

# Microscopic Dynamics and Macroscopic Behavior

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Maryland University, September ..., 2024

# Abstract

The time evolution of out-of-equilibrium macroscopic systems is generally described by time irreversible equations, such as the Navier-Stokes equation. These equations were developed heuristically, based on experimental observations and Newtonian conservation laws, during the nineteenth century. Their rigorous derivation from the reversible dynamics (which we, like the authors of the nineteenth century, will assume to be Newtonian) of the atoms making up the macroscopic system is still a central issue in statistical mechanics. A fundamental advance in this problem was Oscar Lanford's derivation, in the 1970's, of the Boltzmann equation, (for short times) in the Boltzmann-Grad limit. This showed in an explicit example how irreversibility, for typical behavior of macroscopic systems, arises from reversible microscopic dynamics, following an initial nonequilibrium macroscopic state. This still leaves open the question as to what extent the deterministic Boltzmann equation, derived in a certain mathematical limit, gives a good approximation to the time evolution of (turbulent) flows in actual realistic finite systems, where it is argued by some that the Navier-Stokes equations break down. I will discuss these matters in my talk.

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(Much of this work was done jointly with S. Goldstein.)

# Classical Systems

In classical mechanics, the microstate of an isolated system of  $N$  particles confined to a box  $V$  in  $\mathbb{R}^d$  is a point  $X$  in the  $2dN$ -dimensional phase space,  $\Gamma$ ,

$$X = (\mathbf{r}_1, \mathbf{v}_1, \dots, \mathbf{r}_N, \mathbf{v}_N), \quad \mathbf{r}_i \in V \subset \mathbb{R}^d, \quad \mathbf{v}_i \in \mathbb{R}^d \quad (1)$$

Its time evolution is given by a Hamiltonian  $H(X)$  which conserves energy, so  $X(t) = T_t X$  will be confined to the energy surface  $H(X) = E$ . We can take  $H(X)$  to be of the form

$$H(X) = \frac{1}{2} \sum_{j=1}^N \mathbf{v}_j^2 + \sum_{i < j} u(r_{i,j}) \quad (2)$$

with rapidly decaying  $u(r)$ .

## Macrostates

To describe the macroscopic state of such a system,  $M$ , we specify the values of an  $n$ -tuple of macrovariables  $M(X) = \{M_1(X), M_2(X), \dots, M_n(X)\}$ , with resolution  $\Delta M = \{\Delta M_j\}$ . In particular we always choose one of these macro-variables to be the Hamiltonian and replace the energy surface by a thin shell surrounding that surface to which I shall always refer as  $\Gamma_E$ .

The macrostates then partition the energy shell into sets  $\Gamma_M$  of the form:

$$\Gamma_M = \{X | M_j \leq M_j(X) \leq M_j + \Delta M_j, j = 1, \dots, n\}.$$

We then have  $\Gamma_M \subset \Gamma_E$ . I will denote the Liouville volume of  $\Gamma_M$  by  $|\Gamma_M$ .

It can be shown that for all “reasonable” choices of  $M$ , e.g. dividing up the box  $V$  into small regions, but each still containing a large number of particles, and specifying, with some tolerances, the particle, momentum and energy densities in each region of  $V$ , there is in every  $\Gamma_E$  of a macroscopic system one dominant region  $\Gamma_M$  which has most of the volume of  $\Gamma_E$ . This  $M$  is called the equilibrium macrostate  $M_{\text{eq}}$ , and has the property that,

$$\frac{|\Gamma_{M_{\text{eq}}}|}{|\Gamma_E|} = 1 - \varepsilon \quad (3)$$

with  $\varepsilon \ll 1$ , and  $|\Gamma_E|$  the Liouville volume of  $\Gamma_E$ . The existence of a macrostate satisfying (3) is essentially a consequence of the law of large numbers.



Figure 1: Schematic picture of the decomposition of the energy shell  $\Gamma_E$ . Here  $\Gamma_{\text{eq}} \equiv \Gamma_{M_{\text{eq}}}$ .

For classical systems the  $\Gamma_M$  are regions in the energy shell with sizes proportional to their Liouville volume.

The second picture is slightly more faithful. The actual ratio of the sizes is of order  $2^N$  where  $N$  is the number of particles in the system.

A system in a microstate  $X$  is then in macroscopic thermal equilibrium if and only if  $X \in \Gamma_{M_{\text{eq}}}$ . We further note that, for macroscopic systems,  $|\Gamma_M|$  depends strongly on how “close”  $M$  is to  $M_{\text{eq}}$ , the equilibrium macrostate at energy  $E$ , with  $\Gamma_{M_{\text{eq}}}$  occupying almost the whole energy shell  $\Gamma_E$ .

