From the microscopic to the macroscopic world

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Can “Irreversible macroscopic laws”
be deduced from or “reduced to”
“Reversible microscopic laws” ?

(definitions later)

Brief answer (goal of this talk) :

Yes, but in a certain sense, to be made precise.

The basic idea goes back to Boltzmann, but there are also many pseudo-solutions, confused answers etc.

Very little is on firm mathematical grounds

Consider classical mechanics.
Given $\mathbf{x}(t) = (\mathbf{q}(t), \mathbf{p}(t))$
for a (closed) mechanical system,
$\mathbf{q}$ = the positions of the particles
$\mathbf{p}$ = the momenta of the particles,
then ‘everything’ follows.
In particular, macroscopic quantities, like the density or the energy density, are functions of $\mathbf{x}$.

Simple example of macroscopic equation : diffusion

$$\frac{d}{dt}u = \Delta u$$

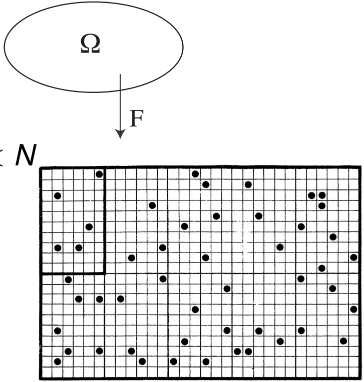
$u = u(x, t), x \in \mathbb{R}^3$.
Let u = density (or energy density).
u = example of 'macroscopic' variable.

Same idea with Navier-Stokes, Boltzmann...

$u(x, t) \to$ constant as $t \to \infty$

Ω = PHASE SPACE $\subset \mathbb{R}^{6N}$

$N \sim$ AVOGADRO



$n << N$

Ex :

n CELLS

$F(\mathbf{x}) = (F_1(\mathbf{x}), ...; F_n(\mathbf{x})) \in \mathbb{R}^n =$ fraction of particles in each cell

$U(x)$ in diffusion equation is a continuous approximation to F.

Simple example
Coin tossing

$\mathbf{x} \rightarrow (H, T, T, H...)$
2^N possible values

$F(\mathbf{x})$ = Number of heads or tails
= N possible values
$N << 2^N$.

$\mathbf{x}(0) \to \mathbf{x}(t) = T^t\mathbf{x}(0)$ Hamilton

$$\begin{array}{ccc} \downarrow & & \downarrow \\ F_0 & \to & F_t \end{array}$$

Is the evolution of F

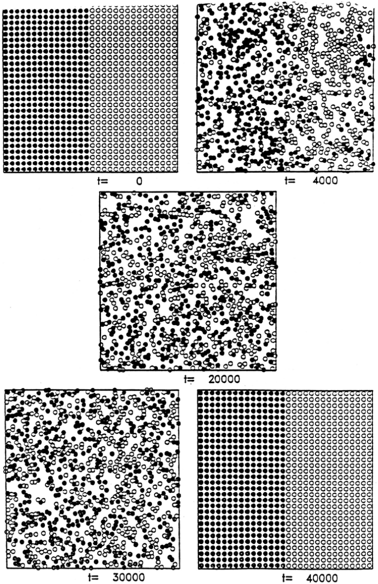
AUTONOMOUS, i.e. independent of the **x** mapped onto F ?

$\mathbf{x}(0) \to \mathbf{x}(t)$
Reversible : $\mathrm{I} T^t \, \mathrm{I} \, \mathbf{x}(t) = \mathbf{x}(0)$
$\mathrm{I}(\mathbf{q}, \mathbf{p}) = (\mathbf{q}, -\mathbf{p})$

But $F_0 \to F_t$ often irreversible, as in the example of diffusion.

$F_t \to$ UNIFORM DISTRIBUTION (in $\mathbb{R}^3$!) There is no I operation that leaves the diffusion equation invariant.

Besides, the evolution of F is NOT autonomous !



