From Time-symmetric Microscopic Dynamics to Time-asymmetric Macroscopic Behavior: An Overview

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Abstract Time-asymmetric behavior as embodied in the second law of thermodynamics is observed in *individual macroscopic* systems. It can be understood as arising naturally from time-symmetric microscopic laws when account is taken of a) the great disparity between microscopic and macroscopic scales, b) a low entropy state of the early universe, and c) the fact that what we observe is the behavior of systems coming from such an initial state—not all possible systems. The explanation of the origin of the second law based on these ingredients goes back to Maxwell, Thomson and particularly Boltzmann. Common alternate explanations, such as those based on the ergodic or mixing properties of probability distributions (ensembles) already present for chaotic dynamical systems having only a few degrees of freedom or on the impossibility of having a truly isolated system, are either unnecessary, misguided or misleading. Specific features of macroscopic evolution, such as the diffusion equation, do however depend on the dynamical instability (deterministic chaos) of trajectories of isolated macroscopic systems.

The extensions of these classical notions to the quantum world is in many ways fairly direct. It does however also bring in some new problems. These will be discussed but not resolved.

1 Introduction

Let me start by stating clearly that I am not going to discuss here—much less claim to resolve—the many complex issues, philosophical and physical, concerning the nature of time, from the way we perceive it to the way it enters into the space-time structure in relativistic theories. I will also not try to philosophize about the "true" nature of probability. My goal here, as in my previous articles [1, 2] on this subject, is much more modest.[a] I will take (our everyday notions of) space, time and probability as primitive undefined concepts and try to clarify the many conceptual and mathematical problems encountered in going from a time symmetric Hamiltonian microscopic dynamics to a time asymmetric macroscopic one, as given for example by the diffusion equation. I will also take it for granted that every bit of macroscopic matter is composed of an enormous number of quasi-autonomous units, called atoms (or molecules).

The atoms, taken to be the basic entities making up these macroscopic objects, will be simplified to the point of caricature: they will be treated, to quote Feynman [3], as "little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another." This crude picture of atoms (a refined version of that held by some ancient Greek philosophers) moving according to non-relativistic classical Hamiltonian equations contains the essential qualitative and even quantitative ingredients of macroscopic irreversibility. To accord with our understanding of microscopic reality it must, of course, be modified to take account of quantum mechanics. This raises further issues for the question of irreversibility which will be discussed in section 9.

Much of what I have to say is a summary and elaboration of the work done over a century ago, when the problem of reconciling time asymmetric macroscopic behavior with the time symmetric microscopic dynamics became a central issue in physics. To quote from Thomson's (later Lord Kelvin) beautiful and highly recommended 1874 article [4], [5] "The essence of Joule's discovery is the subjection of physical [read thermal] phenomena to [microscopic] dynamical law. If, then, the motion of very particle of matter in the universe were precisely reversed at any instant, the course of nature would be simply reversed for ever after. The bursting bubble of foam at the foot of a waterfall would reunite and descend into the water .... Physical processes, on the other hand, are irreversible: for example, the friction of solids, conduction of heat, and diffusion. Nevertheless, the principle of dissipation of energy [irreversible behavior] is compatible with a molecular theory in which each particle is subject to the laws of abstract dynamics."

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[a] The interested reader may wish to look at the three book reviews of which are contained in [1e], [1f]. These books attempt to deal with some fundamental questions about time. As for the primitive notion of probability I have in mind something like this: the probability that when you next check your mail box you will find a package with a million dollars in it is very small, c.f. section 3.

1.1 Formulation of Problem

Formally the problem considered by Thomson in the context of Newtonian theory, the "theory of everything" at that time, is as follows: The complete microscopic (or micro) state of a classical system of N particles is represented by a point X in its phase space Γ, $X = (\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2, ..., \mathbf{r}_N, \mathbf{p}_N)$, $\mathbf{r}_i$ and $\mathbf{p}_i$ being the position and momentum (or velocity) of the ith particle. When the system is isolated its evolution is governed by Hamiltonian dynamics with some specified Hamiltonian $H(X)$ which we will assume for simplicity to be an even function of the momenta. Given $H(X)$, the microstate $X(t_0)$, at time t_0, determines the microstate $X(t)$ at all future and past times t during which the system will be or was isolated: $X(t) = T_{t-t_0}X(t_0)$. Let $X(t_0)$ and $X(t_0 + \tau)$, with τ positive, be two such microstates. Reversing (physically or mathematically) all velocities at time $t_0 + \tau$, we obtain a new microstate. If we now follow the evolution for another interval τ we find that the new microstate at time $t_0 + 2\tau$ is just $RX(t_0)$, the microstate $X(t_0)$ with all velocities reversed: $RX = (\mathbf{r}_1, -\mathbf{p}_1, \mathbf{r}_2, -\mathbf{p}_2, ..., \mathbf{r}_N, -\mathbf{p}_N)$. Hence if there is an evolution, i.e. a trajectory $X(t)$, in which some property of the system, specified by a function $f(X(t))$, behaves in a certain way as t increases, then if $f(X) = f(RX)$ there is also a trajectory in which the property evolves in the time reversed direction. Thus, for example, if particle densities get more uniform as time increases, in a way described by the diffusion equation, then since the density profile is the same for X and RX there is also an evolution in which the density gets more nonuniform. So why is one type of evolution, the one consistent with an entropy increase in accord with the "second law", common and the other never seen? The difficulty is illustrated by the impossibility of time ordering of the snapshots in Fig. 1 using *solely* the microscopic dynamical laws: the above time symmetry implies that if (a, b, c, d) is a possible ordering so is (d, c, b, a).

1.2 Resolution of Problem

The explanation of this apparent paradox, due to Thomson, Maxwell and Boltzmann, as described in references [1]–[17], which I will summarize in this article, shows that *not only is there no conflict* between reversible microscopic laws and irreversible macroscopic behavior, but, as clearly pointed

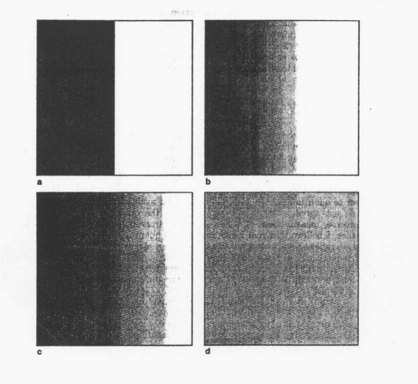

Figure 1: *A sequence of "snapshots", a, b, c, d taken at times* t_a, t_b, t_c, t_d*, each representing a macroscopic state of a system, say a fluid with two "differently colored" atoms or a solid in which the shading indicates the local temperature. How would you order this sequence in time?*

out by Boltzmann in his later writings[b], *there are extremely strong reasons to expect the latter from the former.* These reasons involve several interrelated ingredients which together provide the required distinction between microscopic and macroscopic variables and explain the emergence of definite time asymmetric behavior in the evolution of the latter despite the total absence of such asymmetry in the dynamics of the former. They are: a) the great disparity between microscopic and macroscopic scales, b) the fact that the events we observe in our world are determined not only by the microscopic dynamics, but also by the initial conditions of our system, which, as we shall see later, in section 6, are very much related to the initial conditions of our universe, and c) the fact that it is not every microscopic state of a macroscopic system that will evolve in accordance with the entropy increase predicted by the second law, but only the "majority" of such states—a majority which however becomes so overwhelming when the number of atoms in the system becomes very large that irreversible behavior becomes effectively a certainty. To make the last statement complete we shall have to specify the assignment of weights, or probabilities, to different microstates consistent

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[b] Boltzmann's early writings on the subject are sometimes unclear, wrong, and even contradictory. His later writings, however, are generally very clear and right on the money (even if a bit verbose for Maxwell's taste, c.f. [8].) The presentation here is not intended to be historical.

with a given macrostate. Note, however, that since we are concerned with events which have overwhelming probability, many different assignments are equivalent and there is no need to worry about them unduly. There is however, as we shall see later, a "natural" choice based on phase space volume (or dimension of Hilbert space in quantum mechanics). These considerations enabled Boltzmann to define the entropy of a macroscopic system in terms of its microstate and to relate its change, as expressed by the second law, to the evolution of the system's microstate. We detail below how the above explanation works by describing first how to specify the macrostates of a macroscopic system. It is in the time evolution of these macrostates that we observe irreversible behavior [1]–[17].