The fact that  $|\Gamma_{M_{\text{eq}}}| \simeq |\Gamma_E|$  explains why one can use the microcanonical ensemble which prescribes a uniform probability density,  $\frac{dX}{|\Gamma_E|}$ , for finding the system in  $dX \subset \Gamma_E$ , to compute properties of an equilibrium system despite the fact that  $\Gamma_E$  contains also nonequilibrium states with energy  $E$ . Their contribution is negligible when  $N \gg 1$ . This is independent of whether or not the dynamics is ergodic in a mathematical sense. In particular it is also true for ideal gases.

In computing properties of macroscopic systems from the micro-canonical ensemble (or from the ???) in equilibrium, such as the number of particles in a region  $\omega \subset V$ , we obtain not only their average value but also fluctuations in these values,  $\langle N_{\text{av}} \rangle = \rho|\omega|$ ,  $\langle (N_\omega - \rho|\omega|)^2 \rangle \sim \chi \sqrt{\langle N_{\text{av}} \rangle}$ , where  $\rho = N/|V|$  and  $\chi$  is the compressibility. For a typical system  $X \in \Gamma_E$  these would correspond to variations in  $N_\alpha$  where  $N_\alpha$  are the number of particles in different boxes  $\omega_\alpha$  with the  $|\omega_\alpha| = |\omega|$ . In the grand canonical ensemble. Similarly the empirical average particle velocity in  $\omega$  should have a ??? magnitude of each ???.

I bring this up here because I think that this is similar to what happens in non-equilibrium systems with flows described by some deterministic equations: flow.

## Approach to Equilibrium

Boltzmann (also Maxwell, Kelvin, ...) then argued that given the disparity in the sizes of the  $\Gamma_M$  corresponding to the various macrostates, the evolution of the vast majority of microstates  $X(t_0)$  in  $\Gamma_M$ , will for  $N \gg 1$  be such that  $|\Gamma_{M(X(t))}|$  will not decrease (on a macroscopic scale) for  $t > t_0$  (and  $t$  smaller than the Poincaré recurrence time, which is larger than the age of the universe).

Thus the evolution towards equilibrium of macroscopic systems which start in the region  $\Gamma_M$ ,  $M \neq M_{\text{eq}}$ , and are kept (effectively) isolated afterwards, is “typical” with respect to the micro-canonical measure restricted to  $\Gamma_M$ .

## Boltzmann's Entropy

To make contact with the second law of Clausius which ascribed an entropy for macroscopic systems in equilibrium, and postulated its increase when one such equilibrium state is changed into another after lifting of a constraint Boltzmann found a microscopic interpretation and generalization by defining the entropy of a macroscopic system in a microstate  $X \in \Gamma_M$  as  $S_B = \log |\Gamma_M|$ .

The previous argumentation says that the vast majority of microstates in  $\Gamma_M$  (not all) will evolve in such a way that

$$S_B(X_t) = \log |\Gamma_{M(X_t)}| = S_B(M(X_t)) \quad (4)$$

will increase with time when  $M(X_{t_0}) \neq M_{\text{eq}}$ . This explains the microscopic origin of the second law for individual macroscopic systems.  $S_B(X_t)$  will increase until  $X(t)$  reaches  $\Gamma_{M_{\text{eq}}}$  where it will stay for a very, very long time. Its entropy will then be given by

$$S_B(M_{\text{eq}}) = \log |\Gamma_{M_{\text{eq}}}| \simeq \log |\Gamma_E| \quad (5)$$

its maximum possible value.

An excellent summary of Boltzmann's ideas can be found in Einstein 's description of Planck's reasoning leading to his discovery of the quantization of energy:

*"On the basis of kinetic theory of gases Boltzmann had discovered that, aside from a constant factor, entropy is equivalent to the logarithm of the "probability" of the [macro] state under consideration. Through this insight he recognized the nature of course of events which, in the sense of thermodynamics, are "irreversible". Seen from the molecular-mechanical point of view, however all courses of events are reversible. If one calls a molecular-theoretically defined state a microscopically described one, or, more briefly, micro-state, then an immensely large number ( $Z$ ) of states belong to a macroscopic condition.  $Z$  is then a measure of the probability of a chosen macro-state. **This idea appears to be of outstanding importance also because of the fact that its usefulness is not limited to microscopic description on the basis of mechanics. Planck recognized this and applied the Boltzmann principle to a system which consists of very many resonators of the same frequency.**"<sup>1</sup>*

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<sup>1</sup>Ei49

Boltzmann's great insight was, as Einstein writes, to identify the entropy of an individual macroscopic system, in some micro-state  $X$ , with the log of  $|\Gamma_M|$  the "number" of  $X$ 's giving rise to the macro-state  $M = M(X)$ .

