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Macroscopic laws, microscopic dynamics, time's arrow and Boltzmann's entropy*

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I discuss Boltzmann's resolution of the apparent paradox: microscopic dynamics are time-symmetric but the behavior of macroscopic objects, composed of microscopic constituents, is time-asymmetric. Noting the great disparity between macroscales and microscales Boltzmann developed a statistical approach which explains the observed macroscopic behavior. In particular it predicts the increase with time of the "Boltzmann entropy", $S_B(X)$, for "almost all" microscopic states X, of a nonequilibrium macroscopic system. The quantitative description of the macroscopic evolution, and ipso facto the compatibility between the macroscopic descriptions and microscopic descriptions, is illustrated by an example: the rigorous derivation of a diffusion equation for the typical macroscopic density profile of a Lorentz gas of independent electrons moving according to Hamiltonian dynamics. The role of low entropy "initial states" is emphasized.

1. Introdnction

For the purpose of this article, my notion of space–time is essentially the Newtonian one in which time symmetric basic laws connect the states of a physical system, possibly of the whole universe, at different instants of time. This of course does not take account of relativity, special or general, and is therefore certainly not the whole story. Still I believe that the phenomenon we wish to explain, namely the time asymmetric behavior of spatially localized macroscopic objects, is for all practical purposes the same in a non-relativistic universe. I will therefore focus here on idealized versions of the problem in the simplest context, i.e. look at the evolution in time of a macroscopic system governed by non-relativistic Hamiltonian dynamics. The role of quantum mechanics will be discussed briefly at the end.

The analysis I present here is certainly not novel. It consists mostly of restatements and updatings, in contemporary language, of something important that Boltzmann discovered about the microscopic origin of macroscopic

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behavior [1]. Boltzmann's ideas eliminate the need for devising new theories or new equations, *which are not driven by really novel experiments or insights*, for the sole purpose of dealing with the "problem of irreversibility".

Boltzmann's very original ideas were, perhaps not surprisingly, difficult to grasp for some of his contemporaries. What is surprising is that some of the confusion created by these misunderstandings, the so-called "controversies' with Zermelo and others still persist at present. There is really no excuse for this considering the clarity of Boltzmann's responses and later writings [1]. I strongly recommend reading these papers – they are absolutely beautiful. I only hope that my presentation here retains some of that clarity. In preparing it I have benefited much from refs. [2–5]. I highly recommend these books, and of course ref. [1] as well as Boltzmann's other works [6], for further reading on this subject.

Boltzmann's statistical theory of the nonequilibrium (time asymmetric, irreversible) behavior of macroscopic systems is based on associating to each macrostate M and thus *to each microstate* X which gives rise to M $(=M(X))$ a (Boltzmann) entropy $S_B(M(X))$. This entropy coincides (up to terms negligible in the size of the system), with the ensemble (Gibbs) entropy $S_G(\rho)$ *when* the ensemble density ρ is one of local equilibrium – they are both equal then to the macroscopic thermodynamic entropy. For such ensembles there is essentially no distinction between average and typical values of macroscopic variables. However, unlike S_G, which does not change in time for an isolated system, even when the system is not in equilibrium, S_B typically increases in a way which *explains* and describes qualitatively the evolution towards equilibrium of such systems. This means that S_G, and other quantities like it, are simply not the right objects to look at in the latter context. The constancy of S_G for isolated systems and the resulting disagreement with S_B is therefore not a "problem" of irreversibility or of anything else (despite what is written in many textbooks and articles). It simply reflects the fact that the distinction between microscopic and macroscopic behavior, which is both the problem and the essential ingredient in its resolution, is not captured by S_G. It is however contained in the very definition of S_B, whose increase provides information about the qualitative behavior of macroscopic systems.

The quantitative description of the macroscopic evolution is given by hydrodynamical-type equations which can be derived (explicitly, in some cases) from the microscopic dynamics by utilizing the collective aspect of macrobehavior, i.e. as a law of large numbers arising from the very large macro/micro-ratio [7–9]. These equations describe the typical irreversible behavior of individual macroscopic systems, not just that of ensemble averages. It is this time-asymmetric behavior, manifested in a single typical evolution of macroscopic system, which distinguishes macroscopic irreversibility from the *chaotic* be-

havior of systems with but a few degrees of freedom having good ergodic properties, e.g. two hard spheres in a box.

On the other hand the instabilities induced by "locally" chaotic behavior do play a role in determining the nature of the macroscopic evolution. An example of this is provided by the Lorentz gas consisting of a macroscopic number of non-interacting particles moving among a periodic array of fixed convex scatterers (with finite horizons). Combining results of Bunimovich and Sinai [10], which depend on the "deterministic chaos" in single scatterings, with some work of Lebowitz and Spohn [11], one can derive rigorously a diffusion equation for typical macroscopic particle density profiles of this system in the hydrodynamic scaling limit (macro/micro-ratio goes to infinity).

I want to emphasize again however that the central role in time asymmetric behavior is played by the very large number of degrees of freedom involved in the evolution of macroscopic systems. It is only this which permits statistical predictions to become "certain" ones for *typical individual realizations*, where, after all, we actually observe irreversible behavior. This *typicality* is very robust – the essential features of macroscopic behavior are not dependent on any precise assumptions, such as ergodicity, mixing or "equal a priori probabilities", being strictly satisfied by the statistical distributions. The latter are in fact, for our purposes, nothing more than mathematical tools for describing individual macroscopic behavior.

2. Qualitative aspects of macroscopic behavior

Consider an isolated macroscopic system evolving in time, as exemplified by the schematic macroscopic snapshots of a fluid (or solid) in the four frames in fig. 1. The dots in this figure represent pictorially some excess density variable of the fluid (relative to a baseline represented by the blank space) at different times during the undisturbed evolution of the system. For concreteness let the bottom half of the system in fig. 1a be hotter than the top half (higher kinetic energy density) while in fig. 1d the temperature is uniform. Fig. 2 shows schematic graphs of the same profiles. The question is to identify the time order in which the sequence of snapshots was taken.

The "obvious" answer, based on experience, is that time increases from left to right – any other order is clearly impossible. Now it would be very simple and nice if this answer could be shown to follow directly from the microscopic laws of nature. But this is not the case, for the microscopic laws, as we know them, tell a different story: if the sequence going from left to right is a permissible one, so is the one going from right to left. This is most easily seen in classical mechanics and so I shall use this language for the present. I believe

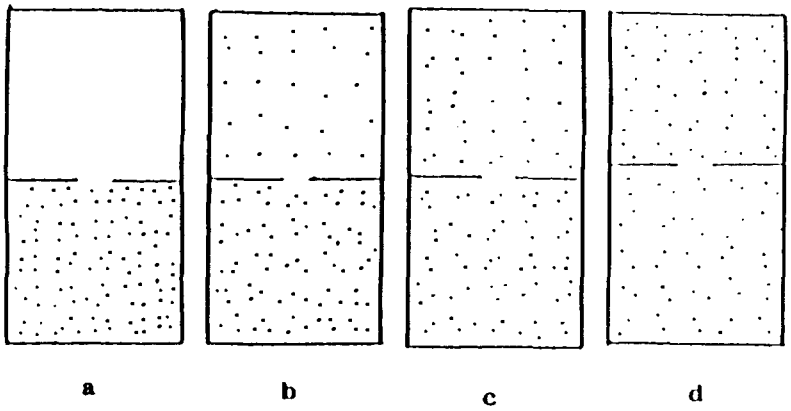

Fig. 1. Snapshots of macroscopic density profiles on an isolated system at four different times.

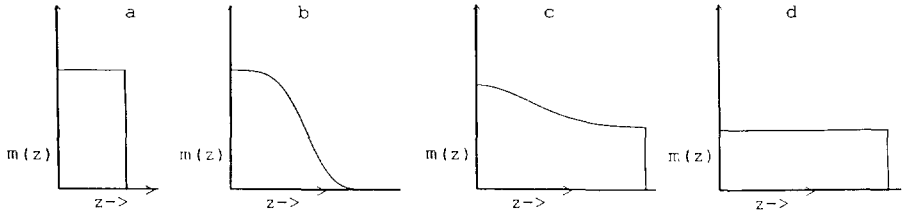

Fig. 2. Plot of the macroscopic density field $m(z)$ for the snapshots in fig. 1.

that the situation is similar in quantum mechanics and will briefly discuss that here, in section 5, cf. ref. [12].