1.3 Macrostates

To describe the macroscopic state of a system of N atoms in a box V, say $N \gtrsim 10^{20}$, with the volume of V, denoted by $|V|$, satisfying $|V| \gtrsim Nl^3$, where l is a typical atomic length scale, we make use of a much cruder description than that provided by the microstate X, a point in the $6N$ dimensional phase space $\Gamma = V^N \otimes \mathbb{R}^{3N}$. We shall denote by M such a macroscopic description or macrostate. As an example we may take M to consist of the specification, to within a given accuracy, of the energy and number of particles in each half of the box V. A more refined macroscopic description would divide V into K cells, where K is large but still $K << N$, and specify the number of particles, the momentum, and the amount of energy in each cell, again with some tolerance. For many purposes it is convenient to consider cells which are small on the macroscopic scale yet contain many atoms. This leads to a description of the macrostate in terms of smooth particle, momentum and energy densities, such as those used in the Navier-Stokes equations [18], [19]. An even more refined description is obtained by considering a smoothed out density $f(\mathbf{r}, \mathbf{p})$ in the six-dimensional position and momentum space such as enters the Boltzmann equation for dilute gases [17]. (For dense systems this needs to be supplemented by the positional potential energy density; see footnote d and reference [2] for details.)

Clearly M is determined by X (we will thus write $M(X)$) but there are many X's (in fact a continuum) which correspond to the same M. Let Γ_M be the region in Γ consisting of all microstates X corresponding to a given macrostate M and denote by $|\Gamma_M| = (N!h^{3N})^{-1} \int_{\Gamma_M} \Pi_{i=1}^{N} d\mathbf{r}_i d\mathbf{p}_i$, its symmetrized $6N$ dimensional Liouville volume (in units of h^{3N}).

1.4 Time Evolution of Macrostates: An Example

Consider a situation in which a gas of N atoms with energy E (with some tolerance) is initially confined by a partition to the left half of of the box V, and suppose that this constraint is removed at time t_a, see Fig. 1. The phase space volume available to the system for times $t > t_a$ is then fantastically enlarged[c] compared to what it was initially, roughly by a factor of 2^N.

Let us now consider the macrostate of this gas as given by $M = \left(\frac{N_L}{N}, \frac{E_L}{E}\right)$, the fraction of particles and energy in the left half of V (within some small tolerance). The macrostate at time $t_a, M = (1, 1)$, will be denoted by M_a. The phase-space region $|\Gamma| = \Sigma_E$, available to the system for $t > t_a$, i.e., the region in which $H(X) \in (E, E + \delta E), \delta E << E$, will contain new macrostates, corresponding to various fractions of particles and energy in the left half of the box, with phase space volumes very large compared to the initial phase space volume available to the system. We can then expect (in the absence of any obstruction, such as a hidden conservation law) that as the phase point X evolves under the unconstrained dynamics and explores the newly available regions of phase space, it will with very high probability enter a succession of new macrostates M for which $|\Gamma_M|$ is increasing. The set of all the phase points X_t, which at time t_a were in Γ_{M_a}, forms a region $T_t\Gamma_{M_a}$ whose volume is, by Liouville's Theorem, equal to $|\Gamma_{M_a}|$. The shape of $T_t\Gamma_{M_a}$ will however change with t and as t increases $T_t\Gamma_{M_a}$ will increasingly be contained in regions Γ_M corresponding to macrostates with larger and larger phase space volumes $|\Gamma_M|$. This will continue until almost all the phase points initially in Γ_{M_a} are contained in $\Gamma_{M_{eq}}$, with M_{eq} the system's unconstrained macroscopic equilibrium state. This is the state in which approximately half the particles and half the energy will be located in the left half of the box, $M_{eq} = (\frac{1}{2}, \frac{1}{2})$ i.e. N_L/N and E_L/E will each be in an interval $\left(\frac{1}{2} - \epsilon, \frac{1}{2} + \epsilon\right)$, $N^{-1/2} << \epsilon << 1$.

M_{eq} is characterized, in fact defined, by the fact that it is the unique macrostate, among all the M_α, for which $|\Gamma_{M_{eq}}|/|\Sigma_E| \simeq 1$, where $|\Sigma_E|$ is the total phase space volume available under the energy constraint $H(X) \in (E, E + \delta E)$. (Here the symbol $\simeq$ means equality when $N \to \infty$.) That there exists a macrostate containing almost all of the microstates in Σ_E is a consequence of the law of large numbers [20], [18]. The fact that N is enormously

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[c] If the system contains 1 mole of gas then the volume ratio of the unconstrained phase space region to the constrained one is far larger than the ratio of the volume of the known universe to the volume of one proton.

large for macroscope systems is absolutely critical for the existence of thermodynamic equilibrium states for any reasonable definition of macrostates, e.g. for any ϵ, in the above example such that $N^{-1/2} << \epsilon << 1$. Indeed thermodynamics does not apply (is even meaningless) for isolated systems containing just a few particles, c.f. Onsager [21] and Maxwell quote in the next section [22]. Nanosystems are interesting and important intermediate cases which I shall however not discuss here; see related discussion about computer simulations in footnote e.

After reaching M_{eq} we will (mostly) see only small fluctuations in $N_L(t)/N$ and $E_L(t)/E$, about the value $\frac{1}{2}$: typical fluctuations in N_L and E_L being of the order of the square root of the number of particles involved [18]. (Of course if the system remains isolated long enough we will occasionally also see a return to the initial macrostate—the expected time for such a Poincaré recurrence is however much longer than the age of the universe and so is of no practical relevance when discussing the approach to equilibrium of a macroscopic system [6], [8].)

As already noted earlier the scenario in which $|\Gamma_{M(X(t))}|$ increase with time for the M_a shown in Fig.1 cannot be true for all microstates $X \subset \Gamma_{M_a}$. There will of necessity be X's in Γ_{M_a} which will evolve for a certain amount of time into microstates $X(t) \equiv X_t$ such that $|\Gamma_{M(X_t)}| < |\Gamma_{M_a}|$, e.g. microstates $X \in \Gamma_{M_a}$ which have all velocities directed away from the barrier which was lifted at t_a. What is true however is that the subset B of such "bad" initial states has a phase space volume which is very very small compared to that of Γ_{M_a}. This is what I mean when I say that entropy increasing behavior is *typical*; a more extensive discussion of typicality is given later.