$|\Gamma_M|$  is proportional to the "probability", with respect to the uniform (micro-canonical) measure, of finding the system in the macro-state  $M$ .

Boltzmann's heuristic argument for the non-decrease of entropy, based on relative phase space volume is, as Einstein says, the correct explanation for the time asymmetric behavior typically observed in actual macroscopic systems. It is, however, very far from a mathematical proof.

A proof would be provided by the rigorous derivation from the microscopic dynamics of the kinetic and hydrodynamic equations such as the heat equation, Navier-Stokes equations, etc. commonly used to describe the time asymmetric, entropy increasing behavior of macroscopic systems out of equilibrium.

This has been achieved so far only for the Boltzmann equation for dilute gases. This equation was derived heuristically by Boltzmann in the 1870's and proven rigorously (in appropriate limits) by Oscar Lanford<sup>2</sup> in 1973. (I particularly recommend his 1976 paper.)

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<sup>2</sup>La 75, 76

To describe Lanford's theorem we have to, following Boltzmann go beyond defining macrostates by the hydrodynamical variables based on dividing  $V \subset \mathbb{R}^d$  into cells and use a more refined description of macrostates. To do that we note that for a system of  $N$  particles in a box  $V$  the microstate  $X = \{\mathbf{r}_i, \mathbf{v}_i\}, i = 1, \dots, N$ , can be described as a set of  $N$  points in six (2d) dimensional one particle space,

$$X \leftrightarrow \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{r}_i) \delta(\mathbf{v} - \mathbf{v}_i), \quad \mathbf{x} \in V, \mathbf{v} \in \mathbb{R}^d. \quad (6)$$

Dividing up this one particle space into cells  $\Delta_\alpha$ ,  $\alpha = 1, \dots, n$ , centered on  $(\mathbf{r}_\alpha, \mathbf{v}_\alpha)$ , of volume  $|\Delta_\alpha|$ , we can, following Boltzmann, describe the macro (meso) states of a gas  $M_f$  by specifying, with some leeway, that the fraction of particles  $N_\alpha(X)/N$  in each  $\Delta_\alpha$  satisfy

$$f_\alpha |\Delta_\alpha| = N_\alpha/N \cong \int_{\Delta_\alpha} f(\mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}. \quad (7)$$

where  $f(\mathbf{x}, \mathbf{v}) \geq 0$  is a smooth distribution in the one particle space. For a dilute gas with negligible potential energy,  $f$  also specifies  $E$ ,  $\Gamma_{M_f} \subset \Gamma_E$ . (When the potential energy is not negligible  $f$  does not specify the energy and we need to add the value of the energy to describe the macrostate, [GL2006].)

## Lanford's Theorem

Consider a gas consisting of  $N$  hard balls of diameter  $d$  in a volume  $V \subset \mathbb{R}^3$  evolving according to Hamiltonian dynamics with elastic collisions.

Keeping  $V$  fixed consider now a sequence of systems with different particle numbers, and different diameters  $d$ , such that  $N \rightarrow \infty$ ,  $d \rightarrow 0$ , while  $Nd^2 \rightarrow b > 0$  (and so  $Nd^3 \rightarrow 0$ ). This is the Boltzmann-Grad (BG) limit:  $b^{-1}$  is proportional to the mean-free-path between collisions.

Choose now a smooth  $f_0(x, v)$  and as  $N$  increases consider microstates  $X_N \subset \Gamma_{M_{f_0}}$  such that the fraction of particles in cubical boxes  $\Delta_\alpha$  is required to satisfy (7) ever more closely, with equality in the BG limit,

$$\lim_{\text{BG}} N_\alpha(X_N)/N = \int_{\Delta_\alpha} f_0(\mathbf{x}, \mathbf{v}) d\mathbf{x}d\mathbf{v}. \quad (8)$$

N.B. The BG limit is required for (8) to hold for arbitrarily small  $\Delta_\alpha$ . The exact distribution of a finite system of  $N$  particles is a sum of  $N$  delta functions, not a smooth  $f$ .

Lanford's theorem then says (roughly):

A typical microstate  $X_N(0) \in \Gamma_{M_{f_0}}$  will evolve, via the Hamiltonian dynamics, to a microstate  $X_N(t)$  such that, in the BG limit

$$\frac{N_\alpha(X_N(t))}{N} = \int_{\Delta_\alpha} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{x}d\mathbf{v} \quad (9)$$

for arbitrarily small  $\Delta_\alpha$ , where  $f(\mathbf{x}, \mathbf{v}, t)$  solves the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = bQ(f, f) \quad (10)$$

with initial condition  $f_0(\mathbf{x}, \mathbf{v})$ .