2.1. *The problem of time asymmetry*

The complete microscopic (or micro) state of an isolated classical system of N particles can be represented by a point X in its phase space Γ, $X = (\boldsymbol{r}_1, \boldsymbol{v}_1, \boldsymbol{r}_2, \boldsymbol{v}_2, \ldots, \boldsymbol{r}_N, \boldsymbol{v}_N)$, $\boldsymbol{r}_i$ and $\boldsymbol{v}_i$ being the position and velocity of the ith particle. The Hamiltonian time evolution of this microstate is described by a flow T_t, i.e. if $X(t_0)$ is the microstate at time t_0, then the state at time t_1 is given by

$$X(t_1) = T_{t_1 - t_0} X(t_0) .$$

Consider now states $X(t_0)$ and $T_\tau X(t_0) = X(t_0 + \tau)$, $\tau > 0$. Reversing (physically or mathematically) all velocities at time $t_0 + \tau$, we obtain a new micro-

scopic state, which we denote by $RX(t_0 + \tau)$. If we now follow the evolution for another interval τ we find that the new microstate at time $t_0 + 2\tau$ is just the state at $X(t_0)$ with all velocities reversed, i.e. $T_\tau R T_\tau X(t_0) = RX(t_0)$.

Let us return now to the sequence of snapshots in fig. 1. These clearly do not specify the microscopic state X of the system; rather they represent macroscopic states, which we denote by M. To each macrostate M there corresponds a set of microstates making up a region Γ_M in the phase space Γ. Thus if we were to divide the box in fig. 1 into say a million little cubs then the macrostate M in each frame could simply specify (within some tolerance) the kinetic energy K_j of particles in cube j, $j = 1, \ldots, 10^6$. In order to properly specify the region Γ_M we need to know also the total energy of this system E, the total particle number N, and any other (macroscopically relevant) constants of the motion (also within some tolerance).

While this specification of the macroscopic state clearly contains some arbitrariness, this need not concern us right now. What is important is that the snapshots shown in the figure would remain unchanged if we reversed all the velocities of the particles so that if $X \in \Gamma_M$ then also $RX \in \Gamma_M$. Now we see the problem with our definite assignment of a time order to the snapshots in the figure: going from a macrostate M_1 at time t_1, to another macrostate M_2 at time $t_2 = t_1 + \tau$, $t > 0$, means that there is a microstate $X \in \Gamma_M$, for which $T_\tau X = Y \in \Gamma_{M_2}$, *but* then also $RY \in \Gamma_{M_2}$ and $T_\tau RY = RX \in \Gamma_{M_1}$. Hence the snapshots depicting M_α, $\alpha =$ a, b, c, d, in fig. 1 could, as far as the laws of mechanics (which we take here to be the laws of nature) go, correspond to a sequence of times going in either direction.

It is thus clear that our judgement of the time order in fig. 1 was not based on the dynamical laws of evolution alone; they permit either order. Rather it was based on experience: one direction is common and easily arranged, the other is never seen. *But why should this be so?*

2.2. *Boltzmann's answer*

The answer given by Boltzmann's statistical theory starts by associating to each macroscopic state M and thus to each phase point X (through the $M(X)$ which it defines) a "Boltzmann entropy", defined (up to multiplicative and additive constants) as

$$S_B(M) = \log|\Gamma_M| , \tag{1}$$

where $|\Gamma_M|$ is the phase space volume associated with the macrostate M, i.e. $|\Gamma_M|$ is the integral of the Liouville volume element $(\Pi_{i=1}^N \mathrm{d}\boldsymbol{r}_i \, \mathrm{d}\boldsymbol{v}_i)$ over Γ_M. Boltzmann's stroke of genius was to make the connection between this

microscopically defined function $S_B(M)$ and the fact or expectation than when a macroscopic constraint is lifted in a system, as when an isolating wall dividing two halves of a box (such as the one in fig. 1) is removed, the dynamical motion of the microscopic phase point will "more likely" wander into newly opened regions of Γ for which Γ_M is large than into those for which Γ_M is small. Thus if we monitor the time evolution of the macrostate $M(t)$ (short for $M(X(t))$) we expect it to change is such a way that $S_B(M(t))$ will "typically" increase as time increases.

To see that this expectation coincides with and in fact explains the observed behavior of macroscopic systems Boltzmann made a direct connection between $S_B(M)$ and the thermodynamic entropy of Clausius, S_{eq}, which is a macroscopically defined, operationally measurable (up to additive constants), extensive function of macroscopic systems in *equilibrium*. For a system in equilibrium at a given energy E and volume V,

$$S_{eq}(E, V, N) = Ns_{eq}(e, n) \simeq S_B(M_{eq}), \qquad e = E/N, \quad n = N/V\ , \tag{2}$$

where $M_{eq}(E, V, N)$ is the macrostate corresponding to the system in equilibrium at a given E and V. By $\simeq$ we mean that for large N, when the system is really macroscopic, the equality holds up to negligible terms when both sides of (2) are divided by N and the additive constant, which is independent of e and n, is suitably fixed. (We require here that the number of cells used to define M_{eq} should grow more slowly than N.) For a lucid discussion of S_B see ref. [3] and also refs. [13,14].

Boltzmann's great insight thus not only gave a microscopic interpretation of the mysterious thermodynamic entropy of Clausius, it also gave a natural generalization of entropy to nonequilibrium macrostates M and with it a plausible explanation of the origin of the second law of thermodynamics – the formal expression of the time-asymmetric evolution of macroscopic states occurring in nature. In particular it explains why the sequence going from left to right in fig. 1 under the action of the system's Hamiltonian is natural; if we posit an initial state M_a where the two parts of the box are in equilibrium at different temperatures then left to right corresponds to a sequence of M's with increasing $S_B(M)$, and hence Γ_M, which is highly likely. Going the other way requires the initial X to evolve in a way which would make $S_B(M)$ and thus Γ_M *decrease*, which is highly unlikely.

To understand why we *never* see the unlikely case it should be noted that when the system in fig. 1 is really macroscopic, say one mole in a one liter container, with a temperature difference between the two halves in fig. 1a of several degrees, the ratio of $\Gamma_{M_{eq}}$ of the unconstrained system and the one constrained in each half of the container (roughly $|\Gamma_{M_d}|/|\Gamma_{M_a}|$) is of order $10^{10^{20}}$.

The "probability" of seeing the unlikely evolution is then roughly the inverse of this number. This also explains why, for systems like these, we do not have to worry too much about the precise specification of macrostates. We thus have "almost" a microscopic derivation of the second law.

2.3. *The use of probabilities*

Boltzmann's ideas are, as Ruelle [5] says, at the same time simple and rather subtle. They introduce into the "laws of nature" notions of probability, as indicated by the use of such words as "likely", "expected", etc., which, certainly at that time, were quite alien to the scientific outlook. Physical laws were supposed to hold without any exceptions, not just almost always. It appears to me that even now Boltzmann's seminal ideas are still not universally understood. Let me try to explain how I understand them.

Let us first consider the system in fig. 1a to be in equilibrium in each half of the box – insulated from the other half by a wall. Observations and analysis show that, for a system in equilibrium, the values of certain types of phase functions $f(X)$ such as the number of particles contained in some subset of the volume, their kinetic energy in that region, will fluctuate in time about some stationary mean value. The single- and multi-time statistics of such observations (obtained by independent repetitions of a specified experiment or situation) will be stationary in time – that is more or less what is meant by the system being in equilibrium. Furthermore the relative magnitude of these fluctuations will decrease as the size of the region increases. A quantitative theory of this fluctuation behavior can be obtained by the use of the Gibbs microcanonical ensemble [3,6,14]. This ensemble assigns probabilities to finding the microstate X of an equilibrium system with energy E and volume V in a phase space region Δ proportional to the volume of Δ. The normalizing factor for these probabilities is the volume of the energy surface – which as indicated later in (5) is, for macroscopic systems, essentially the same as $|\Gamma_{M_{eq}}|$. (As is well known the other commonly used Gibbs ensembles, canonical, grand-canonical, etc., are equivalent in their predictions to the microcanonical one for relevant macroscopic observables and so need not be considered separately here.)

These probabilities can be interpreted either subjectively or as a statement about empirical statistics. Whatever the interpretation we can, using the microcanonical ensemble, compute the probability that the lifting of a constraint from a system in equilibrium will result in a particular evolution of the macrostates. In particular it specifies the notion of typicality: a certain behavior is typical if the set of microscopic states X in Γ_M for which it occurs comprises a region whose volume fraction goes to one as N grows. Thus going back now to

the time ordering of the macrostates in fig. 1 we can say that the sequence going from left to right is typical for a phase point in Γ_{M_a} while the one going from right to left has probability approaching zero with respect to a uniform distribution in Γ_{M_d}, for large N.