2 Boltzmann's Entropy

The end result of the time evolution in the above example, that of the fraction of particles and energy becoming and remaining essentially equal in the two halves of the container when N is large enough (and 'exactly equal' when $N \to \infty$), is of course what is predicted by the second law of thermodynamics. According to this law the final state of an isolated system with specified constraints on the energy, volume, and mole number is one in which the entropy, a measurable macroscopic quantity of equilibrium systems, defined on a purely operational level by Claussius, has its maximum. (In practice one also fixes additional constraints, e.g. the chemical combination of nitrogen and oxygen to form complex molecules is ruled out when considering, for example, the dew point of air in the 'equilibrium' state of air at normal temperature and pressure, c.f. [21]. There are, of course, also very long lived metastable states, e.g. glasses, which one can, for many purposes, treat as equilibrium states even though their entropy is not maximal. I will ignore these complications here.) In our example this thermodynamic entropy would be given by $S = V_L s\left(\frac{N_L}{V_L}, \frac{E_L}{V_L}\right) + V_R s\left(\frac{N_R}{V_R}, \frac{E_R}{V_R}\right)$ defined for all equilibrium states in separate boxes V_L and V_R with given values of N_L, N_R, E_L, E_R. When V_L and V_R are united to form V, S is maximized subject to the constraint of $E_L + E_R = E$ and of $N_L + N_R = N$.

It was Boltzmann's great insight to connect the second law with the above phase space volume considerations by making the observation that for a dilute gas $\log|\Gamma_{M_{eq}}|$ is proportional, up to terms negligible in the size of the system, to the thermodynamic entropy of Clausius. Boltzmann then extended his insight about the relation between thermodynamic entropy and $\log|\Gamma_{M_{eq}}|$ to all macroscopic systems; be they gas, liquid or solid. This provided for the first time a microscopic definition of the operationally measurable entropy of macroscopic systems in *equilibrium*.

Having made this connection Boltzmann then generalized it to define an entropy also for macroscopic systems not in equilibrium. That is, he associated with each microscopic state X of a macroscopic system a number S_B which depends only on $M(X)$ given, up to multiplicative and additive constants (which can depend on N), by

$$S_B(X) = S_B(M(X)) \tag{1a}$$

with

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

which, following O. Penrose [13], I shall call the Boltzmann entropy of a classical system: $|\Gamma_M|$ is defined in section (1.3). N. B. I have deliberately written (1) as two equations to emphasize their logical independence which will be useful for the discussion of quantum systems in section 9.

Boltzmann then used phase space arguments, like those given above, to explain (in agreement with the ideas of Maxwell and Thomson) the observation, embodied in the second law of thermodynamics, that when a constraint is lifted, an isolated macroscopic system will evolve toward a state with greater entropy.[d] In effect Boltzmann argued that due to the large differences in the sizes of Γ_M, $S_B(X_t) = k \log |\Gamma_{M(X_t)}|$ will *typically* increase in a way which *explains* and describes qualitatively the evolution towards equilibrium of macroscopic systems.

These very large differences in the values of $|\Gamma_M|$ for different M come from the very large number of particles (or degrees of freedom) which contribute, in an (approximately) additive way, to the specification of macrostates. This is also what gives rise to typical or almost sure behavior. Typical, as used here, means that the set of microstates corresponding to a given macrostate M for which the evolution leads to a macroscopic increase (or non-decrease) in the Boltzmann entropy during some fixed macroscopic time period τ occupies a subset of Γ_M whose Liouville volume is a fraction of $|\Gamma_M|$ which goes very rapidly (exponentially) to one as the number of atoms in the system increases. The fraction of "bad" microstates, which lead to an entropy decrease, thus goes to zero as $N \to \infty$.

Typicality is what distinguishes macroscopic irreversibility from the weak approach to equilibrium of probability distributions (ensembles) of systems with good ergodic properties having only a few degrees of freedom, e.g. two hard spheres in a cubical box. While the former is manifested in a typical evolution of a single macroscopic system the latter does not correspond to any appearance of time asymmetry in the evolution of an individual system. Maxwell makes clear the importance of the separation between microscopic and macroscopic scales when he writes [22]: "the second law is drawn from our experience of bodies consisting of an immense number of molecules. ... it is continually being violated, ..., in any sufficiently small group of molecules ... . As the number ... is increased ... the probability of a measurable variation ... may be regarded as practically an impossibility." This is also made

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[d] When M specifies a state of local equilibrium, $S_B(X)$ agrees up to negligible terms, with the "hydrodynamic entropy". For systems far from equilibrium the appropriate definition of M and thus of S_B can be more problematical. For a dilute gas (with specified kinetic energy and negligible potential energy) in which M is specified by the smoothed empirical density $f(\mathbf{r}, \mathbf{v})$ of atoms in the six dimensional position and velocity space, $S_B(X) = -k \int f(\mathbf{r}, \mathbf{v}) \log f(\mathbf{r}, \mathbf{v}) d\mathbf{r} d\mathbf{v}$ (see end of Section 4). This identification is, however, invalid when the potential energy is not negligible and one has to add to $f(\mathbf{r}, \mathbf{v})$ also information about the energy density. This is discussed in detail in [2]. Boltzmann's famous H theorem derived from his eponymous equation for dilute gases is thus an expression of the second law applied to the macrostate specified by f. It was also argued in [2] that such an H theorem must hold whenever there is a deterministic equation for the macrovariables of an isolated system.

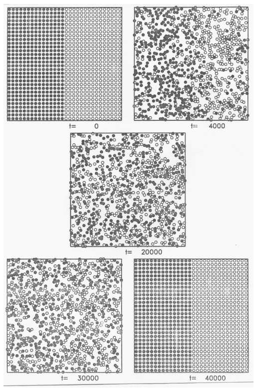

Figure 2: *Time evolution of a system of 900 particles all interacting via the same cutoff Lennard-Jones pair potential using integer arithmetic. Half of the particles are colored white, the other half black. All velocities are reversed at* $t = 20,000$*. The system then retraces its path and the initial state is fully recovered. From Levesque and Verlet, Ref. [23].*

very clear by Onsager in [21] and should be contrasted with the confusing statements found in many books that thermodynamics can be applied to a single isolated particle in a box, c.f. footnote *i*.

On the other hand, because of the exponential increase of the phase space volume with particle number, even a system with only a few hundred particles, such as is commonly used in molecular dynamics computer simulations, will, when started in a nonequilibrium 'macrostate' M, with 'random' $X \in \Gamma_M$, appear to behave like a macroscopic system.[e] This will be so even when integer arithmetic is used in the simulations so that the system behaves as a truly isolated one; when its velocities are reversed the system retraces its steps until it comes back to the initial state (with reversed velocities), after which it again proceeds (up to very long Poincare recurrence times) in the typical way, see section 5 and Figs. 2 and 3 taken from [23] and [24].

We might take as a summary of such insights in the late part of the nineteenth century the statement by Gibbs [25] quoted by Boltzmann (in a German translation) on the cover of his book *Lectures on Gas Theory II*: [7],

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[e] After all, the likelihood of hitting, in the course of say one thousand tries, something which has probability of order 2^{-N} is, for all practical purposes, the same, whether N is a hundred or 10^{23}. Of course the fluctuation in S_B both along the path towards equilibrium and in equilibrium will be larger when N is small, c.f. [2b].

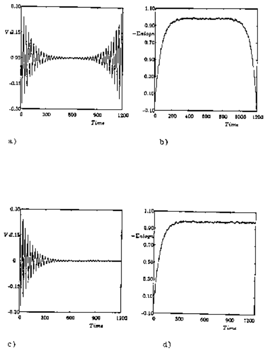

Figure 3: *Time evolution of a reversible cellular automaton lattice gas using integer arithmetic. Figures a) and c) show the mean velocity, figures b) and d) the entropy. The mean velocity decays with time and the entropy increases up to* $t = 600$ *when there is a reversal of all velocities. The system then retraces its path and the initial state is fully recovered in figures a) and b). In the bottom figures there is a small error in the reversal at* $t = 600$*. While such an error has no appreciable effect on the initial evolution it effectively prevents any recovery of the initial state. The entropy, on the scale of the figure, just remains at its maximum value. This shows the instability of the reversed path. From Nadiga et al. Ref. [24].*

"In other words, the impossibility of an uncompensated decrease of entropy seems to be reduced to an improbability."