Time evolution of a system of 900 particles all interacting via the same potential. Half of the particles are colored white, the other half black. All velocities are reversed at $t = 20,000$. The system then retraces its path and the initial state is fully recovered. But at $t = 20,000$, the density is uniform both for the configuration obtained at that time and for the one with the reversed velocities.

So, the evolution of the macroscopic variable CANNOT be autonomous. PARADOX ?

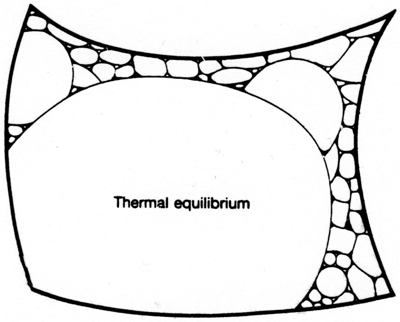
Basis of the **Solution**

The map F is many to one in a way that depends on value taken by F.

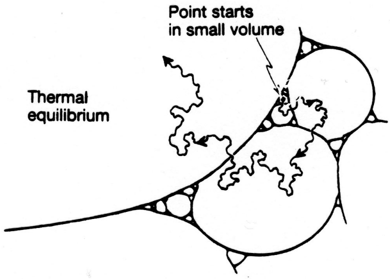
Think of coin tossing

$F = N \to$ one ‘configuration’

$F = \frac{N}{2} \to \simeq \frac{2^N}{\sqrt{N}}$ ‘configurations’



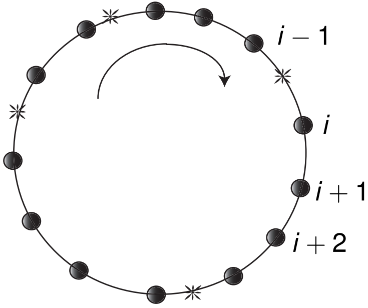
A coarse-graining of phase space into regions corresponding to states that are macroscopically indistinguishable from one another.



As time evolves, the phase-space point enters compartments of larger and larger volume.

CONSIDER A CONCRETE EXAMPLE

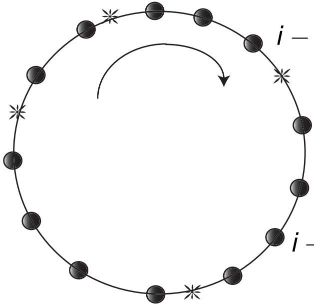
THE KAC RING MODEL



N points
1 particle at each point
"SIGN"
$\eta_i(t) = +1$
$\eta_i(t) = -1$

M CROSSES
= "scatterers"

$\varepsilon_i = +1$
$\varepsilon_{i-1} = -1$



Dynamics – TURN
– CHANGE SIGN
when particle goes through a cross.

So, e.g.

$$\eta_i(t+1) \quad = -\eta_{i-1}(t)$$

$$\eta_{i+1}(t+2) = \eta_i(t+1)$$

$$\eta_i(t) = \eta_{i-1}(t-1)\varepsilon_{i-1}$$

= NEWTON'S EQUATION

– DETERMINISTIC

– ISOLATED

– REVERSIBLE : IF, AFTER TIME t, PARTICLES START TO MOVE BACKWARD, THEY GO BACK TO THE INITIAL STATE IN TIME t.

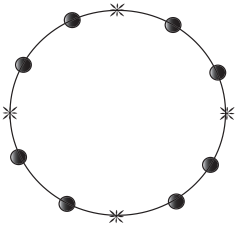
– EVERY CONFIGURATION IS PERIODIC OF PERIOD $2N << 2^N = \#$ STATES
(THIS IS MUCH STRONGER THAN POINCARE'S RECURRENCES OR LACK OF ERGODICITY).

CONVERGENCE TO EQUILIBRIUM ?

$N_+ = N - N_-$ MACROSCOPIC VARIABLES

$$N_+ = N_- = \frac{N}{2} = \text{EQUILIBRIUM}$$

START WITH $N_+(0) = N$



CONFIGURATION OF PERIOD 4

NO CONVERGENCE TO EQUILIBRIUM
$\longrightarrow$ Convergence to equilibrium CANNOT hold for all initial conditions, i.e. for all distributions of crosses.