It is clearly important for our consideration that the microcanonical ensemble is, by Liouville's theorem, time invariant under the dynamics. For ergodic systems one can regard these probabilities as representing the fraction of time (over a sufficiently long time period) which the system spends in Δ. For such systems the microcanonical ensemble is the only stationary measure whose probability density is absolutely continuous with respect to the projection of Liouville measure on the energy surface in Γ [3,15]. Given the ubiquitous presence of deterministic chaos, it is reasonable to assume that real macroscopic systems are *effectively* ergodic.

It should be noted however that there is no experimental evidence that this assignment of equal a priori probabilities to equal phase space volumes (which is also the classical limit of the equal a priori probability assignment to each quantum state), compatible with the macrostate of an equilibrium system specified with a suitable tolerance, exactly describes empirical statistics for every arbitrary small phase space region (or quantum state). How could we tell if the assumption of equal a priori probabilities for equilibrium systems failed for a volume fraction which vanishes rapidly as N increases. Even more to the point, we could not tell a uniform density from a non-uniform one if the domains on which the density differed were sufficiently entangled on the energy surface of a macroscopic system. There is clearly no way we can experimentally analyze the behavior of macrosystems with sufficient accuracy to detect this sort of failure of uniformity. There is also no theoretical necessity for such an assumption in determining the ordering of the sequence in fig. 1. Since the behavior of $S_B(M)$ is typical for points X in Γ_{M_a} and atypical for points in Γ_{M_d} the ordering would not change if we used any other smooth distribution, e.g. one having a piecewise continuous density $\rho(X)$, inside Γ_{M_a} or Γ_{M_d}. Of course when we make mathematical models we naturally want to keep them structurally as simple as possible.

2.4. *Irreversibility and macroscopic stability*

Mechanics itself does not of course rule out having a microstate X, by velocity reversal or otherwise, for which $S_B(M(X_t))$ would be decreasing as t increases. We could, for example, in principle reverse all velocities of the system in figs. 1b, 1c or 1d, although it seems effectively impossible to do so in practice: for some reason (possibly profound), human beings can, as Leggett puts it, "prepare" but not "retropare" states [16]. However even if we

managed to do so, as occurs (at least partially) in spin echo experiments [17], we would not expect to see the sequence in fig. 1 go from right to left. This is related to the following observations: the macroscopic behavior of a system with microstate Y in the state M_b *coming* from M_a which is typical with respect to Γ_{M_a}, i.e. such that $T_{-\tau}Y$ is typical of Γ_{M_a}, and for which therefore $S_B(M(T_{-\tau}Y)) < S_B(M(Y))$, is *stable* against perturbations as far as its future is concerned but very *unstable* as far as its *past* (and thus the future behavior of RY) is concerned. That is, the *macrostate* corresponding to T_tY is stable for $t > 0$ but unstable for $t < 0$. I am thinking here primarily of situations where the equations describing the macroscopic evolution, e.g. the Navier–Stokes equations, are stable. In situations, such as the weather, where the forward macroscopic evolution is chaotic, i.e. sensitive to small perturbations, cf. ref. [5], all evolutions will still have increasing Boltzmann entropies in the forward direction. For the backward evolution of the microstates however, the unperturbed one has decreasing S_B while the perturbed ones have (at least after a very short time) increasing S_B. So even in macroscopically "chaotic" regimes the forward evolution of M is much more stable than the backward one.

This behavior can be understood intuitively by making the natural assumption that almost any perturbation of Y will tend to make the microstate more and not less typical of Γ_{M_b}. It will thus not interfere with the unperturbed behavior of increasing S_B for all $t > 0$. The forward evolution of RY is on the other hand towards a smaller phase space volume which requires "perfect aiming". It can therefore be expected to be derailed by even smaller imprecisions in the reversal and/or tiny random outside influences. This is somewhat analogous to those pinball machine type puzzles where one is supposed to get a small metal ball into a particular small region. You have to do things just right to get it in but almost anything you do gets it out into larger regions. For the macroscopic systems we are considering the disparity between relative sizes of the comparable regions in the phase space is unimaginably larger. The behavior of such systems will therefore be as observed, in the absence of any "grand conspiracy".

The difference between the stability of the macroscopic evolution in the forward, entropy-increasing, direction and its instability in the reverse direction is very relevant to understanding the behavior of systems which are not completely isolated – as is the case in practice with all *physical systems*. In the direction in which the motion is stable this lack of complete isolation interferes very little with our ability to make predictions about macroscopic behavior. It however almost completely hampers our ability to actually observe "back motion" for any extended time following the application of some type of velocity reversal as in the case of spin echo experiments [17]. After a *very short* time in which S_B decreases the imperfections in the reversal and the "outside"

perturbations, such as one coming from a sun flare, a star quake in a distant galaxy (a long time ago) or from a butterfly beating its wings nearby [5], will make it increase again. The same happens also in computer simulations where velocity reversal is easy to accomplish but where roundoff errors play the role of perturbations.

3. Initial conditions

I hope that I have convinced you by now that Boltzmann's explanation of why macroscopic systems evolve in a way which makes S_B increase is very reasonable. I am afraid however that you might wake up in the middle of the night and start worrying and then arguing with me in a form expressed by Schrödinger as follows [18]: "First, my good friend, you state that the two directions of your time variables, from $-t$ to $+t$ and from $+t$ to $-t$ are a priori equivalent. Then by fine arguments appealing to common sense you show that disorder (or 'entropy') must with overwhelming probability increase with time. Now, if you please, what do you mean by 'with time'? Do you mean in the direction $-t$ to $+t$? But if your interferences are sound, they are equally valid for the direction $+t$ to $-t$. If these two directions are equivalent a priori, then they remain so a posteriori. The conclusions can never invalidate the premise. Then your inference is valid for both directions of time, and that is a contradiction."

Put in terms of our example in fig. 1 the point is that on the one hand if we just consider the system with a general non-uniform macroscopic density profile such as shown in fig. 1b, then experience shows that we can predict that its future behavior will be like M_c by assuming that its microstates are typical of Γ_{M_b}, i.e. of local equilibrium consistent with M_b. On the other hand if we use such a local equilibrium state to compute via Newton's equations the antecedent macrostate of a typical micro state $X \in \Gamma_{M_b}$, we get also a macrostate like M_c and not anything resembling M_a. This is of course obvious and inevitable: since the local equilibrium ensemble corresponding to the macrostate M_b, at some time t, gives equal weight to microstates X and RX it must make the same prediction for $t - \tau$ as for $t + \tau$.

We are thus apparently back to something akin to our old problem: Why can we use statistical arguments based on phase space volume (e.g. local equilibrium type ensemble) considerations to make predictions about the future behavior of macroscopic systems but not to make retrodictions? Now in the example of fig. 1 if indeed the macrostate M_b *came* from M_a, and we take its microstate at that *earlier time* to be typical of equilibrium with a constraining wall, i.e. of Γ_{M_a}, then its microstate corresponding to M_b is *necessarily* atypical

of points in Γ_{M_b} since by Liouville's theorem the set of all such phase points has at most volume $|\Gamma_{M_a}|$, which is much smaller than $|\Gamma_{M_b}|$. Nevertheless its *future* but not its *past* behavior, as far as macrostates are concerned, will be similar to that of typical points taken from Γ_{M_b}. It is for this reason that we can use autonomous equations, like the diffusion equation, to predict *future* behavior of real macroscopic systems without worrying about whether their microstates stay typical for their macrostates. They will certainly not be so after the system has been fully isolated for some time while its S_B has been increasing. (The fact that local equilibrium ensembles do not remain such was a great worry to Krilov [19] but it does not appear to me to be a real problem.) Of course in the real world the inevitable small outside perturbations discussed before might in fact push the system towards typicality, particularly if we wait long enough, and have come to an equilibrium macrostate.

The above analysis thus explains why, if shown only the two snapshots M_b and M_c and told that the system was isolated for some time interval which included the time between the two observations, our ordering would be M_b before M_c and not vice versa. This would in fact be based on there being an initial state like M_a, with even lower entropy than M_b, for which the microstate was typical. From such an initial state we get a monotone behavior of $S_B(t)$ with the time ordering M_a, M_b and M_c. If on the other hand we *knew* that the system in fig. 1 had been *completely* isolated for a very long time, compared to the hydrodynamic relaxation time of the system before the snapshots in fig. 1 were taken then (in this *very very very* unlikely case) we would have no basis for assigning an order to the sequence since fluctuations from equilibrium are typically symmetric about times in which there is a local minimum of S_B. In the absence of any knowledge about the history of the system before and after the sequence we use our experience to deduce that the low entropy state M_a was the initial prepared state.