3 The Use of Probabilities

As already noted, typical here means overwhelmingly probable with respect to a measure which assigns (at least approximately) equal weights to regions of equal phase space volume within Γ_M or, loosely speaking, to different microstates consistent with the "initial" macrostate M. (This is also what was meant earlier by the 'random' choice of an initial $X \in \Gamma_M$ in the computer simulations.) In fact, any mathematical statement about probable or improbable behavior of a physical system has to refer to some agreed upon measure (probability distribution). It is, however, very hard (perhaps impossible) to formulate precisely what one means, as a statement about the real world, by an assignment of exact numerical values of probabilities (let alone rigorously justify any particular one) in our context. It is therefore not so surprising that this use of probabilities, and particularly the use of typicality for explaining the origin of the apparently deterministic second law, was very difficult for many of Boltzmann's contemporaries, and even for some people today, to accept. (Many text books on statistical mechanics are unfortunately either silent or confusing on this very important point.) This was clearly very frustrating to Boltzmann as it is also to me, see [1b, 1c]. I have not found any better way of expressing this frustration than Boltzmann did when he wrote, in his second reply to Zermelo in 1897 [6] "The applicability of probability theory to a particular case cannot of course be proved rigorously. ... Despite this, every insurance company relies on probability theory. ... It is even more valid [here], on account of the huge number of molecules in a cubic millimetre... The assumption that these rare cases are not observed in nature is not strictly provable (nor is the entire mechanical picture itself) but in view of what has been said it is so natural and obvious, and so much in agreement with all experience with probabilities ... [that] ... *It is completely incomprehensible to me* [my italics] how anyone can see a refutation of the applicability of probability theory in the fact that some other argument shows that exceptions must occur now and then over a period of eons of time; for probability theory itself teaches just the same thing."

The use of probabilities in the Maxwell-Thomson-Boltzmann explanation of irreversible macroscopic behavior is as Ruelle notes "simple but subtle" [14]. They introduce into the laws of nature notions of probability, 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 and indeed no exceptions were (or are) known to the second law as a statement about the actual behavior of isolated macroscopic systems; nor would we expect any, as Richard Feynman [15] rather conservatively says, "in a million years". The reason for this, as already noted, is that for a macroscopic system the fraction (in terms of the Liouville volume) of the microstates in a macrostate M for which the evolution leads to macrostates M' with $S_B(M') \geq S_B(M)$ is so close to one (in terms of their Liouville volume) that such behavior is exactly what should be seen to "always" happen. Thus in Fig. 1 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}, when N, the number of particles (or degrees of freedom) in the system, is sufficiently large. The situation can be quite different when N is small as noted in the last section: see Maxwell quote there.

Note that Boltzmann's explanation of why $S_B(M_t)$ is never seen to decrease with t does not really require the assumption that over very long periods of time a macroscopic system should be found in every region Γ_M, i.e. in every macroscopic states M, for a fraction of time *exactly* equal to the ratio of $|\Gamma_M|$ to the total phase space volume specified by its energy. This latter behavior, embodied for example in Einstein's formula

$$Prob\{M\} \sim \exp[S_B(M) - S_{eq}] \tag{2}$$

for fluctuation in equilibrium sytems, with probability there interpreted as the fraction of time which such a system will spend in Γ_M, can be considered as a mild form of the ergodic hypothesis, mild because it is only applied to those regions of the phase space representing macrostates Γ_M. This seems very plausible in the absence of constants of the motion which decompose the energy surface into regions with different macroscopic states. It appears even more reasonable when we take into account the lack of perfect isolation in practice which will be discussed later. Its implication for small fluctuations from equilibrium is certainly consistent with observations. In particular when the exponent in (2) is expanded in a Taylor series and only quadratic terms are kept, we obtain a Gaussian distribution for normal (small) fluctuations from equilibrium. Eq.(2) is in fact one of the main ingredients of Onsager's reciprocity relations for transport processes in systems close to equilibrium [26].

The usual ergodic hypothesis, i.e. that the fraction of time spent by a trajectority X_t in any region A on the energy surface $H(X) = E$ is equal to the fraction of the volume occupied by A, also seems like a natural assumption for macroscopic systems. It is however not necessary for identifying equilibrium properties of macroscopic systems with those obtained from the microcanonical ensemble; see Section 7. Neither is it in any way sufficient for explaining the approach to equilibrium observed in real systems: the time scales are entirely different.

It should perhaps be emphasized again here that an important ingredient in the whole picture of the time evolution of macrostates described above is the constancy in time of the Liouville volume of sets in the phase space Γ as they evolve under the Hamiltonian dynamics (Liouville's Theorem). Without this invariance the connection between phase space volume and probability would be impossible or at least very problematic.

For a somewhat different viewpoint on the issues discussed in this section the reader is referred to Chapter IV in [13].

4 Initial Conditions

Once we accept the statistical explanation of why macroscopic systems evolve in a manner that makes S_B increase with time, there remains the nagging problem (of which Boltzmann was well aware) of what we mean by "with time": since the microscopic dynamical laws are symmetric, the two directions of the time variable are *a priori* equivalent and thus must remain so *a posteriori*. This was well expressed by Schrödinger [27]. "First, my good friend, you state that the two directions of your time variable, 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."

In terms of our Fig. 1 this question may be put as follows:[f] why can we use phase space arguments (or time asymmetric diffusion type equations) to predict the macrostate at time t of an *isolated* system whose macrostate at time t_b is M_b, in the future, i.e. for $t > t_b$, but not in the past, i.e. for $t < t_b$? After all, if the macrostate M is invariant under velocity reversal of all the atoms, then the same prediction should apply equally to $t_b + \tau$ and $t_b - \tau$. A plausible answer to this question is to assume that the nonequilibrium macrostate M_b had its origin in an even more nonuniform macrostate M_a, prepared by some experimentalist at some earlier time $t_a < t_b$ (as is indeed the case in Figure 1) and that for states thus prepared we can apply our (approximately) equal a priori probability of microstates argument, i.e. we can assume its validity at time t_a. But what about events on the sun or in a supernova explosion where there are no experimentalists? And what, for that matter, is so special about the status of the experimentalist? Isn't he

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[f] The reader should think of Fig. 1 as representing energy density in a solid: the darker the hotter. The time evolution of the macrostate will then be given by the heat (diffusion) equation.

or she part of the physical universe?

Before trying to answer these "big" questions let us consider whether the assignment of equal probabilities for $X \in \Gamma_{M_a}$ at t_a permits the use of an equal probability distribution of $X \in \Gamma_{M_b}$ at time t_b for predicting macrostates at times $t > t_b > t_a$ when the system is isolated for $t > t_a$. Note that those microstates in Γ_{M_b} which have come from Γ_{M_a} through the time evolution during the time interval from t_a to t_b make up a set Γ_{ab} whose volume $|\Gamma_{ab}|$ is by Liouville's theorem at most equal [g] to $|\Gamma_{M_a}|$; which, as already discussed before, is only a very small fraction of the volume of Γ_{M_b}. Thus we have to show that the overwhelming majority of phase points in Γ_{ab} (with respect to Liouville measure on Γ_{ab}), have *future* macrostates like those typical of Γ_b—while still being very special and unrepresentative of Γ_{M_b} as far as their *past* macrostates are concerned. This property is explicitly proven by Lanford in his derivation of the Boltzmann equation (for short times) [17], and is part of the derivation of hydrodynamic equations [18], [19]; see also [28].

