i.e. starting with configurations distributed by $\mu_{\lambda,0,\beta}$ defined by (2.5)). Numerical evidence shows that in this one-dimensional case $\kappa = +\infty$ ([11], also for $\gamma > 0$, as long as momentum is conserved [2]). In the physics literature there is a long discussion about the nature and the *order* of this superdiffusion. From dimension 3 on, it is expected that formulas corresponding to (3.3) give a finite diffusivity.

Rigorous results can be proven for the harmonic case with $\gamma > 0$ [3, 4]. It turns out that κ is finite if system is pinned or in dimension $d \geq 3$, while the 1 and 2 dimensional unpinned cases are superdiffusive.

4. KINETIC LIMITS: PHONON BOLTZMANN EQUATION

The harmonic case is enough simple to obtain some non-equilibrium results. In [5] we consider the hyperbolic scaling in a weak noise limit. Noise is rescaled by multiplying its strength γ by ϵ . This way the effect of the noise per particle remains finite in the macroscopic scale (that motivates the term *kinetic* in defining this limit). This is in the same spirit as the model of hard sphere with random collision considered in [15]. The right quantity to look here is the Wigner distribution of the energy, formally defined as

$$W^\epsilon(y, k, t) = \frac{1}{2} \int_{-1/2}^{1/2} e^{i2\pi y\eta/\epsilon} \langle \psi(k - \eta/2, t/\epsilon)^* \psi(k + \eta/2, t/\epsilon) \rangle d\eta \quad (4.1)$$

where

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

here $\hat{q}(k, t), \hat{p}(k, t)$ are the Fourier transform of the $q_y(t), p_y(t)$, and $\omega(k)$ is the dispersion relation of the lattice, which in this one-dimensional nearest neighbour case is given by $\omega(k) = c|\sin(\pi k)|$ (*acoustic dispersion*). The result in [5] states that $W^\epsilon(y, k, t)$ converges, as a distribution on $\mathbb{R} \times [0, 1]$, to the solution of the linear transport equation

$$\partial_t W(y, k, t) + \frac{\omega'(k)}{2\pi} \partial_y W(y, k, t) = \gamma \int C(k, k') (W(y, k', t) - W(y, k, t)) dk. \quad (4.2)$$

In the deterministic case ($\gamma = 0$) this result was obtained by Dobrushin et al. in [8], see also [12]. The collision kernel $C(k, k')$ is positive and symmetric. It is computable explicitly (cf. [5]), but the important point is that $C(k, k') \sim k^2$ for small k . This is a consequence of the conservation of momentum: long waves scatter very rarely. Because $C(k, k')$ is positive, (4.2) has a simple probabilistic interpretation: W is the density at time t of the energy of particles (phonons) of mode k . A phonon of mode k moves with velocity $\omega'(k)$ and after an exponentially distributed random time of intensity $\gamma C(k, k')$ changes its mode to k' . Defining a Markov jump process $K(t)$ in $[0, 1]$ with jumping rate γC , the position of the phonons is given by $Y(t) = \int_0^t \omega'(K(s)) ds$.

Thermal conductivity can be computed from (4.2) (cf. [5]) and the results are in accord with the direct calculations done in [4].

5. LEVY'S SUPERDIFFUSION OF ENERGY

As we mention in the previous section, phonons of small k scatter rarely, but their velocity $\omega'(k)$, in the unpinned case, are still of order 1 as $k \rightarrow 0$. This induces a superdiffusive behavior of these phonons. In [10], as application of new limit theorems for functionals of Markov chains and processes, we prove that, for $\alpha = 3/2$,

$$\epsilon Y(\epsilon^{-\alpha} t) \xrightarrow[\text{law}]{} \mathcal{L}(t) \quad (5.1)$$

where $\mathcal{L}(t)$ is a Levy α -stable process, i.e. a stochastic process with independent stationary increments and with $\mathcal{L}(1)$ distributed by a α -stable law. In terms of the solution $W(y, k, t)$ of the equation (4.2) this result implies the convergence

$$\lim_{\epsilon \rightarrow 0} \int |W(\epsilon^{-\alpha} t, \epsilon^{-1} y, k) - \bar{u}(t, y)|^2 dk = 0 \quad (5.2)$$

where $\bar{u}(t, y)$ is the solution of the fractional heat equation

$$\partial_t \bar{u} = -c(-\Delta_y)^{\alpha/2} \bar{u}. \quad (5.3)$$

where c is a positive constant.

In the pinned case all the above result are still valid, but since the velocity of the phonons $\omega'(k) \sim k$ for small k , we have a regular diffusive behavior, and $\alpha = 2$.

It would be very interesting to understand how these results extends to the anharmonic cases. Equation (4.2) will be substituted by the non-linear phonon Boltzmann equation [17]. In the unpinned one-dimensional case this equation still will produce a superdiffusion. Is it again of Levy type, or will have some non-markovian terms?

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