3.1. *Origin of low entropy states*

The origin of low entropy initial states poses no problem in "laboratory situations" such as the one depicted in fig. 1. In such cases systems are prepared in states of low Boltzmann entropy by "experimentalists", who are themselves in low entropy states. Like other living beings they are born in such states and maintained there by eating low entropy foods which in turn are produced by plants using low entropy radiation coming from the sun, etc., cf. ref. [4]. Their macrostates are of course much more complex than those of the fluid in fig. 1 permitting them in particular to deliberately create, in localized spatial regions, certain types of macrostates M with low values of $S_B(M)$, like the state M_a in fig. 1. There are of course some things they cannot do; in

particular it appears that they cannot violate the general rule that the "total S_B", including the entropy of the experimentalists and their instruments, must always increase, i.e. there are no Maxwell demons [20]. (Note however that the reversal of velocities, in which S_B is unchanged, is not ruled out by this requirement.) But what about the origin of these creatures or about events in which there is no human participation, e.g. if instead of fig. 1 we are given snapshots of a meteor and the moon before and after their collision? Surely the time direction is just as obvious as in fig. 1.

To answer this question along the Boltzmann chain of reasoning leads more or less inevitably (depending on considerations outside our domain of discourse) to a consistent picture with an initial "state of the universe" having a very small Boltzmann entropy, i.e. an initial macrostate M_0 for which $|\Gamma_{M_0}|$ is a very small fraction of the "total available" phase space volume. Roger Penrose, in his excellent chapter on the subject of time asymmetry [4], takes that initial state, the macrostate of the universe just after the "big bang", to be one in which the energy density is uniform. He then estimates that $|\Gamma_{M_0}|/|\Gamma_{M_f}| \sim 10^{-10^{123}}$, where M_f is in the state of the "final" crunch, with $|\Gamma_{M_f}| \sim$ total available "phase-space" volume. This is a sufficiently small number (in fact much smaller than necessary) to produce all we observe. The initial "microstate of the universe" can then be taken to be typical of Γ_{M_0}.

In R. Penrose's analysis the low value of $S_B(M_0)$, for a universe with a uniform density, compared to $S_B(M_f)$ is due to the vast amount of the phase space corresponding to macrostates with black holes, in which the gravitational energy is very negative. I do not claim to understand the technical aspects of this estimate, which involves the Bekenstein–Hawking formula for the entropy of a black hole; it certainly goes beyond the realm of classical mechanics being considered here. The general idea, however, that the gravitational energy, which scales like N^2 for a star or galaxy, can overwhelm any non-gravitational terms, which scale like N, seems intuitively clear. It is this pure "high quality" or low entropy form of the gravitational energy which appears to be the source of all organizational order we observe in the universe [21]: including ultimately our consciousness.

3.2. The cosmological initial state problem

I hope that I have convinced you that, as Schrödinger says, "Boltzmann's theory . . . really grants an understanding . . .". It certainly gives a plausible and consistent picture of the evolution of the universe following some initial low entropy state M_0. The question of how M_0 came about is of course beyond my task (or ability) to answer. That would be, as Hawking puts it, "knowing the mind of God". Still, as R. Penrose has pointed out, it would be nice to have a

theory which would force, or at least make plausible, an initial M_0 so special that its phase space volume $|\Gamma_{M_0}|$ is infinitesimally small compared to the proverbial needle in the haystack, see fig. 7.19 in ref. [4]. He and others have searched, and continue to do so, for such a theory. While these theories properly belong to the, for me, esoteric domain of quantum cosmology there is, from a purely statistical mechanical or Boltzmannian point of view, a naturalness to a spatially homogeneous initial state M_0. Such an M_0 would indeed be an equilibrium state in the absence of gravity. It is therefore tempting to speculate that "creation" or the big bang was "just" the turning on of gravity, but I am told by the more knowledgeable that this is quite unreasonable. The initial state problem is thus very much open. It is by far the oldest open problem.

Within the context of special (or singular) origin theories of which the big bang (followed by inflation) is a special example, there is nothing, not even time, before the initial state. There is an alternate suggestion, dating back to much before the advent of the big bang theory, in which one does not have to assume a special singular creation. Boltzmann speculated that a low entropy "initial state" may have arisen naturally as a fluctuation from an "equilibrium universe". This is in some ways a very appealing minimal hypothesis requiring no beginning or end or special creation. All you have to do is wait "long enough" and you will get any state you want, assuming that a microcanonical ensemble and some mild form of ergodicity exist for the universe as a whole. This requires, at the minimum, some short range regularization of gravity. We shall not worry however about such "technical details" since, as we shall argue next, such a hypothesis is very implausible for other entirely conceptual reasons.

While the obvious objection to this hypothesis, that such a fluctuation is enormously unlikely, can be countered by the argument that if indeed the history of the microstate of the universe is typical of trajectories in Γ then, without waiting for some huge fluctuation, we humans would not be here to discuss this problem, there remains a more serious objection. As pointed out by Schrödinger and others and particularly by Feynman [2], the actual "size" of the observed ordered universe is too large by orders and orders of magnitude for what is needed. A fluctuation producing a "universe" the size of our galaxy would seem to be sufficient for us to be around. In fact using *purely* phase space volume arguments the "most likely" fluctuation scenario of how I come to be here is to write this article is one where only "I" or even only my consciousness really exists, i.e. one in which the smallest region possible is out of equilibrium – and this happened just this instant. While irrefutable as an academic debating position this is, of course, even more in conflict with our observed macrostate (e.g. our memories). Merely accepting that what we

observe and deduce logically from our marvelous scientific instruments about the world is really there, the idea of a recent fluctuation seems "ridiculous" and therefore makes the whole fluctuation from equilibrium scenarios seem highly implausible. In fact Feynman, after discussing the problem in some detail, concludes (in the tape of his lecture) that "... it is necessary to add to the physical laws the hypothesis that in the past the universe was more ordered, in the technical sense, than it is today – to make sense, and to make an understanding of the irreversibility" [2].

The "technical sense" in the above statement clearly refers to the initial state M_0 having a smaller S_B. Once we accept such an initial macrostate M_0, then the initial microstate can be assumed to be typical of Γ_{M_0}. We can then apply our statistical reasoning to the further evolution of this initial state despite the fact that it was a very unlikely one. As Schrödinger says in another place when discussing this problem [22] "Never be afraid of dangers that have gone by! It is those ahead that matter." One can of course construct alternative scenarios in which the initial microstate would be *atypical* with respect to M_0. It seems to me however that there is a strong rationale for not accepting such an *additional* improbable beginning without being forced to it by some observational considerations.

4. Boltzmann vs. Gibbs entropies

The Boltzmannian approach described in the last section, which focuses on understanding the observed time-asymmetric evolution of a particular macroscopic system, is conceptually different from the Gibbsian approach, which focuses more on ensembles. Of course the two descriptions (of the same reality) also have much in common and, when used properly, the mathematical elegance of the Gibbsian approach beautifully complements the physical directness of the Boltzmannian one and makes statistical mechanics both mathematically deep and physically precise.

The difference between individual systems and ensemble behavior shows up strikingly when we compare Boltzmann's entropy – defined for a microstate X of a macroscopic system – with the more commonly used (and misused) entropy S_G of Gibbs, defined for an ensemble density $\rho(X)$ by

$$S_G(\{\rho\}) = -\int \rho(X)\,[\log \rho(X)]\,dX\,. \tag{3}$$

Of course if we take $\rho(X)$ to be the generalized microcanonical ensemble associated with a macrostate M,

$$\rho_M(X) \equiv \begin{cases} |\Gamma_M|^{-1}, & \text{if } X \in \Gamma_M, \\ 0, & \text{otherwise}, \end{cases} \tag{4}$$

then clearly

$$S_G(\{\rho_M\}) = \log|\Gamma_M| = S_B(M). \tag{5}$$

The two entropies thus agree with each other, and with the macroscopic thermodynamic entropy, for systems in which the particle density, energy density and momentum density vary slowly on a microscopic scale *and* the system is in each small macroscopic region in equilibrium with the prescribed local densities, i.e. in local equilibrium. This equivalence holds for terms of the order of the size of the regions over which the densities are uniform (see discussion after eq. (2)). The Gibbs ensemble formalism thus provides the right tools also for systems in local thermodynamic equilibrium.