The BE gives a deterministic evolution from the macrostate  $M_{f_0}$  to the macrostate  $M_{f_t}$  in the BG limit. It describes approximately the evolution of the coarse grained empirical distribution for a dilute gas.

Bodineau et al. [xxx] modified and extended Lanford's theorem. Instead of considering an initial microstate  $X_N \in M_{f_0}$  of the system with  $N$  particles they consider an initial probability measure on the grand canonical phase space with probability

$$W_N^\varepsilon(X_N, t = 0) = \frac{1}{Z_\varepsilon} Z_\varepsilon^N \prod_{i=1}^N f^0(x_i, v_i) 1_{D_N^\varepsilon}(X_N) \quad (11)$$

where  $1_{D_N^\varepsilon}(X_N)$  is the characteristic function of the set  $|x_i - x_j| > \varepsilon$ ,  $\varepsilon$  is the diameter of the level spheres and  $Z_\varepsilon = \varepsilon^2$  in three dimensions. Then  $\varepsilon$  equals  $\alpha/\sqrt{6}$  in Lanford. The average particle number will then grow like  $\varepsilon^{-2}$  as  $\varepsilon \rightarrow 0$ . The  $n$ -particles correlation function, multiplied by  $\varepsilon^{-2n}$ ,  $F_N^\varepsilon(X_n, t)$  evolve according to the solution of the Liouville equation for  $t > 0$ .

The grand canonical version of the Lanford Theorem as given by [BGSS] then states, under mild conditions on  $f^0$ , that in the limit  $\varepsilon \rightarrow 0$ , the rescaled one-particle density  $F_1^\varepsilon(t)$  converges, uniformly on compact sets, to the solution  $f(t)$  of the BE on a time interval  $[0, T_0]$ . Furthermore for each  $n$ , the rescaled  $n$ -particle correlation function  $F_n^\varepsilon(t)$  converges almost everywhere (in the  $n$ -particle phase space) to the product  $f^{(\alpha)n}(t)$  on the same time interval.

Going beyond average behavior BGSS show that this behavior is typical. That is with probability approaching 1, with respect to the original distribution, the empirical measure of the microstates  $X_N$  specified by

$$\Pi_t^\varepsilon = \frac{1}{N} \sum \delta(x - x_i(t)) \delta(v - v_i(t)) \quad (12)$$

concentrates on the solution of the Boltzmann equation. This is of course of crucial importance since what we observe is the behavior of typical individual systems. (This has to be emphasized strongly).

Since the limit  $\varepsilon$  with the density going to infinity as  $\varepsilon^{-2}$  is just a mathematical idealization BLSS consider connections to BE for small  $\varepsilon$ . They show that they are stochastic of order  $\varepsilon$ , leading to a fluctuating BE with Gaussian noise. These are described by adding such small Gaussian noise to the linear deviation from the solution of the Boltzmann equation.

The second law generalized to nonequilibrium macrostates now says that for a *typical* microstate of a dilute gas with  $X(0) \in \Gamma_{M_{f_0}}$ ,  $X(t) = T_t X(0) \in \Gamma_{M_{f_t}}$ , the entropy will be non-decreasing with  $t$ .

This is exactly what happens for  $s_{\text{gas}}(f_t)$  defined in (??) for  $f_t$  evolving according to the Boltzmann equation:

Boltzmann's  $\mathcal{H}$ -theorem :

$$\begin{aligned} \frac{d}{dt} s_{\text{gas}}(f_t) &= \frac{d}{dt} \left\{ - \int_V d\mathbf{x} \int_{\mathbb{R}^3} d\mathbf{v} f_t(\mathbf{x}, \mathbf{v}) \log f_t(\mathbf{x}, \mathbf{v}) \right\} \\ &= b\mathcal{I}(f_t) \geq 0. \end{aligned} \quad (13)$$

As put by Boltzmann<sup>3</sup>:

*"In one respect we have even generalized the entropy principle here, in that we have been able to define the entropy in a gas that is not in a stationary [equilibrium] state."*

We note that the rate of increase of entropy in (13) is proportional to  $b = \lim_{\text{BG}} Nd^2$ . If one takes the limit  $N \rightarrow \infty$ ,  $d \rightarrow 0$  in such a way that  $Nd^2 \rightarrow 0$  then  $b = 0$  and the time derivative of  $s_{\text{gas}}(f)$  given in (13) is equal to zero.

