Some models related to the derivation of the Fourier Law

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Corinaldo, 4 June 2010

Here is an heuristic “derivation” of the heat equation:
Imagine that the heat (temperature) u is a fluid, then it must satisfy

$$\partial_t u = \mathrm{div} j$$

where j is the current.
Now assume (Fourier Law, 1822) $j = k\nabla u$, then

$$\partial_t u = \mathrm{div}(k\nabla u)$$

Does this makes any sense?

Not really: Statistical Mechanics states that heat is the average local Kinetic energy per particle in a body.

Thus, to obtain a rigorous (classical) derivation of the heat equation one should write the equations of motion for the N particles of a body, solve them and show that (in some precise technical sense) the local energy density satisfies the heat equation,

$$\text{with } N \sim 10^{24} \text{ !}$$

In the following I will limit the discussion to the a classical microscopic description.

That is, the starting point (at least ideally) are the Newton equations.

First rigorous attempt: Rieder, Lebowitz, and Lieb (1967) studied harmonic crystals

Found anomalous conductivity in $d < 3$ (No Fourier Law!).

Absurd? Maybe not (carbon nanotubes).

Not much progress till now but much related work:

Hydrodynamics limits (Varadhan, ...)

Relation between Non-equilibrium Statistical Mechanics and Dynamical Systems (Sinai, Ruelle, Gallavotti, ...)

Kinetic limit and Boltzmann equation (Lanford, ...)

Enormous amount of numerical simulations
(Fermi–Pasta–Ulam, ...)

A lot of interest lately

Dynamical Systems point of view: Eckmann–Young (2004)

Kinetic Limit point of view: Spohn et al. (2006), Bricmont–Kupiainen (2007), ...

Sistem driven by stochastic heath baths: Eckmann–Pillet–Rey-Bellet (1999), ...

Systems with small random noise: Olla et al. (2005), ...

I have a Dynamical System point of view and I am interested in the role played by nonlinearities and instability.

My goal is to understand a very simple situation:

an insulator made of almost non interacting particles

To simplify further the problem I am willing to consider a situation in which there exists an intermediate time scale between the microscopic and the macroscopic one.

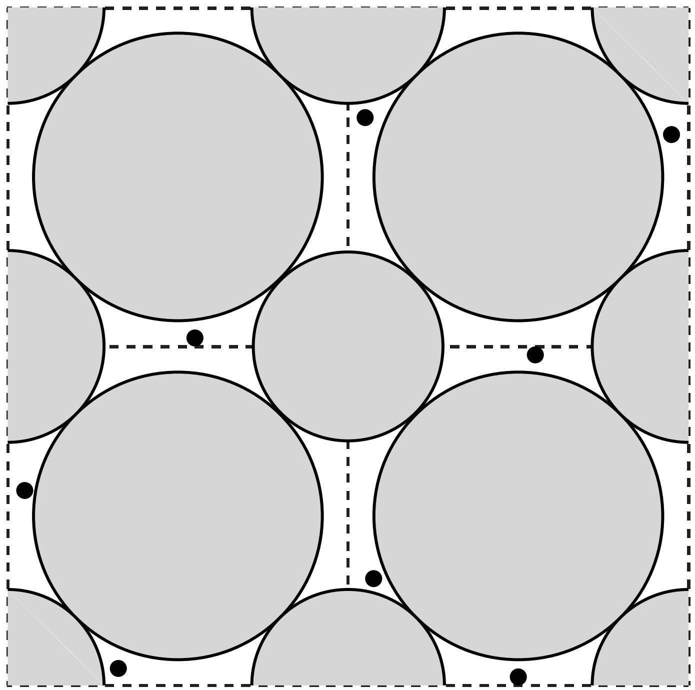
The structure of the models

Consider a Hamiltonian $H(q,p)$ with compact energy levels with good statistical properties and a Lattice or Graph (say $\mathbb{Z}^d$, for simplicity). At each site of the lattice we have a particle with coordinates (q_i,p_i). For each $\Lambda \subset \mathbb{Z}^d$ consider the system

$$\mathcal{H}_\Lambda^\varepsilon(\bar{q},\bar{p}) = \sum_{i\in\Lambda} H(q_i,p_i) + \varepsilon \sum_{|i-j|=1} V(q_i,q_j)$$

A motivating example.

Related to the heuristic work of Gilbert and Gaspard



Obstacles gray, particles black.

What would we like to do?

We are interested in the evolution of $\mathbb{e}_i(t) = \frac{1}{2}p_i^2(t)$.