1. BOLTZMANN

$$N_+(t+1) = N_+(t) - N_+(S,t) + N_-(S,t)$$
$$N_-(t+1) = N_-(t) - N_-(S,t) + N_+(S,t)$$

WHERE $N_+(S,t)$ DENOTES THE NUMBER OF $+$ SIGNS THAT HAVE A CROSS (OR SCATTERER) AHEAD OF THEM (AND, THUS WILL CHANGE SIGN AT THE NEXT TIME STEP). $N_-(S,t)$ IS SIMILAR.

ASSUME

$$N_+(S,t) = \tfrac{M}{N} N_+(t)$$
$$N_-(S,t) = \tfrac{M}{N} N_-(t)$$

$\longleftrightarrow$ MOLECULAR CHAOS : " SIGN UNCORRELATED WITH CROSSES "

$$\Rightarrow \frac{1}{N}\Big(N_+(t+1) - N_-(t+1)\Big)$$

$$= \left(1 - \frac{2M}{N}\right)\Big(N_+(t) - N_-(t)\Big)$$

$$\Rightarrow \frac{1}{N}\Big(N_+(t) - N_-(t)\Big) = \left(1 - \frac{2M}{N}\right)^t$$

$\Big(N_+(0) = N \qquad N_-(0) = 0\Big)$ We may assume $\frac{M}{N} < 1/2$.

$\Rightarrow$ EQUILIBRIUM !

BOLTZMANN'S ENTROPY

$$S_B(t) = \ln \begin{pmatrix} N \\ N_-(t) \end{pmatrix} = \ln \left(\frac{N!}{N_-(t)!N_+(t)!} \right)$$

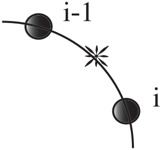
MAXIMUM for $N_- = N_+ = \frac{N}{2}$

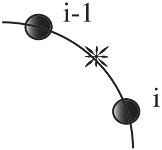
= EQUILIBRIUM

MICROSCOPIC THEORY

1. Eq. of MOTION

$\eta_i(t) = \eta_{i-1}(t-1)\varepsilon_{i-1}$





$\Rightarrow$ SOLUTION

$$\eta_i(t) = \eta_{i-t}(0)\varepsilon_{i-1}\varepsilon_{i-2}\ldots\varepsilon_{i-t} \quad \text{MOD } N$$

BUT MACROSCOPIC VARIABLES
= FUNCTIONS OF THE MICROSCOPIC ONES

$$\frac{1}{N}(N_+(t) - N_-(t))$$

$$= \frac{1}{N}\sum_{i=1}^{N}\eta_i(t)$$

$$= \frac{1}{N}\sum_{i=1}^{N}\eta_{i-t}(0)\varepsilon_{i-1}\varepsilon_{i-2}\dots\varepsilon_{i-t}$$

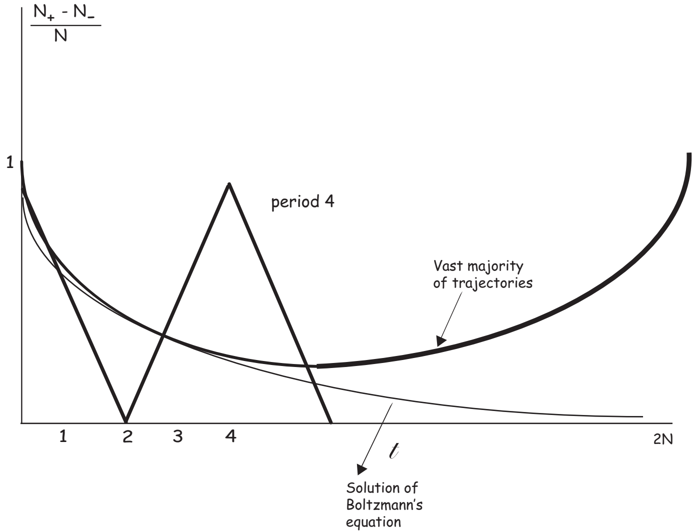
IF we look at $t = 2N$: PROBLEM (PERIODICITY)

TAKE $t << N$, e.g. $t = 10^6$. $N \sim 10^{23}$.

