Heat equation and Non-equilibrium (Classical) Statistical Mechanics

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Many of us have learned and taught the following "derivation" of the heat equation:

Imagine that the heat (temperature) u is a fluid, then it must satisfy

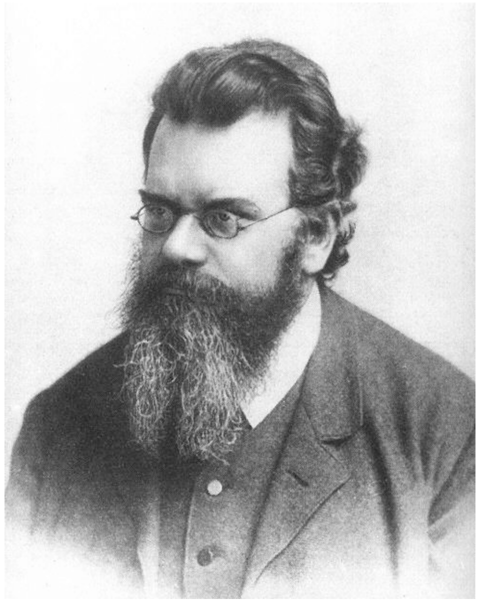
$$\partial_t u = \mathrm{div} j$$

where j is the current.

Now assume (Fourier Law) $j = k\nabla u$, then

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

But



Ludwig Eduard Boltzmann
(1844 –1906)

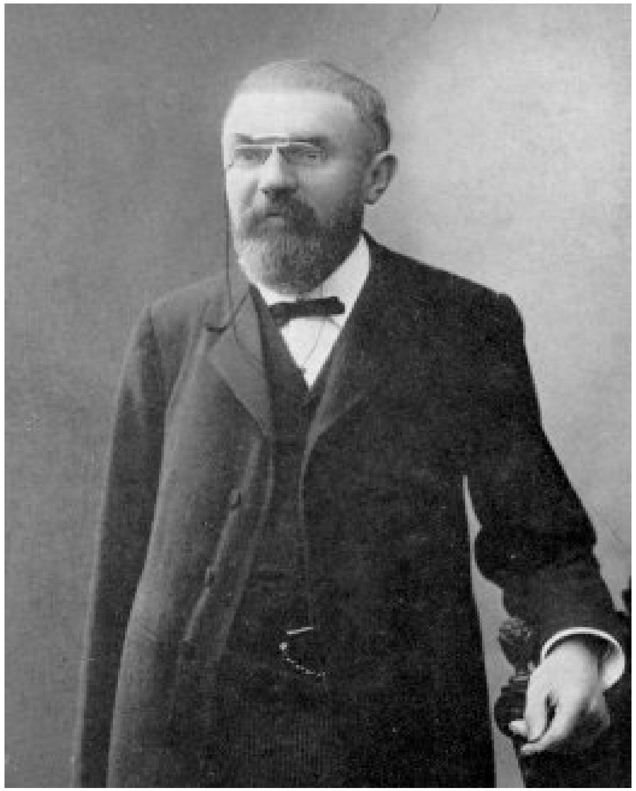
Has explained that heat is not a fluid and, anyway, why should the Fourier Law hold?

Statistical Mechanics states that heat is the average local Kinetic energy per particle in a body.

To obtain a rigorous (classical) derivation of the heat equation one should then write the Newton equations of motion for the N particles of a body, solve them and show that the local energy density satisfies the heat equation,

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

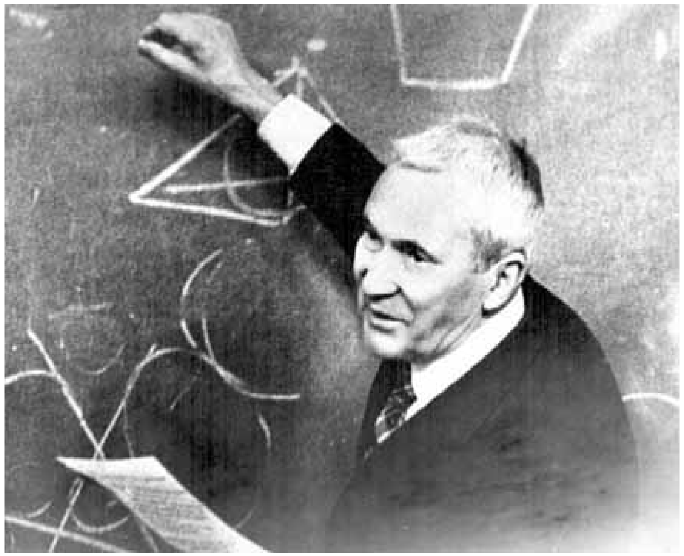
Jules Henri Poincaré (1854 – 1912)



Recognized the phenomenon of instability even in systems with few degree of freedoms (3-dimensional flows)

predictions with 10^{24} is hopeless.

Andrey Nikolaevich Kolmogorov (1903–1987)



Explained the role of probability:
Do statistical predictions or
Look at evolution of measures,
not of points.