The goal is to perform an hydrodynamics limit:

let $\Lambda_L := \{i \in \mathbb{Z}^d \ : \ |i| \le L\}$; consider, for each $\varphi \in \mathcal{C}^\infty$,

$$\frac{1}{L^d} \sum_{i \in \Lambda_L} \varphi(L^{-1}i)\mathbb{e}_i(L^2 t) = \frac{1}{L^d} \sum_{i \in \Lambda_L} \mathbb{e}_i(L^2 t)\delta_{L^{-1}i}(\varphi).$$

We want to prove that, almost surely,

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

where

$$\partial_t u = \mathrm{div}(k \nabla u)$$

Very hard: the motion determined by

$$\mathcal{H}^{\varepsilon}_{\Lambda}(\bar{q},\bar{p}) = \sum_{i\in\Lambda} H(q_i,p_i) + \varepsilon \sum_{|i-j|=1} V(q_i,q_j)$$

is hyperbolic if the energy of the particles is large with respect to ε but if a particle is slow, then ..... elliptic islands are possible.

So, let us introduce an intermediate time scale via

weak coupling.

$$\frac{d}{dt}\mathbb{e}_i(t) = \varepsilon j_i = \varepsilon \sum_{|i-j|=1} \nabla V(p_i + p_j)$$

Consider the energies $\{\mathbb{e}_i(\varepsilon^{-2}t)\}$. The hope is to prove that they converge in law to random variables $\mathcal{E}_i(t)$. In other words, for each smooth function φ

$$\lim_{\varepsilon \to 0} \mathbb{E}(\varphi(\mathbb{e})) = \mathbb{E}(\varphi(\mathcal{E})).$$

But, if so, how would $\mathcal{E}$ look like?

Heuristically we expect a mesoscopic equation where the (q, p) degrees of freedom have been averaged out, namely:

$$d\mathcal{E}_i = \sum_{|i-j|=1} \alpha(\mathcal{E}_i, \mathcal{E}_j)dt + \sum_{|i-j|=1} \gamma(\mathcal{E}_i, \mathcal{E}_j)dB_{\{i,j\}}$$

where the $B_{\{i,j\}} = -B_{\{j,i\}}$ are independent Brownian motions and $\exists\ \phi\ :\ e^{-\beta \sum_i \phi(\mathcal{E}_i)}$ are invariant measures.

Note that, since it must be $\mathcal{E} \geq 0$, necessarily $\gamma(0, x) = \gamma(x, 0) = 0$.

We have then a degenerate diffusion.

The above equation is similar to the Ginzburg-Landau type equation for which Varadhan has already proved the hydrodynamics limit.

Unfortunately, Varadhan approach does not apply directly to the degenerate situation at hand.

Thus: even if one establishes the mesoscopic equation a lot of work remains to be done.

Concrete example

Work in collaboration with Stefano Olla

Consider $\Lambda \subset \mathbb{Z}^d$ and the Hamiltonian

$$H_\varepsilon^\Lambda := \sum_{i\in\Lambda} \frac{1}{2} p_i^2 + \sum_{i\in\Lambda} U(q_i) + \varepsilon \sum_{|i-j|=1} V(q_i - q_j),$$

where $U(0) = U'(0) = 0$ and $c\,\mathrm{Id} \leq U''(x) \leq C\,\mathrm{Id}$ and the same for V.

In addition, consider a random force preserving single sites kinetic energies (i.e. independent diffusions on the spheres $p_i^2 = cost$). We define the diffusion by the generator

$$S = \sum_{i \in \Lambda} \sum_{r,h}^{d} X_{i;r,h}^2$$

where $X_{i;r,h} p_i^2 = 0$ (e.g. $X_{i;r,h} := p_{i,r} \partial_{p_{i,h}} - p_{i,h} \partial_{p_{i,r}}$).

The full generator is thus given by

$$L_{\varepsilon,\Lambda} := \{H_\varepsilon^\Lambda, \cdot\} + \sigma^2 S$$

Theorem 1 (Olla, L.) *The limiting process $\mathcal{E}_i$ is well defined and satisfies the mesoscopic differential stochastic equation*

$$d\mathcal{E}_i = \sum_{|i-k|=1} \alpha(\mathcal{E}_i, \mathcal{E}_k)dt + \sum_{|i-k|=1} \sigma\gamma(\mathcal{E}_i, \mathcal{E}_k)dB_{\{i,k\}}$$

where

$$\alpha(\mathcal{E}_i, \mathcal{E}_k) = C_\sigma e^{\frac{1}{2}\sum_j \phi(\mathcal{E}_j)}(\partial_{\mathcal{E}_i} - \partial_{\mathcal{E}_k})\left(e^{-\frac{1}{2}\sum_j \phi(\mathcal{E}_j)}\gamma^2(\mathcal{E}_i, \mathcal{E}_k)\right).$$

and $\gamma^2(a,b) = abG(ab)$ for some positive symmetric smooth function G.