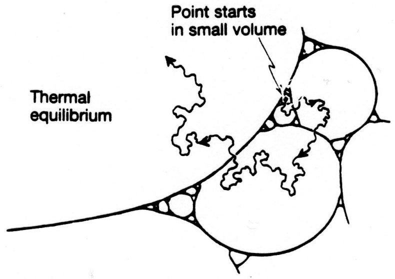
Then, one can show, by the law of large numbers, that, for the overwhelming majority of microscopic initial configurations, i.e. of distributions of crosses,

$$\frac{1}{N}\Big(N_+(t) - N_-(t)\Big) \approx \left(1 - \frac{2M}{N}\right)^t,$$

i.e. the macrostate follows the solution of the Boltzmann approximation. So, the microstate does, in the overwhelming majority of cases, move towards larger regions of phase space.



N+ - N-
N
1
period 4
Vast majority
of trajectories
1
2
3
4
2N
t
Solution of
Boltzmann's
equation



As time evolves, the phase-space point enters compartments of larger and larger volume.

Solution to the reversibility paradox, in general

$\Omega_0 = F^{-1}(F_0)$, given F_0

$\overline{\Omega_0} \subset \Omega_0$ “good” configurations, meaning that

$\forall\ x \in \overline{\Omega_0}$

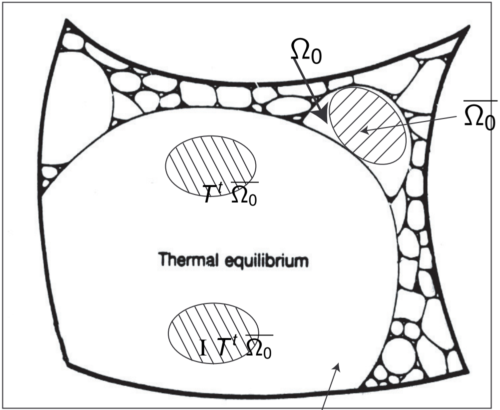
$F_0 = F(\mathbf{x}) \longrightarrow F_t$

ACCORDING TO THE MACROSCOPIC LAW

In Kac's model : $\Omega_0 =$ all signs are $+$ and all configurations of scatterers.

$\overline{\Omega_0} =$ all signs are $+$ and the scatterers belong to that overwhelming majority of configurations of scatterers, discussed above.

$|\Omega_t| \uparrow$ with time
$S_t = k \ \ln |\Omega_t| \ \uparrow$ BOLTZMANN'S ENTROPY
In Kac's model : $S_t = k \ \ln |\Omega_t| = \ln \begin{pmatrix} N \\ N_-(t) \end{pmatrix} = \ln \begin{pmatrix} N \\ N_+(t) \end{pmatrix}$.



$\overline{\Omega_0} \subset \Omega_0$

Ω_t

$\mathrm{I}\ T^t\,\overline{\Omega_0} \not\subset \overline{\Omega_t}$

But $|\mathrm{I}\ T^t\,\overline{\Omega_0}| = |\overline{\Omega_0}| << |\Omega_t|$

$T^t\, \overline{\Omega_0} \subset \overline{\Omega_t}$ for t not too large (BECAUSE OF POINCARE'S RECURRENCE, OR PERIODICITY IN THE KAC MODEL)

$\mathrm{I}\ T^t\, \overline{\Omega_0} \subset \Omega_t$

$\mathrm{I}\ T^t\, \overline{\Omega_0} \not\subset \overline{\Omega_t}$ BECAUSE $\quad T^t\ \mathrm{I}\ T^t \overline{\Omega_0} \subset \Omega_0$

Since $\quad \mathrm{I} T^t\ \mathrm{I}\ T^t \overline{\Omega_0} = \overline{\Omega_0}$, by reversibility.