Note however that unless the system is in complete equilibrium and there is no further systematic change in M or ρ then the time evolutions of S_B and S_G are *very* different. As is well known, $S_G(\{\rho\})$ never changes in time as long as X evolves according to the Hamiltonian evolution, i.e. ρ evolves according to the Liouville equation, while $S_B(M)$ certainly does. In particular, if we consider the microcanonical ensemble corresponding to the macrostate M_a in fig. 1, and then remove the constraint, then S_G would equal S_B at that initial time. Subsequently S_B would typically increase while S_G would not change with time [3]. S_G therefore does not give any indication that the system is evolving towards equilibrium. This reflects the fact, discussed earlier, that the microstate of the system $T_t X$ does not remain typical of the local equilibrium state $M(t)$ for $t > 0$. As long as the system remains truly isolated the state $T_t X$ will contain subtle correlations, which are reflected in the ensemble $\rho(t)$ but which do not affect the future time evolution of M. *Thus the relevant entropy for understanding the time evolution of macrosystems is S_B and not S_G.* The use of S_G in nonequilibrium situations is often a convenient technical tool but is not related directly to the behavior of an individual macroscopic system. In fact when a system with macrostate M is not in local equilibrium then we always have $S_B \geq S_G$.

There are many people, however, who find S_G so nice where it works that they want to keep it for general nonequilibrium situations, even if they have to mutilate it. For this and other reasons many authors, beginning with Gibbs, have introduced the notion of "coarse graining" [3,23]. This means that the ensemble density $\rho(t)$ is replaced by a coarse grained or smoothed out density $\bar{\rho}(t)$, constructed by dividing the phase space Γ into cells and replacing $\rho(t)$ by a constant average density in each cell. When the cells are chosen, as they

usually are, to correspond to macrostates $M(t)$, then, to the extent that one can neglect the dispersion about the average of $M(t)$, the coarse graining can be thought of as replacing the actual $\rho(t)$ by a local equilibrium one, and thus replacing the time independent S_G by the increasing $S_B(M(t))$ at all $t > t_0$ [23]. If the dispersion is not negligible, we still have for the ensemble average of S_B, $\langle S_B(M(t))\rangle \simeq S_G(\{\bar{\rho}(t)\})$. One can thus with some effort get out of the self-inflicted bind caused by the use of S_G but it should be clear that attempts to assign a deep physical significance to S_G and other "entropies" like it can often lead to unnecessary confusion.

5. Quantitative aspects of macroscopic behavior

My discussion so far has dealt with the general qualitative features of the evolution of macroscopic systems: starting with a microstate X_0 typical of a nonequilibrium macrostate, Γ_{M_0}, the successive microstates are characterized by the increase of Boltzmann's entropy,

$$S_B(M(X(t))) \geq S_B(M(X(t'))) , \qquad \text{if } t > t' . \tag{6}$$

We can, however, do much better, at least when we deal with the evolution of relatively simple systems such as the one depicted in figs. 1 and 2. We can then give, for suitably chosen macrodescriptions, highly accurate quantitative descriptions, via purely macroscopic autonomous equations, of the time evolution of $M(t)$. I am sure that most of you have recognized that fig. 2 represents the solution of a diffusion equation for some macroscopic field $m(\boldsymbol{r}, t)$, of the form

$$\frac{\partial m(\boldsymbol{r}, t)}{\partial t} = \frac{\partial}{\partial \boldsymbol{r}} \left(\boldsymbol{D}(m) \cdot \frac{\partial}{\partial \boldsymbol{r}} m(\boldsymbol{r}, t) \right) , \qquad t \geq t_a , \tag{7}$$

with some diffusion tensor $\boldsymbol{D}$ and suitable initial conditions at $t = t_a$.

5.1. *Macroscopic laws: general considerations*

Eq. (7) is an example of an autonomous hydrodynamical law governing the time evolution of macroscopic densities. These laws generally take the form of non-linear partial differential equations,

$$\frac{\partial}{\partial t} M_\alpha(\boldsymbol{r}, t) = F_\alpha(\boldsymbol{M}(\boldsymbol{r}, t), \operatorname{grad} \boldsymbol{M}(\boldsymbol{r}, t), \ldots), \qquad \alpha = 1, 2, \ldots , \tag{8}$$

where $\boldsymbol{M}(\boldsymbol{r}, t) = \{M_\alpha(\boldsymbol{r}, t)\}$ denotes a "full" set of macroscopic densities depending on space and time. While $\boldsymbol{M}$ and $\boldsymbol{F}$ are specific to the phenomena

considered, their dependence on the exact nature of the microscopic constituents of the macroscopic objects studied is in general small. The details of microscopic structure generally enter in $\boldsymbol{F}$ only through the numerical value of some parameters or their functional dependence on the densities, e.g. the dependence of $\boldsymbol{D}$ on m in (7).

The origin of this universality lies in the fact that the hydrodynamical laws are a consequence solely of the existence of different spatial and temporal scales for microscopic and macroscopic phenomena, and some very general features of the microscopic dynamics. The former is just what we already discussed in the previous part. Most important among the latter are the locality and additivity of the interactions and the resulting local conservation laws (local on the macroscale). Consequently, our microscopic models can be rather crude and still give rise to quantitatively correct macroscopic behaviour. All that is necessary, is that the models contain the essential features responsible for the phenomena of interest. Direct visual evidence for this has come recently from computer simulations implementing microscopic dynamics for "large" numbers of particles. These have shown dramatically how similar indeed self-organized macroscopic evolutions are, resulting from very different microscopic models – including Ising-like cellular automata; see the lecture by Bernie Alder in this volume, and references there.

The utility of simple models, e.g. the Ising spin system, is well established for equilibrium behavior and there has been much recent progress in the mathematical derivation of hydrodynamic-type laws of the form of eq. (8) for similarly simple dynamical models [7–9]. I believe that these models capture the essential features of the transition from microscopic to macroscopic evolutions in real physical systems. In all cases the resulting equations describe the typical behavior of a single macroscopic system chosen from a suitable initial ensemble, i.e. there is vanishing dispersion of the values of the macroscopic variables in the limit of micro/macroscale ratio going to zero.

Unfortunately, due to our poor mathematical abilities, the derivation of hydrodynamical laws is far from complete for systems with realistic Hamiltonian dynamics. To make rigorous the arguments leading from the microscopic evolution to the macroscopic one requires, at present, some amount of stochasticity in the microscopic evolution. The only exception I know of is the Lorentz gas, which I shall discuss later. First, however, I want to make a slight detour to tell you about the "best" current results for general Hamiltonian systems. This is due to Olla, Varadhan and Yau [24] and while it is not directly related to irreversibility, as they actually derive the dissipationless Euler equations, it should give you a feel for where this program stands at present.

Olla, Varadhan Yau (OVY) manage to reduce the problem of proving hydrodynamical laws for some systems, including Hamiltonian ones, to a

reasonable, ergodicity type condition on the dynamics. To prove such ergodicity for deterministic Hamiltonian systems is unfortunately still a formidable unsolved problem, so OVY have to add a diffusive noise mimicking "randomizing collisions" between pairs of particles. This noise conserves momentum and energy, but otherwise uniformly spreads the relative momenta. It is sufficiently weak not to affect the hydrodynamical behavior on the time scale on which the Euler equations of hydrodynamics are valid. These are

$$\frac{\partial n(\boldsymbol{r}, t)}{\partial t} = -\boldsymbol{\nabla}\cdot[n\boldsymbol{u}(\boldsymbol{r}, t)]\,, \tag{9a}$$

$$\frac{\partial[n\boldsymbol{u}(\boldsymbol{r}, t)]}{\partial t} = -\boldsymbol{\nabla}\cdot[n\boldsymbol{u}\boldsymbol{u} + p(n, e)]\,, \tag{9b}$$

$$\frac{\partial[ne(\boldsymbol{r}, t)]}{\partial t} = -\boldsymbol{\nabla}\cdot[ne\boldsymbol{u} + \boldsymbol{u}p]\,, \tag{9c}$$

where n, $n\boldsymbol{u}$ and ne are the conserved particle, momentum and energy densities, and $p(n, e)$ is the equilibrium pressure of the system at uniform densities n and e and thus depends on the microscopic interactions. The variables $\boldsymbol{r}$ and t in (9) are measured in macroscopic units which are related to the corresponding microscopic scales, say $\boldsymbol{x}$ and s, by $\boldsymbol{x} = \epsilon^{-1}\boldsymbol{r}$ and $s = \epsilon^{-1}t$. The hydrodynamical scaling limit corresponds to letting the ratio of microscopic to macroscopic length scales $\epsilon \to 0$. Note that time and space are scaled proportionally to each other. This is also the scaling under which eqs. (9) remain invariant.

