Heat equation from a deterministic dynamics

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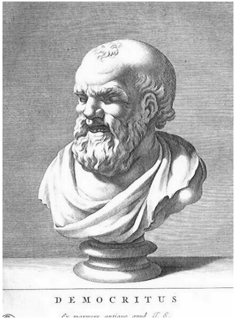
Democrito



Now his principal doctrines were these. That atoms and the vacuum were the beginning of the universe; and that everything else existed only in opinion.

(Diogenes Laërtius, Democritus, Vol. IX, 44, trans. Yonge 1853)

Heat equation from microscopic dynamics: an old problem

Heat equation for the temperature $T(t,x)$

$$C(T)\partial_t T = \partial_x \left(K(T)\partial_x T\right), \qquad C(T) \text{ specific heat, } K(T) \text{ thermal conductivity.}$$

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As a conservative law for the thermal energy:

$$\partial_t e = \partial_x (D(e)\partial_x e), \qquad D(e) = K(T)C(T)^{-1} \text{ thermal diffusivity}$$

How to obtain this from a diffusive rescaling of a microscopic dynamics governed by Hamilton's equations

$$\begin{aligned} \dot{q}_j &= p_j \\ \dot{p}_j &= -\partial_{q_j}\mathcal{H}(q, p) \end{aligned}$$

Connection to the microscopic dynamics

Consider a 1-d chain of anharmonic oscillators (a lattice system):

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

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$$\dot{\mathfrak{e}}_x = J_{x-1,x} - J_{x,x+1}, \qquad J_{x,x+1} = -p_x V'(q_{x+1} - q_x), \qquad \text{energy currents}$$

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then we expect that, under certain conditions on the initial distribution and on the non-linearity of V and W

$$\lim_{\varepsilon \to 0} \varepsilon \sum_x G(\varepsilon x) \mathfrak{e}_x(\varepsilon^{-2} t) = \int G(y)\, e(t,y)\, dy$$

with

$$\partial_t e = \partial_y \left(D(e)\partial_y e\right), \qquad D(e) = \frac{1}{C(T_e) T_e^2} \int_0^\infty dt \sum_x \mathbb{E}_e \left(J_{x,x+1}(t) J_{0,1}(0)\right)$$

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- These relative entropy techniques do not work for the energy for a well known problem: entropy does not control energy.
- For harmonic chains (V and W quadratic) with noise only conserving energy, it is possible to prove heat equation in the diffusive limit, at least in the average (not as a law of large numbers).

A deterministic dynamics

$x = 1, \ldots, N$, $N+1 = 1$, periodic boundary. $q_x, p_x \in \mathbb{R}^2$,

$$\begin{aligned} \dot{q}_x(t) &= p_x(t) \\ \dot{p}_x(t) &= \left(\Delta - \omega_0^2\right) q_x(t) + \varepsilon^{-\frac{1}{2}} b\left(f^{\lfloor t\varepsilon^{-1} \rfloor}\theta_x\right) J p_x(t) \end{aligned}$$

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad \Delta q_x = q_{x+1} + q_{x-1} - 2q_x.$$

f a chaotic map, $\varepsilon = \varepsilon(N) = N^{-a}$, $a > 6$,
$b(\theta)$ of null average wrt the invariant measure of f.

The chaotic maps f

- The easy case: smooth map on the interval

$$f : \mathbb{T} \to \mathbb{T}, \qquad f \in \mathcal{C}^\infty, \qquad f' \geq \lambda > 1.$$

There exists a unique a.c. invariant measure $\rho_\star(\theta)d\theta$ + exponential decay of correlations.

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- An Anosov map on $\mathbb{T}^2$, for example

$$f\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix} = \begin{pmatrix}2 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}\theta_1\\ \theta_2\end{pmatrix}.$$

  This has the advantage to be time reversible.
  Also $\exists!$ $\rho_\star(\theta)d\theta$ + exponential decay of correlations.