Not a paradox, because

$|\mathrm{I}\ T^t\, \overline{\Omega_0}| = |\overline{\Omega_0}|$, by Liouville, and $\quad |\overline{\Omega_0}| \leq |\Omega_0| << |\Omega_t|$, so that $|\Omega_t \backslash \overline{\Omega_t}|$ MAY still be small.

Real mathematical problem : need to show that $|\Omega_t \backslash \overline{\Omega_t}|$ small for all times (not too large).

Easy for the Kac's model, hard for a real dynamical system, but no difference in principle, from a "physical" point of view.

Often misunderstood

Irreversibility is either true on all levels or on none : It cannot emerge as out of nothing, on going from one level to another

I. PRIGOGINE and I. STENGERS

Irreversibility is therefore a consequence of the explicit introduction of ignorance into the fundamental laws

M. BORN

Gibbs was the first to introduce a physical concept which can only be applied to an object when our knowledge of the object is incomplete.

W. HEISENBERG

It is somewhat offensive to our thought to suggest that, if we know a system in detail, then we cannot tell which way time is going, but if we take a blurred view, a statistical view of it, that is to say throw away some information, then we can.

H. BONDI

In the classical picture, irreversibility was due to our approximations, to our ignorance.

I. PRIGOGINE

Misleading ‘solution’

Appeal to ergodicity

(Almost) every trajectory in the ‘big’ phase space Ω will spend in each region of that space a fraction of time proportional to its ‘size’ (i.e. Lebesgue volume).

Shows too much and too little !

Too much : we are not interested in the time spent in every tiny region of the phase space Ω !

Too little : ergodicity, by itself says nothing about time scales. We want the *macroscopic* quantities (and only them !) to ‘reach equilibrium’ reasonably fast.

DOES THIS EXPLAIN
IRREVERSIBILITY
AND THE SECOND LAW ?

WHAT DO YOU MEAN BY “EXPLAIN” ?

IN A DETERMINISTIC FRAMEWORK :

IF THE LAWS IMPLY THAT A STATE A AT TIME ZERO YIELDS A STATE B AT TIME t,

THEN B AT TIME t IS “EXPLAINED” BY THE LAWS AND BY A AT TIME ZERO.

OF COURSE, IT REMAINS TO EXPLAIN A.

IN A PROBABILISTIC FRAMEWORK :

IF F_0 IS A MACROSTATE AT TIME ZERO, THEN THERE IS A “NATURAL” MEASURE (THE ONE WITH MAXIMAL ENTROPY) ON THE CORRESPONDING SET $F^{-1}(F_0)$ OF MICROSTATES $\mathbf{x}_0$.

IF, WITH LARGE PROBABILITY WITH RESPECT TO THAT MEASURE, THE MACROSTATE $F(\mathbf{x}_t)$ OBTAINED FROM THE EVOLUTION OF THE MICROSTATE $\mathbf{x}_t$ EQUALS F_t, THEN F_0 AND THE LAWS “EXPLAIN” F_t.

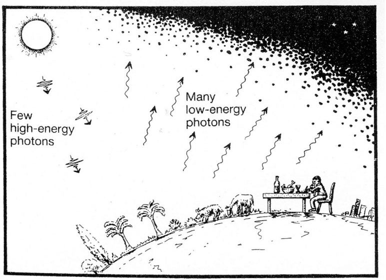
ANOTHER WAY TO SAY THIS, IS THAT ONE EXPLAINS F_t, IF, BY A BAYESIAN REASONING, ONE WOULD HAVE PREDICTED F_t, KNOWING ONLY F_0 AT TIME 0.

WHY DOESN'T THIS ARGUMENT

APPLY TO THE PAST ?

REAL PROBLEM

ORIGIN of the LOW ENTROPY STATES



The sun and the cycle of life

“ God ” choosing the initial conditions of the universe, in a volume of size $10^{-10^{123}}$ of the total volume (according to R. Penrose).
There is no good answer to *that* problem.