To see intuitively the origin of this property we note that for systems with realistic interactions the phase space region $\Gamma_{ab} \subset \Gamma_{M_b}$ will be so convoluted as to *appear* uniformly smeared out in Γ_{M_b}. It is therefore reasonable that the future behavior of the system, as far as macrostates go, will be unaffected by their past history. It would of course be nice to prove this in all cases, "thus justifying" (for practical purposes) the factorization or "Stosszahlansatz" assumed by Boltzmann in deriving his dilute gas kinetic equation for all times $t > t_a$, not only for the short times proven by Lanford [17]. However, our mathematical abilities are equal to this task only in very simple models such as the Lorentz gas in a Sinai billiard. This model describes the evolution of a macroscopic system of independent particles moving according to Newtonian dynamics in a periodic array of scatterers. For this system one can actually derive a diffusion equation for the macroscopic density profile $n(\mathbf{r}, t)$ from the Hamiltonian dynamics [18]; see Section 8.

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[g] $|\Gamma_{ab}|$ may be strictly less than $|\Gamma_{M_a}|$ because some of the phase points in Γ_{M_a} may not go into Γ_{M_b}. There will be approximate equality when M_a at time t_a, determines M_b at time t_b: say via the diffusion equation for the energy density. This corresponds to the "Markov case" discussed in [13]. There are of course situations where the macrostate at time t, depends also (weakly or even strongly) on the whole history of M in some time interval prior to t, e.g. in materials with memory. The second law certainly holds also for these cases - with the appropriate definition of S_B, obtained in many case by just refining the description so that the new macro variables follow autonomous laws [13].

This behavior can also be seen explicitely in a many particle system, each of which evolves independently according to the reversible and area preserving baker's transformation (which can be thought of as a toy version of the above case) see [29]. Here the phase space Γ for N particles is the $2N$ dimensional unit hypercube, i.e. X corresponds to specifying N-points $(x_1, y_1, \ldots, x_N, y_N)$ in the unit square. The discrete time evolution is given by

$$(x_i, y_i) \to \left\{ \begin{array}{c} (2x_i, \frac{1}{2}y_i), 0 \leq x_i < \frac{1}{2} \\ (2x_i - 1, \frac{1}{2}y_i + \frac{1}{2}), x_i \leq \frac{1}{2} < 1 \end{array} \right. .$$

Dividing the unit square into 4^k little squares $\delta_\alpha, \alpha = 1, \ldots, K, K = 4^k$, of side lengths 2^{-k}, we define the macrostate M by giving the fraction of particles $p_\alpha = (N_\alpha/N)$ in each δ_α within some tolerence. The Boltzmann entropy is then given, using (1) and setting $k = 1$, by

$$S_B = \sum_\alpha \log \left[\frac{\delta^{N_\alpha}}{N_\alpha!} \right] \simeq -N \sum_\alpha \left[-1 + p(\alpha) \log \frac{p(\alpha)}{\delta} \right],$$

where $p(\alpha) = N_\alpha/N, \delta = |\delta_\alpha| = 4^{-k}$, and we have used Stirling's formula appropriate for $N_\alpha >> 1$. Letting now $N \to \infty$ followed by $K \to \infty$ we obtain

$$N^{-1} S_B \to -\int_0^1 \int_0^1 \bar{f}(x, y) \log \bar{f}(x, y) dx dy + 1$$

where $\bar{f}(x, y)$ is the smoothed density, $p(\alpha) \sim \bar{f}\delta$, which behaves according to the second law. In particular $p_t(\alpha)$ will approach the equilibrium state corresponding to $p_{eq}(\alpha) = 4^{-k}$ while the empirical density f_t will approach one in the unit square [29]. N. B. If we had considered instead the Gibbs entropy S_G, $N^{-1} S_G = -\int_0^1 \int_0^1 f_1 \log f_1 dx dy$, with $f_1(x, y)$ the marginal, i.e. reduced, one particle distribution, then this would not change with time. See section 7 and [2].

5 Velocity Reversal

The large number of atoms present in a macroscopic system plus the chaotic nature of the dynamics "of all realistic systems" also explains why it is so difficult, essentially impossible, for a clever experimentalist to deliberately put such a system in a microstate which will lead it to evolve in isolation, for any significant time τ, in a way contrary to the second law.[h] Such microstates certainly exist—just reverse all velocities Fig. 1b. In fact, they are readily created in the computer simulations with no round off errors, see Fig. 2 and 3. To quote again from Thomson's article [4]: "If we allowed this equalization to proceed for a certain time, and then reversed the motions of all the molecules, we would observe a disequalization. However, if the number of molecules is very large, as it is in a gas, any slight deviation from absolute precision in the reversal will greatly shorten the time during which disequalization occurs." It is to be expected that this time interval decreases with the increase of the chaoticity of the dynamics. In *addition*, if the system is not perfectly isolated, as is always the case for real systems, the effect of unavoidable small outside influences, which are unimportant for the evolution of macrostates in which $|\Gamma_M|$ is increasing, will greatly destabilize evolution in the opposite direction when the trajectory has to *be aimed* at a very small region of the phase space.

The last statement is based on the very reasonable assumption that almost any small outside perturbation of an "untypical" microstate $X \in \Gamma_{M(X)}$ will tend to change it to a microstate $Y \in \Gamma_{M(X)}$ whose future time evolution is typical of $\Gamma_{M(X)}$, i.e. Y will likely be a typical point in $\Gamma_{M(X)}$ so that typical behavior is not affected by the perturbation [14]. If however we are, as in Figure 1, in a micro-state X_b at time t_b, where $X_b = T_\tau X_a, \tau = t_b - t_a > 0$, with $|\Gamma_{M_b}| >> |\Gamma_{M_a}|$, and we now reverse all velocities, then RX_b will be heading towards a smaller phase space volume during the interval $(t_b, t_b + \tau)$ and this behavior is very untypical of Γ_{M_b}. The velocity reversal therefore requires "perfect aiming" and will, as noted by Thomson [4], very likely be derailed by even small imperfections in the reversal and/or tiny outside influences. After a *very short* time interval $\tau' << \tau$, in which S_B decreases, the imperfections in the reversal and the "outside" perturbations, such as those coming from a sun flare, a star quake in a distant galaxy (a long time ago) or from a butterfly beating its wings [14], will make it increase again. This is clearly illustrated in Fig. 3, which shows how a small perturbation has no effect on the forward macro evolution, but completely destroys the time reversed evolution.

The situation is somewhat analogous to those pinball machine type puzzles where one is supposed to get a small metal ball into a small hole. You have to do things just right to get it in but almost any vibration gets it out

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[h] I am not considering here entropy increase of the experimentalist and experimental apparatus directly associated with creating such a state.

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^e than in the puzzle, as noted in the example in Section 1. In the absence of any "grand conspiracy", the behavior of such systems can therefore be confidently predicted to be in accordance with the second law (except possibly for very short time intervals). This is the reason why even in those special cases such as spin-echo type experiments where the creation of an effective $RT_\tau X$ is possible, the "anti-second law" trajectory lasts only for a short time [30]. In addition the *total* entropy change in the whole process, including that in the apparatus used to affect the spin reversal, is always positive in accord with the second law.

