Energy transport in Hamiltonian systems

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The problem

Derivation of macroscopic laws from microscopic models.

Lot of different instances, today I will concentrate on

energy transport starting from a classical Hamiltonian microscopic model.

In other words:

Is it possible to obtain the Fourier law (or the heat equation) starting from a microscopic Hamiltonian model ?

The problem

Several results are available when the microscopic dynamics has a random part, starting with [Olla-Varadhan-Yau 93], but very little exist in the purely determinist case.

A natural first step is to consider the case with no convection and consisting of weakly interacting systems.

A situation in which one can hope to use some kind of perturbative argument.

The problem

To try to mimic the well established stochastic results, it seems natural to assume that the individual systems have a complex (chaotic) motion.

Yet, before doing perturbations, one needs to understand the weak coupling limit (perturbing the identity does not make much sense).

The model

Consider a Hamiltonian $H(q,p)$ with compact energy levels and a graph or lattice (say $\mathbb{Z}^d$). At each site x of the lattice we have a system with coordinates $(q_x, p_x) \in \mathbb{R}^{2d_*}$. For each $\Lambda \subset \mathbb{Z}^d$ consider the system

$$\mathcal{H}^{\varepsilon}_{\Lambda}(\bar{q}, \bar{p}) = \sum_{x \in \Lambda} H(q_x, p_y) + \varepsilon \sum_{|x-y|=1} V(q_x, q_y)$$

We are interested in the macroscopic distribution of the $\mathbb{e}_x(t) = \frac{1}{2} p_x^2(t)$.

The model

To ensure good statistical properties we assume that H determines a Anosov contact flow on each energy level (e.g. geodesic flow on a compact manifold of strictly negative sectional curvature [triple linkage Hunt, MacKay, 2003]).

Use the coordinates $(q_x, v_x, \mathbb{e}_x)$, $v_x = |p_x|^{-1} p_x$, and consider random initial conditions of the following type

$$\mathbb{E}(f) = \int f(q, v, \bar{\mathbb{e}}) h(q, v) \, dq \, dv$$

for given $h \in \mathcal{C}^1$ and $\bar{\mathbb{e}}_x > 0$.

The current

$$\frac{d}{dt}\mathbb{e}_x = \varepsilon \sum_{|x-y|=1} \nabla V(q_x, q_y)(p_x + p_y) =: \sum_{|x-y|=1} \varepsilon j_{x,y}.$$

The microcanonical measure is symmetric in p, hence in equilibrium $\mathbb{E}_{\mathrm{eq},\mathbb{e}}(j_{x,y}) = 0$.

The effective exchange of energy is due to fluctuations

Hydrodynamics limit

Let $\Lambda_L := \{x \in \mathbb{Z}^d \;:\; |x| \le L\}$, then, for each $\varphi \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{R})$, consider

$$\frac{1}{L^d} \sum_{x \in \Lambda_L} \varphi(L^{-1}x) \mathbb{e}_x(L^2 t) = \frac{1}{L^d} \sum_{x \in \Lambda_L} \mathbb{e}_x(L^2 t) \delta_{L^{-1}x}(\varphi),$$

and assume that

$$\lim_{L \to \infty} \frac{1}{L^d} \sum_{x \in \Lambda_L} \bar{\mathbb{e}}_x \delta_{L^{-1}x}(\varphi) = \int_{\mathbb{R}^d} u_0(x) \varphi(x) dx.$$

The goal is to prove that, for almost all initial conditions,

$$\lim_{L \to \infty} \frac{1}{L^d} \sum_{x \in \Lambda_L} \mathbb{e}_x(L^2 t) \delta_{L^{-1}x}(\varphi) = \int_{\mathbb{R}^d} u(x,t) \varphi(x) dx$$

$$\partial_t u = \mathrm{div}(\kappa(u)\nabla u)$$
$$u(x,0) = u_0(x)$$

and the diffusivity κ is given by the Green-Kubo formula

$$\kappa(u) = \varepsilon^2 \int_0^\infty \sum_x \mathbb{E}_{\mathsf{eq},u}(j_{x,x+1}(t) j_{0,1}(0))dt.$$

We are VERY far from proving something like this.

Weak coupling limit

As a first step let us define, for L fixed, the variables $\mathcal{E}_{\varepsilon,x}(t) = \mathbb{e}_x(\varepsilon^{-2}t)$ and consider the limit $\varepsilon \to 0$.

The hope is that the limit is a process for the energy alone to which the ideas developed to study the Hydrodynamics limit for stochastic systems (starting with [Guo, Papanicolaou, Varadhan, 88] and [Varadhan, 93]) can be applied.