First rigorous attempt: Rieder, Lebowitz, and Lieb (1967) studied harmonic crystals (no chaos!)

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

Absurd? Maybe not (carbon nanotubes).

Not much progress till this century.

Yet, much has happened extremely relevant to our story:

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, ...)

Prompting a new wave of attempts.

Let me mention a few

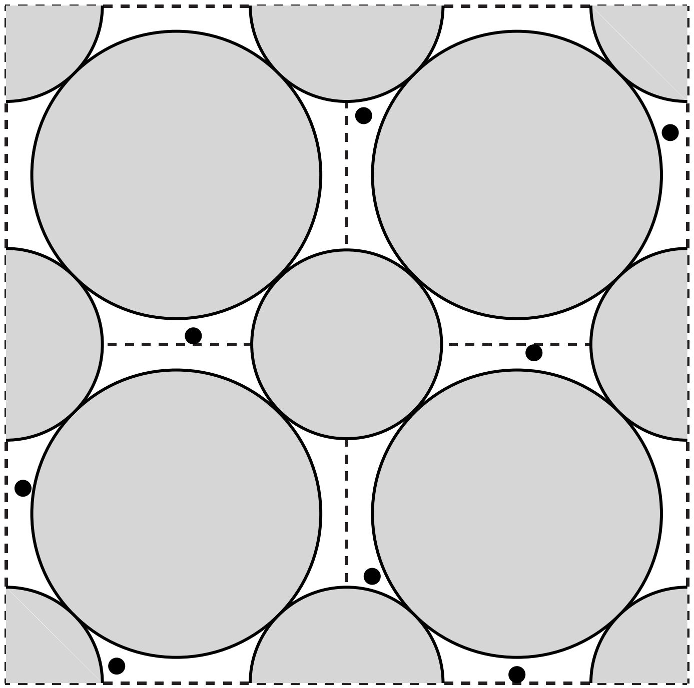
Dynamical Systems point of view: Eckmann-Young (2004)

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

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

All very interesting ideas that will be part of our journey.

I have a dream (destination).



Obstacles gray, particles black.

ergodicity? no!

no interaction $\Rightarrow$ energy cons.

Perturbation Theory? How?

What to do ?

Toy Models

Itinerary and some amusing stops:

Toys 1) Non interacting models with a conserved quantity

(a) Random model (discrete time)

(b) Deterministic models (discrete time)

Toys 2) Interacting models in the weak interaction regime

(a) Random models (continuous time)

(b) Deterministic models (discrete time)

Toys 3) Weakly interacting hyperbolic flows (destination)

Toys 1

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 1 (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* $\mathbf{P}_\theta$.

Toys 2

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 $c\,\mathrm{Id} \leq U''(x) \leq C\,\mathrm{Id}$.

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 be 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

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

The single particles energies are the random variables

$$e_i(t) = \frac{1}{2}\|p_i(t)\|^2 + U(q_i(t)).$$

We look at the kinetic limit

$$\tilde{e}_i(t) = \lim_{\varepsilon \to 0} e_i(\varepsilon^{-2} t).$$

The limit is in distribution.

Theorem 2 (Olla, L.) *The limiting process* $\tilde{e}_i$ *is well defined and satisfies the mesoscopic differential stochastic equation*

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

where

$$\sigma^2(\partial_{\tilde{e}_i} - \partial_{\tilde{e}_k})\gamma^2(\tilde{e}_i, \tilde{e}_k) = \alpha(\tilde{e}_i, \tilde{e}_k)$$

and $B_{\{i,k\}} = -B_{\{k,i\}}$ *are independent random walks.*
All the measures $\prod_i \beta e^{-\beta\tilde{e}_i}$ *are invariant.*

The next step is to take the hydrodynamic limit:

- Let $\Lambda \subset \mathbb{R}^d$ and $\Lambda_L := \{i \in \mathbb{Z}^d \ : \ L^{-1} i \in \Lambda\}$
- $\{\tilde{e}_i^L(t)\}_{\Lambda_L}$ be the solution of the mesoscopic equation with initial condition $\tilde{e}_i(0) = g(L^{-1}i)$, $g \in \mathcal{C}^\infty(\Lambda, \mathbb{R})$.
- $u(x,t)$ is the HL of $\tilde{e}_i^L$ if, $\forall\ \varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

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

$\{\tilde{e}_i^L(t)\}_{\Lambda_L}$ converges to the heat equation if

- the hydrodynamic limit u exists.
- u satisfies $\partial_t u = \mathrm{div}(k \nabla u)$.

The weak interaction (kinetic) limit for choatic systems should yield the same mesoscopic equation

........Work in progress ....

Toys 3: Things to come

Deterministic case in which the local dynamics is symplectic.

Very hard but maybe possible by twisting present technology.

Avoid the two limit step and obtain heat equation taking immediately the Hydrodynamic limit: at the moment is

. . . . .science fiction. . . . .