Another example

Work in progress with Dmitry Dolgopyat

Let M be the a manifold of negative curvature and TM its cotangent bundle. Then, for $\Lambda \subset \mathbb{Z}^d$, consider the Hamiltonian on TM

$$H_\varepsilon^\Lambda := \sum_{i \in \Lambda} \frac{1}{2} p_i^2 + \varepsilon \sum_{|i-j|=1} V(q_i, q_j),$$

Theorem(well, almost)**2 (Dolgopyat, L.)** *The limiting process $\mathcal{E}_i$ is well defined and satisfies the mesoscopic differential stochastic equation*

$$d\mathcal{E}_i = \sum_{|i-k|=1} \alpha(\mathcal{E}_i, \mathcal{E}_k)dt + \sum_{|i-k|=1} \gamma(\mathcal{E}_i, \mathcal{E}_k)dB_{\{i,k\}}$$

where

$$\alpha(\mathcal{E}_i, \mathcal{E}_k) = \frac{1}{2}(\partial_{\mathcal{E}_i} - \partial_{\mathcal{E}_k})\gamma^2(\mathcal{E}_i, \mathcal{E}_k) + \frac{d+1}{4}(\mathcal{E}_i^{-1} - \mathcal{E}_k^{-1})\gamma^2(\mathcal{E}_i, \mathcal{E}_k).$$

and $\gamma^2(a,b) = abG(\sqrt{a}, \sqrt{b})$ *for some positive symmetric smooth function* G*. The measures* $\prod_{x\in\Lambda} \mathcal{E}_x^{\frac{d-2}{2}} e^{-\beta\mathcal{E}_x}$ *are invariant. Moreover, zero energy is unreacheable.*

Attempts to awoid weak coupling

I be the state space of the single site system.

$\Omega = I^{\mathbb{Z}^d} \times \mathbb{R}_+^{\mathbb{Z}^d}$ the state space of the full system (body)

$(x_i(n), E_i(n)) \in \Omega$ be the state at time $n \in \mathbb{N}$.

The x_i evolve independently from the E_i, while

$$E_i(n+1) = [1 - \varepsilon\pi_0(x(n))]E_i(n) + \frac{\varepsilon}{2d}\sum_{|z|=1}\pi_z(x(n))E_{i+z}(n)$$

- $1 \geq \pi_z \geq 0$, energy is positive
- $\frac{1}{2d}\sum_{|z|=1}\pi_z = \pi_0$, total energy is conserved.

If $\sum_{i\in\mathbb{Z}^d} E_i(0) < \infty$, we can renormalize the variables so that $\sum_{i\in\mathbb{Z}^d} E_i(0) = 1$ then $\sum_{i\in\mathbb{Z}^d} E_i(n) = 1$ for all $n \in \mathbb{N}$.

IDEA:

Think of the $E_i(n)$ as the probability of having an imaginary particle at site i at time n. Then the particle performs a random walk in random environment

Fact	Energy	RWRE
$E_i(0) = \delta_{i,0}$	all energy at 0	start walk at 0
$\mathbb{E}(E_{Lx}(L^2)) \sim Ze^{-\sigma x^2}$	heat equation in averaged HL	annealed CLT
$E_{Lx}(L^2) \sim Ze^{-\sigma x^2}$ $\mathbb{P}$-a.s.	a.s. heat equation in HL	quenched CLT

Random: $x_i(n)$ independent (or weakly coupled) Markov chains [Dolgopyat-Keller-L. (2007)] true in all dimensions

Deterministic: $x_i(n+1) = Tx_i$, $T : I \to I$ piecewise expanding (chaotic) maps [Dolgopyat-L. (2008)] true in all dimensions

Quenched CLT

The map $F : I^{\mathbb{Z}^d} \to I^{\mathbb{Z}^d}$, $(F(\theta))_i := T(x_i)$, $i \in \mathbb{Z}^d$, has a unique *natural* invariant measure μ^e.

Theorem 3 (Dolgopyat-L.) *There exists $\varepsilon_0 > 0$: for all $\varepsilon < \varepsilon_0$, $d \in \mathbb{N}^*$ and for μ^e almost all $\{x_i(0)\}_{i \in \mathbb{Z}^d}$,*

(a) $\frac{1}{N} X_N \to v \quad \mathbf{P}_\theta \; a.s.$;

(b) $\frac{X_N - vN}{\sqrt{N}} \Rightarrow \mathcal{N}(0, \Sigma^2)$ *under* $\mathbf{P}_\theta$.