Theorem (Dolgopyat, L. (2011))**.** *For each* $d_* \geq 3$ *and* $T \in \mathbb{R}_+$ *the process* $\{\mathcal{E}_{\varepsilon,x}(t)\}_{t \leq T}$ *converges in law to a limit* $\{\mathcal{E}_x(t)\}_{t \leq T}$ *satisfying the mesoscopic SDE*

$$d\mathcal{E}_x = \sum_{|x-y|=1} \boldsymbol{b}(\mathcal{E}_x, \mathcal{E}_y)dt + \sum_{|x-y|=1} \boldsymbol{a}(\mathcal{E}_x, \mathcal{E}_y)dB_{x,y}$$

$$\mathcal{E}_x(0) = \bar{\mathbb{e}}_x$$

where $\boldsymbol{b}(\mathcal{E}_x, \mathcal{E}_y) = -\boldsymbol{b}(\mathcal{E}_y, \mathcal{E}_x)$, $\boldsymbol{a}(\mathcal{E}_x, \mathcal{E}_y) = \boldsymbol{a}(\mathcal{E}_y, \mathcal{E}_x)$ *and* $B_{x,y} = -B_{y,x}$ *are independent standard Brownian motions.*

The result includes the fact that the SDE is well posed (uniqueness of the Martingale problem) since zero is unreachable and

$\boldsymbol{b}, \boldsymbol{a}^2 \in \mathcal{C}^\infty((0,\infty)^2)$ and, for $\mathcal{E}_x \le \mathcal{E}_y$,

$$\boldsymbol{a}(\mathcal{E}_x, \mathcal{E}_y)^2 = \frac{A\mathcal{E}_x}{\sqrt{2\mathcal{E}_y}} + \mathcal{O}\left(\mathcal{E}_x^{\frac{3}{2}} \mathcal{E}_y^{-1}\right)$$

$$\boldsymbol{b}(\mathcal{E}_x, \mathcal{E}_y) = \frac{Ad}{2\sqrt{2\mathcal{E}_y}} + \mathcal{O}\left(\mathcal{E}_x^{\frac{1}{2}} \mathcal{E}_y^{-1}\right),$$

$d_* = 2$ should also work, but it is harder to prove.

The only invariant measures are absolutely continuous w.r.t. Leb. with density $h_\beta = \prod_{x\in\Lambda} \mathcal{E}_x^{\frac{d}{2}-1} e^{-\beta\mathcal{E}_x}$.

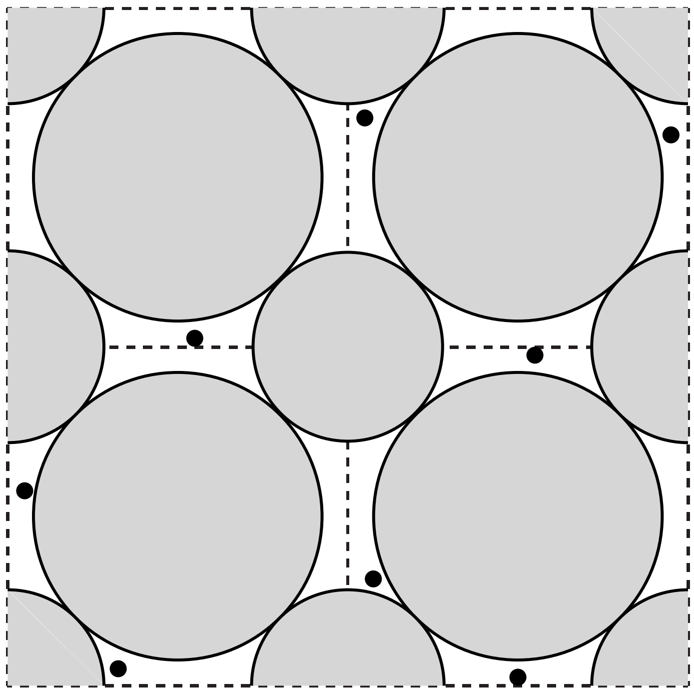
The SDE corresponds to a parabolic PDE with generator

$$\mathcal{L} = \frac{1}{2h_0} \sum_{|x-y|=1} (\partial_{\mathcal{E}_x} - \partial_{\mathcal{E}_y}) h_0 \boldsymbol{b}^2 (\partial_{\mathcal{E}_x} - \partial_{\mathcal{E}_y}).$$

The basic ingredient to take the hydrodynamic limit (or, at least, study the fluctuations in equilibrium) on the mesoscopic equation, is a spectral gap of size L^{-2} for the operator $\mathcal{L}$ acting on a region of volume L^d.

It has been obtained for similar models by [Sasada, 2015], but for our model there is a problem at high energies due to soft interactions.

Hard core interactions



Obstacles gray, particles black.

Introduced in [Bunimovich, L., Pellegrinotti, Suhov, 1992] and used to heuristically study energy transport by [Gaspard, Gilbert, 2008-9].

Summary

I have proposed a two step strategy. In one case (soft interations) one can complete the first step, but not yet the second. In the second case (hard core interactions) one can complete the second step, but not yet the first.

This is already sad, in addition one can have doubts about the strategy itself.

Green-Kubo

A (non trivial) formal computation [Bernardin, Huveneers, Lebowitz, L., Olla, 2015] shows that if κ is the diffusivity for the original model and κ_M the diffusivity for the mesoscopic equation, then

$$\kappa = \varepsilon^2 \kappa_M + \mathcal{O}(\varepsilon^3).$$

This gives some hope that the mesoscopic equation indeed describes the right behaviour of the system.