The thermodynamic entropy obtained by assuming that the fluid, confined to a macroscopic region V, is in local thermodynamic equilibrium is given by

$$S_{\mathrm{l.eq}} = \int_V \mathrm{d}\boldsymbol{r}\, n(\boldsymbol{r}, t)\, s_{\mathrm{eq}}(e(\boldsymbol{r}, t), n(\boldsymbol{r}, t)) \simeq S_{\mathrm{B}}(M(t))\,, \tag{10}$$

with $s_{\mathrm{eq}}(e, n)$ defined in (2). The equality on the right is to be understood as holding up to order ϵ, ϵ^{-1} being the length on the microscopic scale over which the system is in a uniform equilibrium state. As is well known $S_{\mathrm{l.eq}}$ does not change in time under the Euler evolution (9), as long as the flow is smooth, i.e. no shocks. The constancy in time of the Boltzmann entropy for a smooth solution of the Euler equations (9) is to be understood also as corresponding to S_{B}/V, V being of order ϵ^{-3}, in the limit $\epsilon \to 0$. The existence of smooth solutions of (9) for times $t' \leq t$ is in fact one of the requirements of OVY for the validity of (9) at time t. The derivation, but presumably not the result, breaks down at a time t_{s}, when the solution of (9) develops a shock. (There are

also some "technical" requirements on the Hamiltonian which are irrelevant here.)

It is interesting to note that the derivation of OVY uses the fact that for microscopic times $s = \epsilon^{-1}t$, $t < t_s$, there are no dissipative effects, i.e. S_B is unchanged to leading order, ϵ^{-3}. Thus starting from a local equilibrium ensemble $\rho_{M(0)}$, $M(0)$ corresponding to the densities, $n(\boldsymbol{r}, 0)$, $\boldsymbol{u}(\boldsymbol{r}, 0)$ and $e(\boldsymbol{r}, 0)$, the Gibbs and Boltzmann entropies (per particle) agree at $t = 0$ and since neither changes for $t < t_s$ they have to continue to agree. On the other hand $S_B(M(t))$ agrees with $S_G(\{\rho_{M(t)}\})$ for some $M(t)$. Thus if $\rho(t)$ is the actual ensemble density, starting with $\rho(0) = \rho_{M(0)}$, then $S_G(\{\rho(t)\}) = S_G(\{\rho_{M(t)}\})$, which in fact implies (using a lot of deep mathematics) that $M(t)$ evolves, for $t < t_s$, according to (9).

It should be emphasized again that the artificial stochasticity added to the Hamiltonian dynamics by OVY disappears in the hydrodynamical scaling limit $\epsilon \to 0$. The results of OVY were extended by Fritz [25] to prove Euler type equations for hydrodynamical lattice gases of the type discussed by Alder. The randomness needed here is more "short range" and thus in some sense "more physical" than that needed by OVY; Fritz, Funaki and Lebowitz [26] have investigated similar mechanisms, for Hamiltonian systems. Ultimately one hopes of course to do away with any need for artificial randomness and derive (9) directly from Hamiltonian dynamics in the limit $\epsilon \to 0$.

This is the current situation for general fluids – we understand the origin of the non-dissipative equations (9); they arise from the macro space-time scaling $\boldsymbol{r} = \epsilon \boldsymbol{x}$, $t = \epsilon s$ when $\epsilon \to 0$, but some mathematical details are still missing. To see dissipation, as expressed by the Navier–Stokes equations for a fluid, in which the rhs of (9b) and (9c) are modified by the addition of viscous and heat conduction terms, we need to take account of the fact that in reality ϵ is not zero; it is roughly of the same order as the ratio of interatomic spacings to the distance over which the macroscopic densities change significantly, say angströms to millimeters. The irreversible changes in which S_B increases significantly then require microscopic times of order ϵ^{-2}, the time scale appropriate for diffusion, for gradients of order ϵ. However, unlike the pure diffusion equation (6), which remains invariant under the transformation $\boldsymbol{r} \to \lambda \boldsymbol{r}'$, $t \to \lambda^2 t'$, the Navier–Stokes equations have no such scaling behavior. It is therefore unclear at present whether they are exact in some limit or are just the leading correction to the Euler equations. The situation is somewhat different for the incompressible Navier–Stokes equations for the velocity field $\boldsymbol{u}(\boldsymbol{r}, t)$ with n and e taken as constant. These have the form

$$\frac{\partial \boldsymbol{u}}{\partial t} = -\boldsymbol{\nabla} \cdot [\boldsymbol{u}\boldsymbol{u} + \boldsymbol{\Pi}] + \nu \nabla^2 \boldsymbol{u}\,, \qquad \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0\,, \tag{11}$$

where ν is the kinetic viscosity and $\boldsymbol{\Pi}$ is the stress tensor computed from the velocity field. Eq. (11) is invariant when $\boldsymbol{r} \to \lambda \boldsymbol{r}'$, $t \to \lambda^2 t'$ and $\boldsymbol{u} \to \lambda^{-1} \boldsymbol{u}'$. This means that it can in principle be obtained from the microscopic dynamics when the macroscopic velocity is small, i.e. of order ϵ compared to thermal velocities. At the present time such a derivation can in fact be made starting from the Boltzmann equation [27] whose status I shall discuss briefly later. First, however, I want to describe an example in which we can derive an irreversible macroscopic diffusion equation from a reversible microscopic Hamiltonian dynamics without any additional assumptions.

5.2. *The Lorentz gas*

We consider the Lorentz model of a classical gas of non-interacting particles moving in a fixed periodic array of hard convex scatterers, e.g. hard spheres in three dimensions or hard discs in two. This model, also known as the Sinai billiard, possesses very strong hyperbolic properties; we assume that the particle can travel only a uniformly bounded distance between collisions. This allows the diffusive Brownian motion of a single particle to be rigorously established in the long-length- and time-scale limit. More precisely, what Bunimovich and Sinai [10] proved for two dimensions and Chernov [28] extended to higher dimensions, is the following: Let $\boldsymbol{x}(t; \theta_0, \boldsymbol{x}_0)$ be the position at time t of a particle with initial position $\boldsymbol{x}_0$ and initial unit velocity in the direction θ_0. (Since the magnitude of the velocity is not changed by the dynamics we consider a particle with unit speed.) If there is an uncertainty in the initial position $\boldsymbol{x}_0$ given by the probability density $p(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ then this will induce a probability distribution on the trajectories $\boldsymbol{x}(t; \cdot)$. Define now the "macroscopic" position $\boldsymbol{y}_\epsilon$ at the macroscopic time t, as

$$\boldsymbol{y}_\epsilon(t; \cdot) = \epsilon \boldsymbol{x}(t/\epsilon^2; \cdot)\,. \tag{12}$$

Then, as $\epsilon \to 0$, a "typical" trajectory looks, on the macroscopic scale, just like Brownian motion, i.e.

$$\boldsymbol{y}_\epsilon(t; \cdot) \underset{\text{weakly}}{\longrightarrow} \boldsymbol{W}_{\boldsymbol{D}}(t)\,. \tag{13}$$

Here $\boldsymbol{W}_{\boldsymbol{D}}(t)$ is d-dimensional Brownian motion starting at the origin with a positive diffusion tensor $\boldsymbol{D}$, given by the Green–Kubo formula. Weak convergence means roughly that on the macroscopic scale the behavior of the trajectory, e.g. the correlations between its position in different regions of space at different times, is indistinguishable from that of a Brownian path.

Let us consider now the case where we have a Lorentz gas in a macroscopic

box, say a cube with sides of length $2bL$ where b is a fixed number, say ten, and L is the macrolength unit, $L = \sigma/\epsilon$, σ some unit of microscopic distance, e.g. the diameter of a scatterer, which is kept fixed, and $\epsilon \ll 1$. Let X represent a microscopic phase point in the phase space region Γ in which all particles have unit speed and let the macrostate M corresponding to X be specified by a smooth initial density $n_0(\boldsymbol{r})$ on the macroscale $\boldsymbol{r}$, $-b \leq r_\alpha \leq b$, $\alpha = 1, 2, 3$. This could be our system in fig. 1, in which the scatterers are invisible, and in which $n_0(\boldsymbol{r}) = c_1$ for $-b \leq r_3 < 0$, $n_0(\boldsymbol{r}) = c_2$ for $0 < r_3 < b$, $c_1 > c_2$. Since this many-body system is very far from being ergodic, the kinetic energy of every particle being separately conserved, we consider the Gibbs ensemble with uniform density on the phase space region $\Gamma_M \subset \Gamma$ in which *each* particle has unit speed and the macrodensity is given by $n_0(\boldsymbol{r})$. Let now $\epsilon^d \mathcal{N}(\omega/\epsilon^d, t/\epsilon^d)$ be the number of particles in a macroscopic region ω of volume $|\omega|$, having volume $|\omega|/\epsilon^d$ in microunits, at the microscopic time t/ϵ^2. Then it follows from the work of Lebowitz and Spohn [11] that as $\epsilon \to 0$, the random variable $\epsilon^d \mathcal{N}(\omega/\epsilon^d, t/\epsilon^2)$ approaches a deterministic value

$$\epsilon^d \mathcal{N}(\omega/\epsilon^d, t/\epsilon^2) \xrightarrow[\epsilon \to 0]{} \int_\omega n(\boldsymbol{r}, t)\, \mathrm{d}\boldsymbol{r}\,, \tag{14}$$

where $n(\boldsymbol{r}, t)$ satisfies (6) with $n(\boldsymbol{r}, 0) = n_0(\boldsymbol{r})$ and the $\boldsymbol{D}$ obtained by Bunimovich and Sinai via the Kubo formula. The approach in (14) is with probability one, i.e., it holds for every typical point X of the initial ensemble.