6 Cosmological Considerations

Let us return now to the big question posed earlier: what is special about t_a in Fig. 1 compared to t_b in a world with symmetric microscopic laws? Put differently, where ultimately do initial conditions, such as those assumed at t_a, come from? In thinking about this we are led more or less inevitably to introduce cosmological considerations by postulating an initial "macrostate of the universe" having a very small Boltzmann entropy, (see also $1e$ and $1f$). To again quote Boltzmann [31]: "That in nature the transition from a probable to an improbable state does not take place as often as the converse, can be explained by assuming a very improbable [small S_B] initial state of the entire universe surrounding us. This is a reasonable assumption to make, since it enables us to explain the facts of experience, and one should not expect to be able to deduce it from anything more fundamental". While this requires that the initial macrostate of the universe, call it M_0, be very far from equilibrium with $|\Gamma_{M_0}| << |\Gamma_{M_{eq}}|$, it does not require that we choose a special microstate in Γ_{M_0}. As also noted by Boltzmann elsewhere "we do not have to assume a special type of initial condition in order to give a mechanical proof of the second law, if we are willing to accept a statistical viewpoint...if the initial state is chosen at random...entropy is almost certain to increase." This is a very important aspect of Boltzmann's insight, it is sufficient to assume that this microstate is typical of an initial macrostate M_0 which is far from equilibrium.

This going back to the initial conditions, i.e. the existence of an early state of the universe (presumably close to the big bang) with a much lower

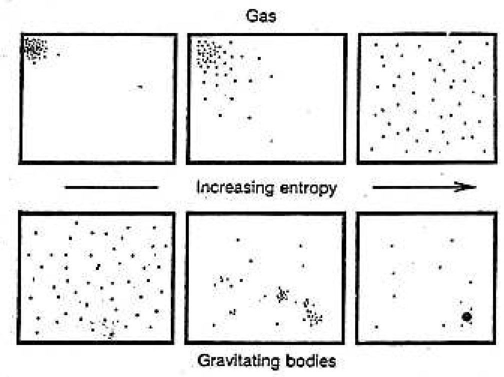

Figure 4: *With a gas in a box, the maximum entropy state (thermal equilibrium) has the gas distributed uniformly; however, with a system of gravitating bodies, entropy can be increased from the uniform state by gravitational clumping leading eventually to a black hole. From Ref. [16].*

value of S_B than the present universe, as an ingredient in the explanation of the observed time asymmetric behavior, bothers some physicists. It really shouldn't since the initial state of the universe plus the dynamics determines what is happening at present. Conversely, we can deduce information about the initial state from what we observe now. As put by Feynman [15], "it is necessary to add to the physical laws the hypothesis that in the past the universe was more ordered, in the technical sense, [i.e. low S_B] than it is today...to make an understanding of the irreversibility." A very clear discussion of this is given by Roger Penrose in connection with the "big bang" cosmology [16]. He takes for the initial macrostate of the universe the smooth energy density state prevalent soon after the big bang: an equilibrium state (at a very high temperature) **except** for the gravitational degrees of freedom which were totally out of equilibrium, as evidenced by the fact that the matter-energy density was spatially very uniform. That such a uniform density corresponds to a nonequilibrium state may seem at first surprising, but gravity, being purely attractive and long range, is unlike any of the other fundamental forces. When there is enough matter/energy around, it completely overcomes the tendency towards uniformization observed in ordinary objects at high energy densities or temperatures. Hence, in a universe dominated, like ours, by gravity, a uniform density corresponds to a state of very low entropy, or phase space volume, for a given total energy, see Fig. 4.

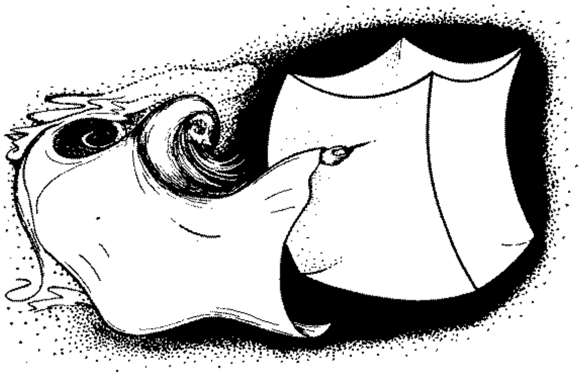

Figure 5: *The creator locating the tiny region of phase-space—one part in* $10^{10^{123}}$*—needed to produce a* 10^{80}*-baryon closed universe with a second law of thermodynamics in the form we know it. From Ref. [16]. If the initial state was chosen randomly it would, with overwhelming probability, have led to a universe in a state with maximal entropy. In such a universe there would be no stars, planets, people or a second law.*

The local ‘order’ or low entropy we see around us (and elsewhere)—from complex molecules to trees to the brains of experimentalists preparing macrostates—is perfectly consistent with (and possibly even a necessary consequence of, i.e. typical of) this initial macrostate of the universe. The value of S_B at the present time, t_p, corresponding to $S_B(M_{t_p})$ of our current clumpy macrostate describing a universe of planets, stars, galaxies, and black holes, is much much larger than $S_B(M_0)$, the Boltzmann entropy of the “initial state”, but still quite far away from $S_B(M_{eq})$ its equilibrium value. The ‘natural’ or ‘equilibrium’ state of the universe, M_{eq}, is, according to Penrose [16], one with all matter and energy collapsed into one big black hole. Penrose gives an estimate $S_B(M_0)/S_B(M_{t_p})/S_{eq} \sim 10^{88}/10^{101}/10^{123}$ in natural (Planck) units, see Fig. 5. (So we may still have a long way to go.)

I find Penrose’s consideration about the very far from equilibrium uniform density initial state quite plausible, but it is obviously far from proven. In any case it is, as Feynman says, both necessary and sufficient to assume a far from equilibrium initial state of the universe, and this is in accord with all cosmological evidence. The question as to why the universe started out in such a very unusual low entropy initial state worries R. Penrose quite a lot (since it is not explained by any current theory) but such a state is just accepted as a given by Boltzmann. My own feelings are in between. It would certainly be nice to have a theory which would explain the "cosmological initial state" but I am not holding my breath. Of course, if one believes in the "anthopic principle" in which there are many universes and ours just happens to be right or we would not be here then there is no problem – but I don't find this very convincing [32].

7 Boltzmann vs. Gibbs Entropies

The Boltzmannian approach, which focuses on the evolution of a single macroscopic system, is conceptually different from what is commonly referred to as the Gibbsian approach, which focuses primarily on probability distributions or ensembles. This difference shows up strikingly when we compare Boltzmann's entropy—defined in (1) 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

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

Here $\rho(X)dX$ is the probability (obtained some way or other) for the microscopic state of the system to be found in the phase space volume element dX and the integral is over the phase space Γ. 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,

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

The probability density $\rho_{M_{eq}}$ for a system in the equilibrium macrostate M_{eq} is, as already noted, essentially the same as that for the microcanonical (and equivalent also to the canonical or grandcanonical) ensemble when the system is of macroscopic size. Generalized microcanonical ensembles $\rho_M(X)$, or their canonical versions, are also often used to describe 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 which we have local equilibrium [18]. In such cases $S_G(\{\rho_M\})$ and $S_B(M)$ agree with each other, and with the macroscopic hydrodynamic entropy, to leading order in system size^d. (The ρ_M do not however describe the fluxes in such systems: the average of $J(X)$, the microscopic flux function, being zero for ρ_M [18].)

The time evolutions of S_B and S_G subsequent to some initial time when $\rho = \rho_M$ are *very* different, unless $M = M_{eq}$ when there is no further systematic change in M or ρ. As is well known, it follows from the fact (Liouville's thoerem) that the volume of phase space regions remains unchanged under the Hamiltonian time evolution (even though their shape changes greatly) that $S_G(\{\rho\})$ never changes in time as long as X evolves according to the Hamiltonian evolution, i.e. ρ evolves according to the Liouville equation. $S_B(M)$, on the other hand, certainly does change. Thus, if we consider the evolution of the microcanonical ensemble corresponding to the macrostate M_a in Fig. 1a after removal of the constraint, S_G would equal S_B initially but subsequently S_B would increase while S_G would remain constant. S_G therefore does not give any indication that the system is evolving towards equilibrium.