The exterior force

$$\dot{q}_x(t) = p_x(t) \qquad \dot{p}_x(t) = \left(\Delta - \omega_0^2\right) q_x(t) + \varepsilon^{-\frac{1}{2}} b\left(f^{\lfloor t\varepsilon^{-1} \rfloor}\theta_x\right) J p_x(t), \qquad x = 1, \dots, N.$$

$$\int_{\mathbb{T}} b(\theta)\rho_\star(\theta)\, d\theta = 0,$$

and there exists a periodic orbit $\{\theta_n\}_{n=1}^{p}$, $p \in \mathbb{N}$, $\theta_{n+1} = f\theta_n$, $\theta_p = \theta_1$, such that

$$\sum_{n=1}^{p} b(\theta_n) \neq 0 \quad \Longrightarrow \quad \gamma := \int_{\mathbb{T}} b(\theta)^2 \rho_\star(\theta)\, d\theta + 2\sum_{k=1}^{\infty} \int_{\mathbb{T}} b(\theta) b(f^k\theta)\rho_\star(\theta)\, d\theta > 0,$$

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$$\frac{1}{\sqrt{n}}\sum_{k=1}^{n} b(f^k\theta) \xrightarrow[n\to\infty]{\text{law}} \mathcal{N}(0,\gamma), \qquad \frac{1}{\sqrt{n}}\sum_{k=1}^{\lfloor nt\rfloor} b(f^k\theta) \xrightarrow[n\to\infty]{\text{law}} \sqrt{\gamma}W(t) \ \text{ Wiener process}$$

Assumptions on the initial distribution

$$q = (q_1, \dots, q_N), p = (p_1, \dots, p_N), \theta = (\theta_1, \dots, \theta_N), \ (q, p, \theta) \in \mathbb{R}^N \times R^N \times \mathbb{T}^N.$$

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The initial distribution $d\mu_N(q, p, \theta)$ is a probability measure on $\mathbb{R}^N \times R^N \times \mathbb{T}^N$ such that

$$d\mu_N(q, p, \theta) = \rho_N(\theta)\mu_{\theta,N}(dq, dp)d\theta,$$

$$\rho_N(\theta) = \prod_{x=1}^N \rho_x(\theta_x), \qquad \sup_x \sup_{\theta_x \in \mathbb{T}} \frac{|\partial_{\theta_x}\rho_x(\theta_x)|}{\rho_x(\theta_x)} \leq C_0.$$

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It is important that there is a certain smoothness in the initial distribution of θ, while $\mu_{\theta,N}(dq, dp)$ can also be singular.

$$\lim_{N\to\infty} \mathbb{E}_{\mu_N}\left[\frac{1}{N}\sum_{x=1}^N \varphi\left(\frac{x}{N}\right)\mathfrak{e}_x(0)\right] = \int_{\mathbb{T}} \varphi(y)e_0(y)dy, \quad \text{initial macroscopic profile}$$

The limit theorem

Let $e(t,y)$ the solution of

$$\partial_t e = \frac{D}{\gamma}\,\partial_x^2 e, \qquad e(0,y) = e_0(y), \qquad y \in \mathbb{T}.$$

with

$$D = \frac{2}{2 + \omega_0^2 + \omega_0\sqrt{\omega_0^2 + 4}},$$

then for any smooth test function φ on $\mathbb{T}$:

$$\lim_{N\to\infty} \mathbb{E}_{\mu_N}\left[\frac{1}{N}\sum_{x=1}^{N} \varphi\left(\frac{x}{N}\right) \mathfrak{e}_x(N^2 t)\right] = \int_{\mathbb{T}} \varphi(y) e(t,y) dy,$$

Error control and longer time scales

$$\left| \mathbb{E}_{\mu_N}\left[\frac{1}{N}\sum_{x=1}^{N} \varphi\left(\frac{x}{N}\right) \mathfrak{e}_x(N^2 t) \right] - \int_{\mathbb{T}} \varphi(y) e(t,y) dy \right| \le \frac{C \|\varphi\|_{\mathcal{C}^8}}{N^{\frac{\alpha}{6}-1}}$$