The reason for this lack of change in  $s_{\text{gas}}(f)$  when  $b = 0$  is that  $s_{\text{gas}}(f)$ , defined in terms of a smooth  $f(x, v, t)$  does not capture all the features of the evolution of macrostates, defined in terms of coarse graining,  $|\Delta_\alpha| > 0$ . Keeping  $|\Delta_\alpha| > 0$  is essential for seeing the increase of the Boltzmann entropy from spreading in physical space.

To see the increase of  $s_B(M_f)$  when  $b = 0$  Chakraborti et al. investigated numerically the time evolution of a spatially nonuniform ideal gas in one dimension<sup>4</sup>. They started the system in a microstate  $X$  randomly chosen from  $\Gamma_{M_{eq}}$  of a system of  $N$  particles confined to an interval of length  $L$ , and then, let the gas expand to an interval of length  $2L$ . They chose cells  $\Delta_\alpha$  all of equal size  $\Delta = |\Delta_x||\Delta_v|$  with cutoff on the maximal speed  $|v|$ . They computed the change in

$$s_B^f(t) = \frac{1}{N} S_B(M_f) = \sum_{\alpha} |\Delta_\alpha| f_\alpha \log f_\alpha + \text{Const} \quad (14)$$

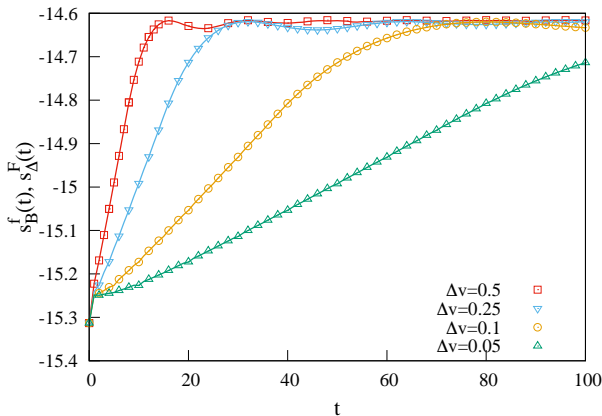
as this system evolved in time without any collisions, see also<sup>5</sup>.

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<sup>4</sup>[Ch21]

<sup>5</sup>[Ch23]

We found, to our surprise, that the time “ $t_{\text{eq}}$ ” it took the system with initial entropy  $S_{\text{eq}}(L)$  to reach the new entropy,  $S_{\text{eq}}(2L) = S_{\text{eq}}(L) + N \log 2$ , depended strongly on the width  $|\Delta v|$  of the single-particle phase space cells used to define the macrostate  $M_f$  and thus the Boltzmann entropy  $S_B(M_f)$ . The smaller  $|\Delta v|$ , the slower the entropy production, see Fig. 2.

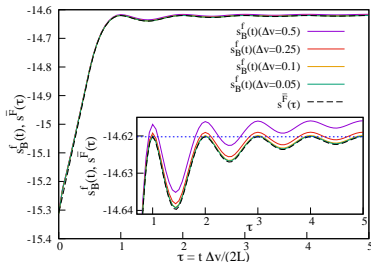


**Figure 2:** The time evolution of  $s_B^f(t)$  when  $X_0$  is chosen at random from an initial  $\Gamma_{M_0}$  corresponding to the phase space region where all  $N$  particles are in the left half of the box with energy  $E \simeq N\epsilon_0$ ,  $\epsilon_0 = 1.25$  corresponding to a temperature 2.5,  $N = 10^7$ . (The continuous line  $s_\Delta^F(t)$ . will be explained later.)

The reason for this strong dependence on  $|\Delta v|$  is that for the ideal gas the only mechanism for uniformizing the velocity distribution over all of space is via the difference between the total distance traveled in a time  $t$  by the particles with velocity  $v$  versus those with velocity  $v + \Delta v$ . In order for the systems to approach equilibrium, this distance must exceed  $L$ , which only occurs after time  $t_{\text{eq}} \sim L/|\Delta v|$ .

The time evolution of the entropy is much less sensitive to the spatial size  $\Delta x$  of the cells. The time scale for the initial uniformization of the spatial density (ignoring the local velocity distributions) is of order  $L/v_{\text{th}}$ , where  $v_{\text{th}}$  is the mean speed, this time is much shorter than  $t_{\text{eq}}$ . It accounts for the apparent jump in  $s$  at  $t = 0$ .

The different curves  $s_B^f(t)$  collapse to a single curve when  $t$  is rescaled as  $t = \frac{2L\tau}{|\Delta v|}$ , where  $2L$  is the circumference of the circle to which our system can be mapped.



**Figure 3:** The figure shows a collapse of the data presented in the previous figure for different values of  $\Delta v$ , on plotting the entropy as a function of the scaled time  $\tau = t\Delta v/(2L)$ . The dashed line in the insert is the graph of  $s^F(\tau)$ , will be defined defined below. The oscillations have period 1 with maxima at  $\tau = 1, 2, \dots$ , the time it takes “ $\Delta v$ ” to go around the circle.