This reflects the fact, discussed earlier, that the probabililty density $\rho_t(X)$ does not remain uniform over the domain corresponding to the macrostate $M_t = M(X_t)$ for $t > 0$. I am thinking here of the case in which M_t evolves deterministicaly so that almost all X initially in Γ_{M_0} will be in Γ_{M_t} at time t, c.f. [2]. As long as the system remains truly isolated $\rho_t(X)$ will contain memories of the initial ρ_0 in the higher order correlations, which are reflected in the complicated shape which an initial region Γ_{M_0} takes on in time but which do not affect the future time evolution of M (see the discussion at end of section 4). *Thus the relevant entropy for understanding the time evolution of macroscopic systems is S_B and not S_G.*

Of course, if we do, at each time t, a "coarse graining" of ρ over the cell Γ_{M_t} then we are essentially back to dealing with ρ_{M_t}, and we are just defining S_B in a backhanded way. This is one of the standard ways, used in many textbooks, of reconciling the constancy of S_G with the behavior of the entropy in real systems. I fail to see what is gained by this except to obscure the fact that the microstate of a system is specified at any instant of time by a single phase point X_t and that its evolution in time is totally independent of how well we know the actual value of X_t. Why not use S_B from the beginning? We can of course still use ensembles for computations. They will yield correct results whenever the quantities measured, which may involve averages over some time interval τ, have small dispersion in the ensemble considered.

8 Quantitative Macroscopic Evolution

Let me now describe briefly the very important but very daunting task of actually rigorously deriving time asymmetric hydrodynamic equations from reversible microscopic laws [18], [19]. While many qualitative features of irreversible macroscopic behavior depend very little on the positivity of Lyapunov exponents, ergodicity, or mixing properties of the microscopic dynamics, such properties are important for the existence of a quantitative description of the macroscopic evolution via time-asymmetric *autonomous* equations of hydrodynamic type. The existence and form of such equations depend on the rapid decay of correlations in space and time, which requires chaotic dynamics. When the chaoticity can be proven to be strong enough (and of the right form) such equations can be derived rigorously from the reversible microscopic dynamics by taking limits in which the ratio of macroscopic to microscopic scales goes to infinity. Using the law of large numbers one shows that these equations describe the behavior of almost all individual systems in the ensemble, not just that of ensemble averages, i.e. that the dispersion goes to zero in the scaling limit. The equations also hold, to a high accuracy, when the macro/micro ratio is finite but very large [18].

As already mentioned, an example in which this can be worked out in detail is the periodic Lorentz gas. This consists of a *macroscopic number of non-interacting particles* moving among a periodic array of fixed convex scatterers, arranged in the plane in such a way that there is a maximum distance a particle can travel between collisions (finite horizon Sinai billiard). The chaotic nature of the microscopic dynamics, which leads on microscopic time scales to an approximately isotropic local distribution of velocities, is directly responsible for the existence of a simple autonomous deterministic description, via a diffusion equation, for the macroscopic particle density profile of this system [18]. A second example is a system of hard spheres at very low densities for which the Boltzmann equation has been shown to describe (at least for short times) [17] the evolution of $f_t(\mathbf{r}, \mathbf{v})$, the empirical density in the six dimensional position and velocity space. I use these examples, despite their highly idealized nature, because here (and unfortunately only here) all the mathematical i's have been dotted. They thus show *ipso facto*, in a way that should convince even (as Mark Kac put it) an "unreasonable" person, not only that there is no conflict between reversible microscopic and irreversible macroscopic behavior but also that, in these cases at least, *for almost all initial microscopic states consistent with a given nonequilibrium* *macroscopic state*, the latter follows from the former—in complete accord with Boltzmann's ideas.

9 Quantum Mechanics

While the above analysis was done, following Maxwell, Thomson and Boltzmann, in terms of classical mechanics, the situation is in many ways similar in quantum mechanics. Formally the reversible incompressible flow in phase space is replaced by the unitary evolution of wave functions in Hilbert space and velocity reversal of X by complex conjugation of the wavefunction Ψ. In particular, I do not believe that quantum *measurement* is a *new* source of irreversibility. Rather, real measurements on quantum systems are time-asymmetric because they involve, of necessity, systems with a very large number of degrees of freedom whose irreversibility can be understood using natural extensions of classical ideas [33]. There are however also some genuinely new features in quantum mechanics relevant to our problem; for a more complete discussion see [34].

Similarities

Let me begin with the similarities. The analogue of the Gibbs entropy of an ensemble, Eq (3), is the well known von Neumann entropy of a density matrix $\hat{\mu}$,

$$\hat{S}_{vN}(\hat{\mu}) = -kTr\hat{\mu}\log\hat{\mu}. \tag{6}$$

This entropy, like the classical $S_G(\rho)$, does not change in time for an isolated system evolving under the Schrödinger time evolution [13], [35]. Furthermore it has the value zero whenever $\hat{\mu}$ represents a pure state. It is thus, like $S_G(\rho)$, not appropriate for describing the time asymmetric behavior of an isolated macroscopic system. We therefore naturally look for the analog of the Boltzmann entropy given by Eq (1). We shall see that while the quantum version of (1b) is straight forward there is no strict analog of (1a) with X replaced by Ψ which holds for all Ψ.

In a surprisingly little quoted part of his famous book on quantum mechanics [35], von Neumann discusses what he calls the macroscopic entropy of a system. To begin with, von Neumann describes a macrostate M of a macroscopic quantum system[i] by specifying the values of a set of "rounded

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[i] von Neumann unfortunately does not always make a clear distinction between systems

off" commuting macroscopic observables, i.e. operators $\hat{M}$, representing particle number, energy, etc., in each of the cells into which the box containing the system is divided (within some tolerence). Labeling the set of eigenvalues of the $\hat{M}$ by M_α, $\alpha = 1, ...$, one then has, corresponding to the collection $\{M_\alpha\}$, an orthogonal decomposition of the system's Hilbert space $\mathcal{H}$ into linear subspaces $\hat{\Gamma}_\alpha$ in which the observables $\hat{M}$ take the values of M_α. (We use here the subscript α to avoid confusion with the operators $\hat{M}$.)

Calling E_α the projection into $\hat{\Gamma}_\alpha$, von Neumann then defines the *macroscopic entropy* of a system with a density matrix; $\hat{\mu}$ as,

$$\hat{S}_{mac}(\hat{\mu}) = k \sum_{\alpha=1}^{L} p_\alpha(\hat{\mu}) \log |\hat{\Gamma}_\alpha| - k \sum_{\alpha=1}^{L} p_\alpha(\hat{\mu}) \log p_\alpha(\hat{\mu}) \tag{7}$$

where $p_\alpha(\hat{\mu})$ is the probability of finding the system with density matrix $\hat{\mu}$ in the macrostate M_α,

$$p_\alpha(\hat{\mu}) = Tr(E_\alpha \hat{\mu}), \tag{8}$$

and $|\hat{\Gamma}_\alpha|$ is the dimension of $\hat{\Gamma}_\alpha$ (Eq (6) is at the bottom of p 411 in [35]; see also Eq (4) in [36]). An entirely analogous definition is made for a system represented by a wavefunction Ψ: we simply replace $p_\alpha(\hat{\mu})$ in (7) and (8) by $p_\alpha(\Psi) = (\Psi, E_\alpha \Psi)$. In fact $|\Psi >< \Psi|$ just corresponds, as is well known, to a particular (*pure*) density matrix $\hat{\mu}$.