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At a larger time scale we get a global equilibrium:

$$\lim_{N\to\infty}\mathbb{E}_{\mu_N}\left[\frac{1}{N}\sum_{x=1}^{N}\varphi\left(\frac{x}{N}\right)\mathfrak{e}_x(N^{2+\beta} t)\right] = \mathcal{E}_0\int_{\mathbb{T}}\varphi(y)dy,$$

$$\mathcal{E}_0 = \int_{\mathbb{T}} e_0(y)dy.$$

The equivalent stochastic dynamics

$$\dot{q}_x(t) = p_x(t),$$
$$dp_x(t) = \left(\Delta - \omega_0^2\right) q_x(t)dt - \gamma p_x(t)dt + \sqrt{2\gamma} J p_x(t) dw_x(t), \quad x = 1, \dots, N.$$

where $\{w_x(t)\}$ are i.i.d. standard Wiener processes (one dimensional).

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In fact this has the same macroscopic equation for the energy:

$$\partial_t e = \frac{D}{\gamma} \partial_x^2 e, \qquad D = \frac{2}{2 + \omega_0^2 + \omega_0 \sqrt{\omega_0^2 + 4}}.$$

Strategy of the proof

$$\mathbb{E}\left(\frac{1}{N}\sum_x \varphi\left(\frac{x}{N}\right)\left[\mathfrak{e}_x(N^2 t) - \mathfrak{e}_x(0)\right]\right) = \sum_x \varphi'\left(\frac{x}{N}\right)\int_0^t \mathbb{E}\left(j_{x,x+1}(N^2 s)\right) ds + o_N$$

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We want to show that the time average of the energy currents:

$$\int_0^t \mathbb{E}\left(j_{x,x+1}(N^2 s)\right) ds = -\int_0^t \mathbb{E}\left(p_x(N^2 s)\cdot q_{x+1}(N^2 s)\right) ds + \int_0^t \mathbb{E}\left(p_x(N^2 s)\cdot q_x(N^2 s)\right) ds$$

is close to the same quantity of the stochastic dynamics,
then we proceed as in the stochastic dynamics.

Covariance Matrix evolution

$$\mathbf{S}^{q}_{x,x'} = \int_0^t \mathbb{E}\left(q_x(N^2 s)\cdot q_{x'}(N^2 s)\right) ds, \qquad \mathbf{S}^{q,p}_{x,x'} = \int_0^t \mathbb{E}\left(q_x(N^2 s)\cdot p_{x'}(N^2 s)\right) ds$$

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after calculations, we have

$$\begin{aligned}
&\mathbf{S}^{(p,q)} + \mathbf{S}^{(q,p)} = R_N^{(q)} \\
&\mathbf{S}^{(q)}(\omega_0^2 I - \Delta) + \gamma \mathbf{S}^{(q,p)} - \mathbf{S}^{(p)} = R_N^{(q,p)} \\
&(\omega_0^2 I - \Delta)\mathbf{S}^{(q)} + \gamma \mathbf{S}^{(p,q)} - \mathbf{S}^{(p)} = R_N^{(p,q)} \\
&(\omega_0^2 I - \Delta)\mathbf{S}_N^{(q,p)} + \mathbf{S}_N^{(p,q)}(\omega_0^2 I - \Delta) + 2\gamma \mathbf{S}^{(p)} - 2\gamma \Sigma\left(\mathbf{S}^{(p)}\right) = R_N^{(p)}.
\end{aligned}$$

where $R_N^{(\alpha)}$ is a negligeable matrix for $N \to \infty$.