So, let us be bold, and ask:

can we say something for $\varepsilon > 0$?

Two basic questions:

- Can one establish the converge to the limit, for $\varepsilon \to 0$ for time scales longer than ε^{-2}?
- Can one establish the Green-Kubo formula ?

To answer is needed

- control on error terms in the limit theorem (Local central limit theorem with errors).
- control on the decay of correlations.

At the moment, I do not see how to address rigorously such questions in the Hamiltonian setting. So, to build up some understanding, it seems a good idea to start with a much much simpler model.

Simplifying to the point of being ridiculous:

- reduce the lattice from $\mathbb{Z}^d$ to a point
- reduce the fast variable from an Anosov flow to an expanding map of the circle
- reduce the space in which the conserved quantity lives from $\mathbb{R}_+$ to $\mathbb{T}^1$ (compact !)
- reduce the current to some artificial mechanism that changes the conserved quantity

Simplified model

Then, you get the dynamical systems $F_\varepsilon \in C^3(\mathbb{T}^2, \mathbb{T}^2)$

$$F(x, \theta) = (f(x, \theta), \theta + \varepsilon\omega(x, \theta))$$

with $\partial_x f \geq \lambda > 1$. We consider initial conditions $\theta_0 = \theta_*$ and x_0 to be a random variable so that

$$\mathbb{E}(\varphi(x_0, \theta_0)) = \int_{\mathbb{T}^1} \varphi(x, \theta_*)\rho(x)dx$$

with $\rho \in \mathcal{C}^\infty$.

Simplified model

Let $(x_n, \theta_n) = F^n(x, \theta)$, then $\omega(x_n, \theta_n) = \varepsilon^{-1}(\theta_{n+1} - \theta_n)$ plays the role of the current. It is known that, for each $\theta \in \mathbb{T}$, $f(\cdot, \theta)$ has a unique a.c.i.m. μ_θ.

We should then ask

$$\bar{\omega}(\theta) = \mu_\theta(\omega(\cdot, \theta)) = 0.$$

Too hard!

Suppose instead that $\bar{\omega}$ has only two non degenerate zeroes.

Define $\Theta_\varepsilon(t) = \theta_{\lceil t\varepsilon^{-1} \rceil}$.

Averaging ([Anosov, '60], [Bogolyubov-Mitropolskii, '61])

$\lim_{\varepsilon \to 0} \Theta_\varepsilon(t) = \Theta(t)$, where

$$\dot{\Theta} = \bar{\omega}(\Theta)$$
$$\Theta(0) = \theta_*.$$

Fluctuations around average (CLT) ([Dolgopyat, 2004])

Let $\xi_\varepsilon(t) = \varepsilon^{-\frac{1}{2}}(\Theta_\varepsilon(t) - \Theta(t))$, then, for $t \in [0, T]$, ξ_ε converges in law to a random variable satisfying

$$d\xi = b(\Theta(t))dt + a(\Theta(t))dW$$
$$\xi(0) = 0.$$

Non-linear SDE

$\Theta_\varepsilon \sim \overline{\Theta} + \sqrt{\varepsilon}\zeta$ but $\overline{\Theta} + \sqrt{\varepsilon}\zeta \sim \eta_\varepsilon$ where

$$d\eta_\varepsilon = \bar{\omega}(\eta_\varepsilon)dt + \sqrt{\varepsilon}\sigma(\eta_\varepsilon)dB$$
$$\eta_\varepsilon(0) = \theta.$$

Such SDE were introduced by [Hasselmann, 1976] and extensively studied by Wentzell–Freidlin and Kifer in the 70's-80's.

Local CLT with error

Theorem (De Simoi, L., preprint 2015; De Simoi-L.-Poquet-Volk, 2016). *For all* $\beta \in (0, 1/2)$ *there exists* $C, \varepsilon_0 > 0$ *and a coupling* $\mathbb{P}_c$ *such that, for all* $\varepsilon < \varepsilon_0$ *and* $t \in [\varepsilon \ln \varepsilon^{-1}, \varepsilon^{-\beta}]$*, we have*

$$\mathbb{P}_c(|\Theta_\varepsilon(t) - \eta_\varepsilon(t)| \geq C\varepsilon)| \leq C\varepsilon^\beta.$$

Hence, if we do measurements up to the scale ε the stochastic and deterministic process are close with high probability for a time of order $o(\varepsilon^{-1/2})$.

Decay of correlations

Theorem (De Simoi, L.). *If the central Lyapunov exponent is negative, then there exists* $\varepsilon_0 > 0$ *such that, for all* $\varepsilon \in (0, \varepsilon_0)$*, the system has a unique* physical measure μ. *Moreover, for each* $f, g \in C^1(\mathbb{T}^2, \mathbb{R})$

$$|\mu(f \circ F_\varepsilon^n \cdot g) - \mu(f)\mu(g)| \leq C_\# e^{-C_\# \frac{\varepsilon}{\ln \varepsilon^{-1}} n}.$$

The last results are far form proving that it is possible to study the original Hamiltonian system with $\varepsilon > 0$.

However, I believe they can be considered as a proof of concept that the proposed strategy is not totally crazy.