Von Neumann justifies (7) by noting that

$$\hat{S}_{mac}(\hat{\mu}) = -kTr[\tilde{\mu} \log \tilde{\mu}] = S_{vN}(\tilde{\mu}) \tag{9}$$

for

$$\tilde{\mu} = \sum (p_\alpha / |\hat{\Gamma}_\alpha|) E_\alpha \tag{10}$$

and that $\tilde{\mu}$ is macroscopically indistinguishable from $\hat{\mu}$. This is analogous to the classical "coarse graining" discussed at the end of section 7, with $\tilde{\mu}_\alpha = E_\alpha / |\hat{\Gamma}_\alpha| \leftrightarrow \rho_{M_\alpha}$ there.

It seems natural to make the correspondence between the partitioning of classical phase space Γ and the decomposition of the Hilbert space $\mathcal{H}$ and to define the natural quantum analogue to Boltzmann's definition of $S_B(M)$ in (1), as

$$\hat{S}_B(M_\alpha) = k \log |\hat{\Gamma}_{M_\alpha}| \tag{11}$$

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of macroscopic size and those consisting of only a few particles and this leads I believe to much confusion, c.f. article by Kemble [36]. See also articles by Bocchieri and Loinger [37], who say it correctly.

where $|\hat{\Gamma}_M|$ is the dimension of $\hat{\Gamma}_M$. This is in fact done more or less explicitely in [35], [37], [13], [38] and is clearly consistent with the standard prescription for computing the von Neumann quantum entropy of an equilibrium systems, with $\hat{\mu} = \hat{\mu}_{eq}$, where $\hat{\mu}_{eq}$ is the microcanonical density matrix; $\hat{\mu}_{eq} \sim \tilde{\mu}_\alpha$, corresponding to $M_\alpha = M_{eq}$. This was in fact probably standard at one time but since forgotten. In this case the right side of (11) is, to leading order in the size of the system, equal to the von Neumann entropy computed from the microcanonical density matrix (*as it is for classical systems*) [13].

With this definition of $\hat{S}_B(M)$, the first term on the right side of equation (7) is just what we would intuitively write down for the expected value of the entropy of a classical system of whose macrostate we were unsure, e.g. if we saw a pot of water on the burner and made some guess, described by the probability distribution p_α, about its temperature or energy. The second term in (7) will be negligible compared to the first term for a macroscopic system, classical or quantum, going to zero when divided by the number of particles in the system.

One can give arguments for expecting $\hat{S}_B(M_t)$ to increase (or stay constant) with t after a constraint is lifted in a macroscopic system until the system reaches the macrostate M_{eq} [38]. [37], [34]. These arguments are on the heuristic conceptual level analogous to those given above for classical systems, although there are at present no worked out examples analogous to those described in the last section. This will hopefully be remedied in the near future.

Differences

We come now to the differences between the classical and quantum pictures. While in the classical case the actual state of the system is described by $X \in \Gamma_\alpha$, for some α, so that the system is always definitely in one of the macrostates M_α, this is not so for a quantum system specified by $\hat{\mu}$ or Ψ. We thus do not have the analog of (1a) for general $\hat{\mu}$ or Ψ. In fact, even when the system is in a microstate $\hat{\mu}$ or Ψ corresponding to a definite macrostate at time t_0, only a classical system will always be in a unique macrostate for all times t. The quantum system may evolve to a superposition of different macrostates, as happens in the well known Schrödinger cat paradox: a wave function Ψ corresponding to a particular macrostate evolves into a linear combination of wavefunctions associated with very different macrostates, one corresponding to a live and one to a dead cat (see references [38] - [41]).

The possibility of superposition of wavefunctions is of course a general, one might say the central, feature of quantum mechanics. It is reflected here by the fact that whereas the relevant classical phase space can be partitioned into cells Γ_M such that every X belongs to exactly one cell, i.e. every microstate corresponds to a unique macrostate, this is not so in quantum mechanics. The superposition principle rules out any such meaningful partition of the Hilbert space: all we have is an orthogonal decomposition. Thus one cannot associate a definite macroscopic state to an arbitrary wave function of the system. This in turn raises questions about the connection between the quantum formalism and our picture of reality, questions which are very much part of the fundamental issues concerning the interpretation of quantum mechanics as a theory of events in the real world; see [16], and [38]–[44] and references there for a discussion of these problems.

Another related difference between classical and quantum mechanics is that quantum correlations between separated systems arising from wave function entanglement render very problematic, in general, our assigning a wave function to a subsystem $\mathcal{S}_1$ of a system $\mathcal{S}$ consisting of parts $\mathcal{S}_1$, and $\mathcal{S}_2$ even when there is no direct interaction between $\mathcal{S}_1$ and $\mathcal{S}_2$. This makes the standard idealization of physics— an isolated system—much more problematical in quantum mechanics than in classical theory. In fact any system, considered as a subsystem of the universe described by some wavefunction Ψ, will in general not be described by a wavefunction but by a density matrix, $\mu^\Psi = Tr|\Psi >< \Psi|$ where the trace is over $\mathcal{S}_2$.

It turns out that for a small system coupled to a large system, which may be considered as a heat bath, the density matrix of the small system will be the canonical one, $\hat{\mu}_s = \hat{\mu}_\beta \sim \exp[-\beta \hat{H}_s]$ [45], [46]. To be more precise, assume that the (small) system plus heat bath $(s + B)$ are described by a microcanonical ensemble, specified by giving a uniform distribution over all normalized wave functions Ψ of $(s+B)$ in an energy shell $(E, E+\delta E)$. Then the reduced density matrix of the system $\hat{\mu}_s = Tr_B|\Psi >< \Psi|$ obtained from any typical Ψ will be close to $\hat{\mu}_\beta$, i.e. the difference between them will go to zero (in the trace norm) as the number of degrees of freedom in the bath goes to infinity. This is a remarkable property of quantum systems which has no classical analogue. All one can say classically is that if one averges over the microstates of the bath one gets the canonical Gibbs distribution for the system. This is of course also true and well known for quantum systems, but what is new is that this is actually true for almost all pure states Ψ, [45], [46] see also references there to earlier work in that direction, including [37].

One can even go further and find the dsitribution of the "wave function"

φ of the small system described by $\hat{\mu}_\beta$ [47]. For ways of giving meaning to the wavefunction of a subsystem, see [41] - [42] and [48].

10 Final Remarks

As I stated in the beginning, I have here completely ignored relativity, special or general. The phenomenon we wish to explain, namely the time-asymmetric behavior of macroscopic objects, has certainly many aspects which are the same in the relativistic (real) universe as in a (model) non-relativistic one. The situation is of course very different when we consider the entropy of black holes and the nature of the appropriate initial cosmological state where relativity is crucial. Similarly the questions about the nature of time mentioned in the beginning of this article cannot be discussed meaningfully without relativity. Such considerations may yet lead to entirely different pictures of the nature of reality and may shed light on the interpretation of quantum mechanics, discussed in the last section, c.f. [16]. Still it is my belief that one can and in fact one must, in order to make any scientific progress, isolate segments of reality for separate analysis. It is only after the individual parts are understood, on their own terms, that one can hope to synthesize a *complete picture*.

To conclude, I believe that the Maxwell-Thomson-Boltzmann resolution of the problem of the origin of macroscopic irreversibility contains, in the simplest idealized classical context, the essential ingredients for understanding this phenomena in real systems. Abandoning Boltzmann's insights would, as Schrödinger says[j] be a most serious scientific regression. I have yet to see any good reason to doubt Schrödinger's assessment.

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[j] Schrödinger writes [26], "the spontaneous transition from order to disorder is the quintessence of Boltzmann's theory ... This theory really grants an understanding and does not ... reason away the dissymmetry of things by means of an a priori sense of direction of time variables... No one who has once understood Boltzmann's theory will ever again have recourse to such expedients. It would be a scientific regression beside which a repudiation of Copernicus in favor of Ptolemy would seem trifling."

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