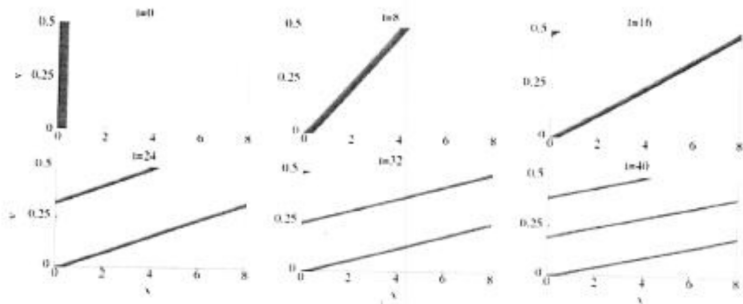


Figure 4: Plot showing the evolution of one of the boxes used earlier,  $N = 10^6$  particles, in the  $(x, v)$  plane, where the particles move on a circle of length  $2L = 8$ . The particles were initially distributed uniformly in a small box with  $\Delta x = 0.25$ ,  $\Delta v = 0.5$ . With time the box gets continually stretched and, at times that are multiples of  $2L/\Delta v = 16$ , the stretched pieces wind completely around the box. Comparing with Fig 3 we see that the maxima in  $s_B^f(t)$  occur at times  $\approx 16, 32$ , at which the winding around the length  $2L$  is complete. [Ch21]

To study analytically the curves in Figures 4 and 5 [Ch21] define

$$F(x, v, 0) = \sum_{i=1}^N \langle \delta(x - r_i) \delta(v - v_i) \rangle, \quad (15)$$

where the average is over the  $\{r_i, v_i\}$  in canonical distribution (equivalent to the microcanonical one with the same energy) for the given density and temperature. We then evolve  $F$  according to Eq. (10) with  $b = 0$ ,  $F(x, v, t) = F(x - vt, v, 0)$ , periodic over the circle. We then integrate  $F(x, v, t)$  over cells  $\Delta_\alpha$  to obtain an averaged  $N_\alpha$  and thus the entropy  $s_\Delta^F(t)$ . This is plotted as a continuous line in Fig2. We see in the figure that  $s_\Delta^F(t)$  coincides with  $s_B^f(t)$ , the entropy computed for a single typical microstate.

Taking the limit  $|\Delta_\alpha| \rightarrow 0$  we obtain  $s^{\bar{F}}(\tau)$  given by

$$s^{\bar{F}}(\tau) = -\frac{1}{N} \int \bar{F}(x, v, \tau) \ln \bar{F}(x, v, \tau) dx dv \quad (16)$$

where

$$\bar{F}(x, v, \tau) = \frac{1}{2L\tau} \int_0^{2L\tau} F(x - x', v, 0) dx'. \quad (17)$$

## Setting

$$F(x, \nu, 0) = \rho h(\nu)[1 + \phi(x, \nu)], \quad \text{with } 2L = 1 \quad (18)$$
$$\phi(x, \nu) = \phi(x + 1, \nu), \quad \int_0^1 \phi(x, \nu) dx = 0.$$

we obtain

$$\begin{aligned} \bar{F}(x, \nu) &= \rho h(\nu) \left[ 1 + \frac{1}{\tau} \int_0^\tau \phi(x - x', \nu) dx' \right] \\ &= \rho h(\nu) \left[ 1 + \frac{1}{\tau} \psi(x, \nu, \tau) \right], \end{aligned} \quad (19)$$

where  $\psi(x, \nu, \tau)$  is periodic in  $\tau$  with period 1 with

$$\psi(x, \nu, n) = 0, \quad \text{for } n = 1, 2, 3, \dots \quad (20)$$

This yields the  $s\bar{F}(\tau)$  plotted in the insert of Figure 3 for the initial condition used. The maxima, all of equal height, occur at  $\tau = 1, 2, \dots$

## Time evolution of the Boltzmann entropy for hard discs

To elucidate the time evolution of  $S_B(M)$  for different choices of  $|\Delta_\alpha|$  when the interaction between the particles is not neglected but the mean free path is still large comparable to the scale of the spatial inhomogeneity Garrido et al. have carried out molecular dynamics computations for the time evolutions of a two-dimensional system of  $N$  hard discs<sup>6</sup>.