5.3. *Dilute gases and Boltzmann's h-function*

The Boltzmann equation is a deterministic, time-asymmetric, integro-differential equation for the time evolution of the density of particles $f_1(\boldsymbol{r}, \boldsymbol{v})$ in the six-dimensional position and velocity space of the system, the so-called μ-space (μ for molecule, Γ for gas). It was "derived" by Boltzmann, using intuitively appealing heuristic reasoning, *for a dilute gas in which the potential energy is negligible.* While f_1 is usually referred to as a "mesoscopic" description, intermediate between the microdescriptions and macrodescriptions described so far, we can in fact sometimes usefully think of f_1 as describing the macroscopic state M of such a system, cf. ref. [7]. The Boltzmann equation is then another type of macroscopic equation to be derived from the microscopic dynamics in some suitable scaling limit. This requires in addition to the hydrodynamical scaling of the Euler type discussed earlier, also a reduction in the particle density as a function of ϵ so that on the "macroscopic scale" the density is of order ϵ. This keeps the mean free path between collisions finite while the pressure and energy become those of a non-interacting system (ideal

gas). In this limit, which is equivalent to what is usually referred to as the Boltzmann–Grad limit [7], Lanford was able to derive rigorously the irreversible Boltzmann equation from the reversible Hamiltonian dynamics of a system of hard spheres (or more general finite range interactions) [29]. The results (which, at present, are unfortunately restricted to "short" times) are for typical microscopic phase points with respect to a suitable initial measure [7,29].

Forgetting about limits and just talking physically, we note that for the choice of the macrostate M corresponding to $f_1(\boldsymbol{r}, \boldsymbol{v})$ the Boltzmann entropy $S_B(f_1)$ coincides (up to constants) with the negative of Boltzmann's famous h-function,

$$S_B(f_1) = -h_B(f_1) = \int\int f_1(\boldsymbol{r}, \boldsymbol{v}) \log f_1(\boldsymbol{r}, \boldsymbol{v})\, d\boldsymbol{r}\, d\boldsymbol{v} . \tag{15}$$

Now according to the Boltzmann equation, S_B will keep on increasing until the system reaches equilibrium when $S_B(f_1)$ is equal to $Ns_{eq}(e, n)$ given in (2). This is correct as long as the potential energy is really negligible. When this is not the case however then it is possible to create experimentally a situation, see ref. [30], in which $h_B(f_1)$ decreases with time. To see this let the macroscopic system of N particles in volume V with total energy E start out, at $t = 0$, with a Maxwellian distribution of velocities, $f_1(\boldsymbol{r}, \boldsymbol{v}, 0) = f_M(n, T_0; \boldsymbol{v})$ with uniform particle density $n = N/V$ and kinetic temperature T_0, where

$$f_M(n, T; \boldsymbol{v}) = n(2\pi k_B T/m)^{-3/2} \exp(-mv^2/2k_B T) . \tag{16}$$

Now if the initial T_0 is greater than the equilibrium temperature of this system, $T_{eq}(E)$, determined by the total energy E (and volume V), then the system will evolve toward a state in which $f_1(\boldsymbol{R}, \boldsymbol{v}, t) \to f_M(n, T_{eq}; \boldsymbol{v})$ with $T_{eq} < T_0$ and $-h_B(f_1)$ will decrease since

$$h_B(f_1(\infty)) - h_B(f_1(0)) = \tfrac{3}{2} N \log[T_0/T_{eq}(E)] > 0 . \tag{17}$$

The choice of an initial Maxwellian is of course inessential. All that is required is that $h_B(f_1(\boldsymbol{r}, \boldsymbol{v}, 0))$ be smaller than $h_B(f_M(n, T_{eq}; \boldsymbol{v}))$, see ref. [30].

On the other hand, for any reasonable initial f_1 the correct $S_B(f_1)$, defined by eq. (1), will of course (almost) never decrease. There is no contradiction here since when the potential energy is not negligible, $S_B(f_1) \neq -h_B(f_1)$. Of course, the Boltzmann equation is not valid in the case when the potential energy is not negligible since it assumes from the beginning conservation of kinetic energy and an ideal gas equation of state.

The existence and efficiency of the interaction terms is what leads to the Euler equations, rather than the Boltzmann equation, when the density is not

taken to zero as $\epsilon \to 0$. Note also that there is no contradiction in S_B staying constant for the Euler evolution but increasing for the Boltzmann equation. In the low density limit required for the validity of the Boltzmann equation $\epsilon^2 S_B \to 0$ and the entropy given by (15) is of lower order in ϵ.

6. Quantum mechanics

The analysis given above in terms of classical mechanics can be rephrased, formally at least, in terms of quantum mechanics. We make the following correspondences:

(i) microstate $X \Leftrightarrow$ wave function $\psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$;
(ii) time evolution $T_t X \Leftrightarrow$ unitary Schödinger evolution $U_t \psi$;
(iii) velocity reversal $RX \Leftrightarrow$ complex conjugation $\bar{\psi}$;
(iv) phase space volume of macrostate $|\Gamma_M| \Leftrightarrow$ dimension of projector on macrostate M.

This correspondence clearly preserves the time symmetry of classical mechanics. It does not however take into account the non-unitary or "wave function collapse" (measurement) part of quantum mechanics, which on the face of it appears time asymmetric. In fact it is sometimes said that quantum theory "is concerned exclusively with the prediction of probabilities of specific outcomes of future measurements on the basis of the results of earlier observations. Indeed the reduction of the wave packet has as its operational contents nothing but this probabilistic connection between successive observations." The above quote is taken from an old article by Aharonov, Bergmann and Lebowitz (ABL) [12], which to me still seems reasonable now. In fact I will now quote the whole abstract of that article:

"We examine the assertion that the "reduction of the wave packet", implicit in the quantum theory of measurement, introduces into the foundations of quantum physics a time-asymmetric element, which in turn leads to irreversibility. We argue that this time asymmetry is actually related to the manner in which statistical ensembles are constructed. If we construct an ensemble time symmetrically by using both initial and final states of the system to delimit the sample, then the resulting probability distribution turns out to be time symmetric as well. The conventional expressions for prediction as well as those for "retrodiction" may be recovered from the time-symmetric expressions formally by separating the final (or the initial) selection procedure from the measurements under consideration by sequences of "coherence destroying" manipulations. We can proceed from this situation, which resembles prediction, to true prediction (which does not involve any postselection) by adding to the time-symmetric theory a postulate which asserts that ensembles with unambiguous

probability distributions may be constructed on the basis of preselection only. If, as we believe, the validity of this postulate and the falsity of its time reverse result from the macroscopic irreversibility of our universe as a whole, then the basic laws of quantum physics, including those referring to measurements, are as completely time symmetric as the laws of classical physics. As a by-product of our analysis, we also find that during the time interval between two noncommuting observations, we may assign to a system the quantum state corresponding to the observation that follows with as much justification as we assign, ordinarily, the state corresponding to the preceding measurement."

Aharonov[#1] has emphasized and developed further the idea described in the last sentence of the abstract. He assigns two wave functions to a system – one coming from the past and one from the future measurement. It is not clear to me whether this will lead to new insights into the nature of time. Aharonov does think so and there are others too who feel that there are new fundamental discoveries to be made about the nature of time [31]. While this is certainly something interesting to think about, it definitely goes beyond my premises so I will not pursue this further here.

Quite aside from that I believe that the ABL analysis shows that one can conceptually and usefully separate the measurement formalism of conventional quantum theory into two parts, a time symmetric part and a second-law type asymmetric part – which can be traced back, using Boltzmann type reasoning, to the initial low entropy state of the universe. (Of course it is not clear how to discuss meaningfully the concept of measurement in the context of the evolution of the universe as a whole, but see the recent works by Gell-Mann and Hartle [32] and Hartle [33].)