Closing the heat equation

After diagonalizing in Fourier coordinates and more esplicit calculations we obtain

$$\sum_x \varphi'\left(\frac{x}{N}\right)\int_0^t \mathbb{E}\left(j_{x,x+1}(N^2 s)\right) ds = -\sum_x \varphi'\left(\frac{x}{N}\right)\left(\boldsymbol{S}^{(q,p)}_{x,x+1} - \boldsymbol{S}^{(q,p)}_{x,x}\right)$$

$$= \frac{D}{\gamma}\frac{1}{N}\sum_x \varphi''\left(\frac{x}{N}\right)\boldsymbol{S}^{(p)}_{x,x} + o_N = \frac{D}{\gamma}\frac{1}{N}\sum_x \varphi''\left(\frac{x}{N}\right)\int_0^t \mathbb{E}(p_x^2(N^2 s))ds + o_N$$

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$$= \frac{D}{\gamma}\frac{1}{N}\sum_x \varphi''\left(\frac{x}{N}\right)\boldsymbol{S}^{(p)}_{x,x} + o_N = \frac{D}{\gamma}\frac{1}{N}\sum_x \varphi''\left(\frac{x}{N}\right)\int_0^t \mathbb{E}(p_x^2(N^2 s))ds + o_N$$

and we conclude with the asymptotic equipartition of potential and kinetic energies:

$$\frac{D}{\gamma}\frac{1}{N}\sum_x \varphi''\left(\frac{x}{N}\right)\int_0^t \left[\mathbb{E}(p_x^2(N^2 s)) - \mathbb{E}(\mathfrak{e}_x(N^2 s))\right] ds \underset{N\to\infty}{\longrightarrow} 0.$$

From the deterministic to the random evolution

Let $\mathcal{G}$ the generator of the random evolution:

$$
\begin{aligned}
\mathcal{G} &= \mathcal{A} + \gamma \mathcal{S} \\
\mathcal{A} &= \sum_x \left(p_x \cdot \partial_{q_x} + \left(\Delta q_x - \omega_0^2 q_x \right) \cdot \partial_{p_x} \right) \\
\mathcal{S} &= \sum_x \left(p_{x,2} \partial_{p_{x,1}} - p_{x,1} \partial_{p_{x,2}} \right)^2 = \sum_x \left(J p_x \cdot \partial_{p_x} \right)^2 ,
\end{aligned}
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For the random evolution we obtain the equation for the covariance matrix from

$$\int_0^t \mu_N(\mathcal{G}A(N^2 s))ds = \frac{\mu_N(A(N^2 t)) - \mu_N(A(0))}{N^2} = o_N$$

for $A = A(p,q)$ quadratic function.

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For the deterministic evolution we want then

$$\int_0^t \mu_N(\mathcal{G}A(N^2 s))ds = \frac{\mu_N(A(N^2 t)) - \mu_N(A(0))}{N^2} + o(N, \varepsilon_N) = o_N$$

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From the deterministic to the random evolution

The (natural) idea is to split the macroscopic time interval $[0, N^2 t]$ in intervals of length h, long enough for the maps f_x to be close to equilibrium and CLT variances close to the equilibrium one (i.e. γ), but short enough so that the configuration (q, p) has moved very little.

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The main difficulty is to prove that, after each time step, the distributions of the angles θ_x, when conditioned on the positions, has still enough smoothness to ensure a new convergence in the following step.

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The mathematical tool to control this is called *standard pairs* (developped by Dolgopyat, from ideas of Sinai, L.S. Young, ...). Intuitively, standard pairs are the measures closer to a δ function for which the deterministic dynamics still exhibit statistical properties.