The system is started in a microstate  $X$  chosen at random from a canonical Gibbs ensemble with temperature  $T = 1$  (setting  $K_B = 1$ ) in a rectangular box of size  $L_x = 1/2$ ,  $L_y = 1$  with periodic boundary conditions along the  $y$  direction and hard walls constraining the system along the  $x$  direction. The disc's radius  $r$  is fixed in such a way that the system has a given initial areal density  $\eta = \pi r^2 N / |V|$  where  $V = L_x L_y = 1/2$ . The corresponding mean free path when the system is dilute is  $\lambda \sim (\eta N)^{-1/2}$ .

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<sup>6</sup>P. Garrido, S. Goldstein, D. Huse and J.L.L (in preparation)

At time  $t = 0$  we remove the hard walls and let this gas of discs expand to a box of size  $L_x = L_y = L = 1$  with now periodic boundary conditions along both directions. We study the time evolution of this system until it reaches an equilibrium state  $X \in \Gamma_{M_{\text{eq}}}$  in this larger periodic box.

The degrees of freedom associated with  $y$  and  $v_y$ , along which direction the system does not expand, remain near thermal equilibrium. Therefore the Boltzmann entropy associated with these  $y, v_y$  degrees of freedom remains approximately constant in time while the system expands along the  $x$  direction and approaches the new thermal equilibrium.

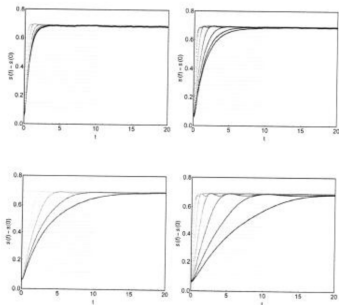
We will consider only the entropy due to the degrees of freedom associated with  $x$  and  $v_x$ , since it is this part of the entropy that is most out of equilibrium and changing with time.

Thus we divide the four-dimensional one-particle phase space  $(x, v_x; y, v_y)$  into cells  $\Delta_\alpha$  of extent  $\Delta x$  and  $\Delta v_x$  in the  $(x, v_x)$  plane with each cell including the full range of  $y$  and  $v_y$ . We count  $N_\alpha(t)$ , the number of particles in  $\Delta_\alpha$  at time  $t$  and evaluate the

$$s(t; \Delta, N, \eta) = -\frac{\Delta}{N} \sum_{\alpha} \frac{N_{\alpha}(t)}{\Delta} \log \frac{N_{\alpha}(t)}{\Delta}. \quad (21)$$

All cells have equal “area”  $|\Delta_\alpha| = |\Delta x| |\Delta v_x| = \Delta$  in the  $(x, v_x)$  plane.

## Results for different values of the mean free path $\lambda$ :



**Figure 5:** Boltzmann entropy for  $N = 10^5$  and areal densities  $\eta = 10^{-6}$  (upper left),  $\eta = 10^{-7}$  (upper right),  $\eta = 10^{-8}$  (lower left) and  $\eta = 10^{-9}$  (lower right) for 16 cells along the  $x$  direction and different values of  $|\Delta v_x|$ .

The mfp for the different boxes are  $\lambda \approx .7$ ,  $\lambda \approx 2.2$ ,  $\lambda \approx 5$ ,  $\lambda \approx 22$ . For  $\lambda \approx 22$  the dependence on  $|\Delta v_x|$  is the same as for the ideal gas,  $\lambda = \infty$ , while for  $\lambda = .7$  there is almost no dependence on  $|\Delta v_x|$ . It is this latter case for which  $s_{\text{gas}}(f)$  is a good approximation to the entropy of the dilute gas. This is surely what Boltzmann had in mind.

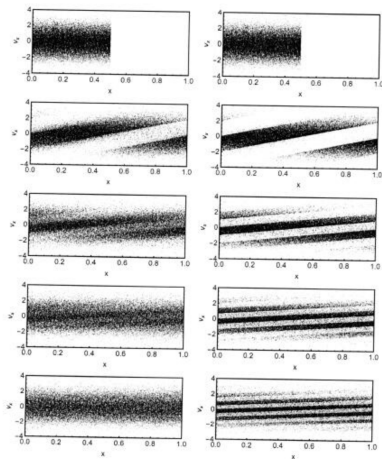
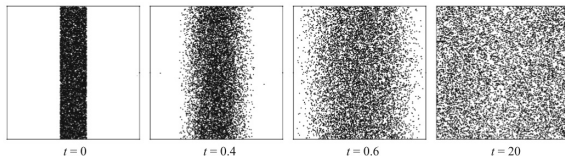


Figure 6:  $(x, v_x)$ -phase space typical evolution of a system in the  $x, v_x$  plane with  $N = 10^5$  discs with areal densities  $\eta = 10^{-4}$  (left column) and  $\eta = 10^{-6}$  (right column) for times (from top to bottom)  $t = 0.0, 0.5, 1.0, 1.50$  and  $2.0$ .