7. Concludiug remarks

The reader who has gotten to this point will have noticed that my discussion has focused almost exclusively on what is usually referred to as the thermodynamic arrow of time and on its connection with the cosmological arrow. I did not discuss the asymmetry between advanced and retarded electromagnetic potentials or "causality" [31]. It is my general feeling that these and other arrows, like the one in the wave packet reduction discussed in the last section, are all manifestations of Boltzmann's general principle, and of the low entropy initial state of the universe. For this reason I also agree with most physicists that there would be no change in the monotone increase of entropy if and when the universe stops expanding and starts contracting.

[#1] In lectures and private conversations.

7.1. Typical vs. averaged behavior

I would like to emphasize again in as strong terms as I can that having results for typieal microstates rather than averages is not just a mathematical nicety but goes to the heart of the problem of understanding the microscopic origin of observed macroscopic behavior – *we do not have or need ensembles when we carry out observations like those illustrated in fig. 1.* What we need and can expect to have is typical behavior. Ensembles are therefore useful mathematical tools as long as the dispersion, in the quantities we are interested in, is sufficiently small. This is always the case for properly defined macroscopic variables in equilibrium Gibbs ensembles: they have the property of "self-averaging". We can therefore use these ensembles to calculate, with great confidence and precision, the equilibrium properties of macroscopic systems. Also, in the overwhelming majority of cases, i.e. with probability approaching one as N grows large, the evolution of $M(t)$, following the lifting of a constraint from a macroscopic system in equilibrium at some time t_0, will be the same for different $X(t_0)$. It makes therefore sense to use such an ensemble as the initial "statistical state" of the system at t_0.

There is no such typicality with respect to ensembles describing the time evolution of a system with a few degrees of freedom. This is an important distinction (unfortunately frequently overlooked or misunderstood) between irreversible and chaotic behavior of Hamiltonian systems. The latter, which can be observed in systems consisting of only a few particles, will not have a uni-directional time behavior in any particular realization. Thus if we had only a few hard spheres in the box of fig. 1, we would get plenty of chaotic dynamics and very good ergodic behavior (mixing, K-system, Bernoulli) but we could not tell the time order of any sequence of snapshots.

7.2. Other uses of entropy

Let me close by noting the existence of many well known and some obscure connections between "entropy" and degree of order or organization in various physical and abstract systems far removed from the simple gas in fig. 1. It is my feeling that, at least when dealing with physical objects containing many microscopic constituents, e.g. macroscopic or mesoscopic systems, the distinction between Boltzmannian and Gibbsian entropies, made earlier for simple systems, is always important and needs to be explored. I am therefore suggesting that there is interesting work to be done on obtaining more refined definitions of such concepts for complex systems like a Rembrandt painting, a beer can, or a human being. It is clear that the difference in S_B between a Rembrandt and a similar size canvas covered with the same amount and type of paint by some child is orders of magnitude smaller than the entropy

differences we have been talking about earlier. The same is true, I am afraid, for the entropy difference, if at all definable, between a living and a dead person. We therefore need more refined, logically consistent and physically meaningful definitions of organization for a *given* complex system than those currently available in information or complexity theory.

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References

[1] L. Boltzmann, Ann. Phys. (Leipzig) 57 (1896) 773; Sitzungsberichte Akad. Wiss., Vienna, part II, 75 (1877) 67 (translated and reprinted in: S.G. Brush, Kinetic Theory 2, (Pergamon, Oxford, 1966) pp. 218, 188.
[2] R. Feynman, The Character of Physical Law, (MIT Press, Cambridge, MA., 1967) ch. 5: The Feynman lectures on physics, 46-3,4,5.
[3] O. Penrose, Foundations of Statistical Mechanics (Pergamon, Oxford, 1970) cf. in particular ch. 5.
[4] R. Penrose, The Emperor's New Mind (Oxford Univ. Press, Oxford, 1990) ch. 7.
[5] D. Ruelle, Chance and Chaos (Princeton Univ. Press, Princeton, NJ, 1991) chs. 17, 18.
[6] L. Boltzmann, Wissenschaftliche Abhandlungen (J.A. Barth, Leipzig, 1909) 3 vols. [reprinted by: (Chelsea, New York, 1968)]; for a history of the subject see S.G. Brush, The Kind of Motion We Call Heat, vol. 2, Studies in Statistical Mechanics, vol. VI, E.W. Montroll and J.L. Lebowitz, eds. (North-Holland, Amsterdam, 1976).
[7] H. Spohn, Large Scale Dynamics of Interacting Particles (Springer, Berlin, 1991).
[8] A. DeMasi and E. Presutti, Mathematical Methods for Hydrodynamic Limits, Lecture Notes in Mathematics, vol. 1501 (Springer, Berlin, 1991).
[9] J.L. Lebowitz, E. Presutti and H. Spohn, J. Stat. Phys. 51 (1988) 841.
[10] L. Bunimovich and Y. Sinai, Commun. Math. Phys. 78 (1981) 479; L.A. Bunimovich, Y. Sinai and N. Chernov, Russ. Math. Surveys 45 (1990) 105.
[11] J.L. Lebowitz and H. Spohn, J. Stat. Phys. 28 (1982) 539; 29 (1982) 39.
[12] Y. Aharonov, P.G. Bergmann and J.L. Lebowitz, Phys. Rev. B 134 (1964) 1410.
[13] H.B. Callen, Thermodynamics (Wiley, New York, 1960) appendix B.
[14] A. Martin-Löf, Statistical Mechanics and the Foundation of Thermodynamics, Lecture Notes in Mathematics, vol. 101 (Springer, Berlin, 1979).
[15] J.L. Lebowitz and O. Penrose, Phys. Today 26 (1973) 155.
[16] A.J. Leggett, The Problems of Physics (Oxford Univ. Press, Oxford, 1987) ch. 5.
[17] E.L. Hahn, Phys. Rev. 80 (1950) 580; S. Zhang, B.H. Meier and R.R. Ernst, Phys. Rev. Lett. 69 (1992) 2149, and references therein.

[18] E. Schrödinger, What is Life? and Other Scientific Essays, sec. 6, The spirit of science (Doubleday Anchor Books, 1965).
[19] N.S. Krylov, Works on the Foundations of Statistical Physics, with appendix by Y. Sinai (Princeton Univ. Press, Princeton, NJ, 1979).
[20] C.H. Bennett, Sci. Am. 257 (November 1987) 108; R. Landauer, Physica A 194 (1993) 551, these Proceedings.
[21] F. Dyson, Energy in the Universe, in: From Eros to Gaia (Pantheon, 1992).
[22] E. Schrödinger, Irreversibility, Proc. R. Irish Acad. 53 (1950) 53.
[23] P.G. Bergmann, Phys. Rev. 84 (1951) 1026; N.G. van Kampen, Physica 20 (1954) 603; in: Fundamental Problems in Statistical Mechanics, E.G.D. Cohen, ed. (North-Holland, Amsterdam, 1962).
[24] S. Olla, S.R.S. Varadhan and H.T. Yau, Hydrodynamical limit for a Hamilton system with weak noise, Commun. Math. Phys., to appear.
[25] J. Fritz, preprint.
[26] J. Fritz, T. Funaki and J.L. Lebowitz, Stationary states of random Hamilton systems, preprint (1991).
[27] A. DeMasi, R. Esposito and J.L. Lebowitz, Comm. Pure and Appl. Math. XLII (1989) 1189.
[28] N. Chernov, Statistical properties of the periodic Lorentz gas: multidimensional case, J. Stat. Phys., to appear.
[29] O. Lanford, Time Evolution of Large Classical Systems, J. Moser, ed., Lecture Notes in Physics, vol. 38 (Springer, Berlin, 1975) pp. 1–111; Physica A 106 (1981) 70.
[30] E.T. Jaynes, Phys. Rev. A 4 (1971) 747.
[31] A.J. Leggett, The Arrow of Time in Quantum Mechanics, in: The Encyclopedia of Ignorance, R. Duncan and M. Weston-Smith, eds. (Pergamon, Oxford, 1977) [reprinted in: The Enigma of Time, P.T. Landsberg, ed. (Adam Hilger, London, 1982)].
[32] M. Gell-Mann and J.B. Hartle, Time symmetry and asymmetry in quantum mechanics and quantum cosmology, to appear; Quantum mechanics in the light of quantum cosmology, in: Complexity, Entropy and the Physics of Information, W.H. Zureck, ed. (Addison–Wesley, New York, 1990).
[33] J.B. Hartle, Phys. Rev. D 44 (1991) 3173, and references therein.