Standard Pair $\ell = (G_\ell, \rho_\ell)$

Given a small $\delta > 0$,

$$\theta_x \in [a_x, b_x], \quad |b_x - a_x| \in [\delta/2, \delta], x = 1, \dots, N$$

$$G_\ell : \bigtimes_{x=1}^{N} [a_x, b_x] \to \mathbb{R}^N \times \mathbb{R}^N,$$

$$G(\theta) = \left\{ G_x(\theta) = \left(G_{q_x^1}(\theta), G_{q_x^2}(\theta), G_{p_x^1}(\theta), G_{p_x^2}(\theta) \right), x = 1, \dots, N \right\}$$

$$\sum_x \mathfrak{e}_x(G(\theta)) = E \qquad \text{constant energy}$$

The configuration $G(\theta)$ changes little for $\theta \in \bigtimes_{x=1}^{N} [a_x, b_x]$:

$$\| DG \|_\infty = \sup_{x,\theta} \left[\sum_y \left(\partial_{\theta_x} G_y(\theta) \right)^2 \right]^{1/2} \le \bar{C} \sqrt{E \varepsilon}$$

Standard Pair $\ell = (G_\ell, \rho_\ell)$

The *standard probability density* ρ_ℓ

$$\rho_\ell(\theta) = \prod_x \rho_x(\theta_x), \qquad \int_{a_x}^{b_x} \rho_x(\theta_x) d\theta_x = 1, \quad \left\| \frac{\rho_x'}{\rho_x} \right\|_{\mathcal{C}^0} \le C_0.$$

There exists C_0 large enough such that this property is conserved by the map f.

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There exists C_0 large enough such that this property is conserved by the map f. The standard pair $\ell = (G_\ell, \rho_\ell)$ depends on the parameters $N, E, \delta, \varepsilon, \bar{C}, C_0$.

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A standard pair ℓ induces the probability measure

$$\mu_\ell(g) = \int_{\times_x [a_x, b_x]} g(\theta, G_\ell(\theta)) \rho_\ell(\theta) d\theta,$$

for $g(\theta, q, p)$.

Evolution of standard pairs

Fact: the evolution of a standard pair is a convex combination of standard pairs with the same parameters.

It also allow, for a proper choice of the parameters and the time step h, to control the error in the calculation of the covariances uniformly in N. It turns out that $\varepsilon(N) < N^{-6}$ is enough for the speeding of the external field.

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- $\rho_\star$ density of the stationary measure of the chaotic maps, and let $\rho_{\star,N}(d\theta) = \prod_x \rho_\star(\theta_x) d\theta_x$
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assume the initial distribution has density

$$d\mu_N(q,p,\theta) = g_0(q,p,\theta)\ \nu_{\beta,N}(q,p)\rho_{\star,N}(d\theta)\ dq_x\ dp_x := g_0(q,p,\theta)\ d\mu_{eq}(\theta,q,p)$$

with finite entropy:

$$H(0) := \int g_0(q,p,\theta) \log g_0(q,p,\theta)\nu_{\beta,N}(q,p) \leq CN.$$

Entropy evolution

At (macroscopic) time t we have density $g_t(q,p,\theta)$, with entropy

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same as time 0 (as in Joel's and others talks).
We need to loose some information. Consider the marginal

$$\bar{g}_t(q,p) = \int g_t(\theta,q,p) \rho_{\star,N}(d\theta),$$

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The time derivative of this marginal entropy is not 0, and

$$\frac{d}{dt}\bar{H}(t) = N^2\sum_x \int \left(\varepsilon^{-1/2}\int b(\theta_x)\, Jp_x\cdot\partial_{p_x} g_t(\theta,q,p)\rho_{\star,N}(d\theta)\right)\log\bar{g}_t(q,p)\ \nu_{\beta,N}(q,p)\prod_x dq_x\, dp$$

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I do not know about the sign of this derivative, but there is no reason that it is always negative.

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I do not know about the sign of this derivative, but there is no reason that it is always negative. How is this related with the same entropy production of the stochastic dynamics? For $t > s$

$$\bar{H}(t) - \bar{H}(s) \underset{n\to\infty}{\sim} -N^2\gamma\int_s^t\sum_x\int \frac{(Jp_x\cdot\partial_{p_x}\bar{g}_r)^2}{\bar{g}_r}\nu_{\beta,N}(q,p)\prod_x dq_x\, dp_x < 0.$$