The spatial time evolution of an ideal gas in a torus is analyzed in detail in a very nice paper by S. De Bievre and P.E. Parris<sup>7</sup>. They consider an initial distribution of  $N$  point particles with a product measure  $\prod f_0(r_i, v_i)$ , corresponding to a uniform density in part of a unit torus and a “smooth” velocity distribution, say Maxwellian with variance 1.



**Figure 7:** (From BP) Numerical simulation of the free expansion on the 2-torus of a non-interacting gas of  $10^4$  particles having a thermal distribution of momenta with mean thermal speed equal to unity, initially confined in the horizontal direction to the region  $0.4 < x < 0.6$ , at the sequence of times indicated.

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<sup>7</sup>BiPa17

To define the macro state  $M_f$  BP divide the unit torus into  $\mathcal{L}$  squares,  $D_j$ ,  $j = 1, \dots, \mathcal{L}$ , of area  $D$  each, and specify the fraction of particles in each region with uncertainty  $\epsilon$ .  $M_{\text{eq}}$  then corresponds to “uniform density”, i.e. the fraction  $f_j$  of particles in  $D_j$ , satisfy  $|f_j - D| < \epsilon$ ,  $\epsilon > 0$ , for **every**  $j$ .

Fixing  $\mathcal{L}$  and  $\epsilon$ , BP prove that a system picked at random from the initial  $\Gamma_{M_f}$  will, with probability,  $P \geq 1 - \delta_N$ ,  $\delta_N = Le^{-\frac{1}{4}\epsilon^2 N}$ , uniformly spread out, i.e. will be in equilibrium, for an exponentially long time period  $t$ ,  $\tau_1 < t < \tau_2$ . Here  $\tau_1$  is of order 1 and  $\tau_2$  is exponentially large in  $N$ , corresponding to Poincaré recurrence time.

This is what is meant by the approach to equilibrium, i.e. a uniform distribution, being **typical** behavior for phase points in the initial macrostate.

I highly recommend this paper.

## More General Macroscopic Equations

Going beyond the examples described above suppose, more generally, that the time evolution of the macrostate  $M$ , given by  $M(X(t)) = M_t$ , effectively satisfies an autonomous deterministic time asymmetric equation, such as the diffusion or the heat equation. (I shall consider here for simplicity macrostates  $M$  which are invariant under velocity reversal.)

Having such an equation means that if  $t_3 > t_2 > t_1$ , then the microscopic dynamics  $T_t$  carries almost all of  $\Gamma_{M_{t_1}} = \Gamma_{M_1}$ , inside  $\Gamma_{M_2}$  and  $\Gamma_{M_2}$  inside  $\Gamma_{M_3}$ , i.e.  $T_{t_2-t_1}\Gamma_{M_1} \subset \Gamma_{M_2}$  and  $T_{t_3-t_2}\Gamma_{M_2} \subset \Gamma_{M_3}$ , with *negligible error*. Put otherwise a typical phase point in  $\Gamma_{M_1}$  will go to  $\Gamma_{M_2}$  and then to  $\Gamma_{M_3}$ , i.e.  $T_{t_3-t_1}\Gamma_{M_1} \subset \Gamma_{M_3}$ , c.f. [Go04].

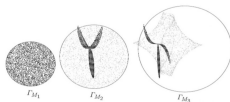


Figure 8: Time evolution of  $\Gamma_{M_1}$

The fact that phase space volume is conserved by the Hamiltonian time evolution implies that  $|\Gamma_{M_1}| \leq |\Gamma_{M_2}| \leq |\Gamma_{M_3}|$ , and thus that  $S_B(M_3) \geq S_B(M_2) \geq S_B(M_1)$ .

Hence the solution of any deterministic macroscopic equation for  $M_t$  has to satisfy the inequality<sup>8</sup>  $\frac{d}{dt} S_B(M_t) \geq 0$ , exactly what Boltzmann showed for the BE.

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<sup>8</sup>Go04,Pe70

We note that the existence of such a macroscopic equation implies (at least insofar as the macro-variables are concerned) that the phase points in the region in  $\Gamma_2$  coming from  $\Gamma_1$  behave, forward in time, as microstates typical of  $\Gamma_2$ .

They are, however, very atypical backwards in time. Thus if we reverse all the velocities in  $\Gamma_2$ , then at a later time,  $t' = t_2 + (t_2 - t_1)$  all of the points initially in  $\Gamma_{M_1}$  will again be in  $\Gamma_{M_1}$  (with their velocities reversed), a smaller region than  $\Gamma_{M_2}$ , while  $|\Gamma_{M_{t'}}| \geq |\Gamma_{M_2}|$ .

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