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Physica A 263 (1999) 516–527

**PHYSICA A**

# Microscopic Origins of Irreversible Macroscopic Behavior <sup>\*</sup>

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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 in accord with the ideas of Thompson, Maxwell and Boltzmann. Alternate explanations based on equating irreversible macroscopic behavior with the mixing type of behavior already present in the time evolution of ensembles (probability distributions) of certain systems having only a few degrees of freedom are, in my opinion, unnecessary, misguided and misleading.

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## Formulation of Problem

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. My goal is much more modest. Using as a working hypothesis, a) the Newtonian notions of space and time as primitive undefined concepts and b) that matter is composed of atoms that move according to classical dynamics, I will try to clarify the many conceptual and technical problems encountered in going from a time symmetric description of the dynamics of atoms to a time asymmetric description of the evolution of macroscopic systems.<sup>1</sup> This passage involves a change from Hamiltonian equations to hydrodynamical ones, e.g. the diffusion equation.

The problem of reconciling the latter description with the former became a central issue in physics during the last part of the nineteenth century. It was also, in my opinion (but clearly not in that of all scientists) resolved at that time. To quote from Thompson's (later Lord Kelvin) 1874 article [1], "The essence of Joule's discovery is the subjection of physical phenomena to dynamical law. If, then, the motion of every particle of matter in

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<sup>\*</sup> Much of the material is taken from my review article which will appear in the special March 1999 issue of Reviews of Modern Physics celebrating the centennial of the American Physical Society.

<sup>1</sup> The reason why this simplified model contains the essential ingredient of macroscopic irreversibility even though it neglects relativistic effects and how it needs to be extended to take account of quantum mechanics will be discussed briefly later.

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 [read irreversible behavior] is compatible with a molecular theory in which each particle is subject to the laws of abstract dynamics.”

Formally the problem considered by Thomson is as follows: The complete microscopic (or micro)state of an isolated classical system of  $N$  particles is represented by a point  $X$  in its phase space  $\Gamma$ ,  $X = (\mathbf{r}_1, \mathbf{p}_1, \mathbf{r}_2, \mathbf{p}_2, \dots, \mathbf{r}_N, \mathbf{p}_N)$ ,  $\mathbf{r}_i$  and  $\mathbf{p}_i$  being the position and momentum of the  $i$ th particle. The evolution is governed by Hamiltonian dynamics which, given the microstate  $X(t_0)$  at some time  $t_0$  determines the microstate  $X(t)$  at all other times  $t$ ,  $-\infty < t < \infty$ . Let  $X(t_0)$  and  $X(t_0 + \tau)$ , with  $\tau$  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  $\tau$  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;  $RX = (\mathbf{r}_1, -\mathbf{p}_1, \mathbf{r}_2, -\mathbf{p}_2, \dots, \mathbf{r}_N, -\mathbf{p}_N)$ . Hence, if there is an evolution, i.e. a trajectory  $X(t)$  in which some property of the system, described by some function  $f(X)$  for which  $f(X) = f(RX)$ , increases as  $t$  increases, e.g. particle densities get more uniform by diffusion, there is also one in which the property, e.g. the density profile, evolves in the opposite direction, since the density is the same for  $X$  and  $RX$ . So why is one type of evolution, identified with “entropy” increase by the second “law”, common and the other never seen?

### Resolution of Problem

The explanation of this apparent paradox, due to Thomson, Maxwell and Boltzmann, which I will now describe, shows that not only is there no conflict between reversible microscopic laws and irreversible macroscopic behavior, but, as clearly pointed out by Boltzmann in his later writings <sup>2</sup>, there are extremely strong, albeit subtle, reasons to expect the latter from the former. These involve several interrelated ingredients which together provide the sharp distinction between microscopic and macroscopic variables required for the emergence of definite time asymmetric behavior in the evolution of the latter despite the total absence of such asymmetry in the dynamics of individual atoms. They are: a) the great disparity between microscopic and macroscopic scales, b) the fact that events are, as put by Boltzmann, determined not only by differential equations, but also by initial conditions, and c) the use of probabilistic reasoning: it is not every microscopic state of a macroscopic system that will evolve in accordance with the second law, but only the “majority” of states – a majority which however becomes so overwhelming when the number of atoms in the system becomes very large that irreversible behavior becomes a near certainty. (The characterization of the set whose “majority” we are describing will be discussed later.)

To see how the explanation works let us denote by  $M$  the macrostate of a macroscopic system. For a system containing  $N$  atoms in a box  $V$ , the microstate  $X$  is a point in the

<sup>2</sup> Boltzmann’s early writings on the subject are sometimes unclear, wrong, and even contradictory. His later writings, however, are superbly clear and right on the money (even if a bit verbose for Maxwell’s taste). I strongly recommend the references cited at the end.

$6N$  dimensional phase space  $\Gamma$  while  $M$  is a much cruder description, e.g. the specification, to within a given accuracy, of the energy of the system and of the number of particles in each half of the box. (A more refined (hydrodynamical) description would divide  $V$  into  $K$  cells, where  $K$  is large, but still  $K \ll N$ , and specify the number of particles and energy in each cell, again with some tolerance.) Thus, while  $M$  is determined by  $X$  there are many  $X$  which correspond to the same  $M$ . We will call  $\Gamma_M$  the region in  $\Gamma$  consisting of all microstates  $X$  corresponding to a given macrostate  $M$  and take as a measure of the “number” of microstates corresponding to a subset  $A$  of  $\Gamma_M$  to be equal to the  $6N$  dimensional Liouville volume of  $A$ , normalized by the volume of  $\Gamma_M$  denoted by  $|\Gamma_M|$ :  $|\Gamma_M| = \int_{\Gamma_M} \prod_{i=1}^N d\mathbf{x}_i d\mathbf{p}_i$ . (This “number” corresponds to the classical limit of the number of states in quantum mechanics.)

Consider now a situation in which there is initially a wall confining a dilute gas of  $N$  atoms to the left half of the box  $V$ . When the wall is removed at time  $t_a$ , the phase space volume available to the system is fantastically enlarged, roughly by a factor of  $2^N$ . (If the system contains 1 mole of gas in a container then the volume ratio of the unconstrained region to the constrained one is of order  $10^{10^{20}}$ ). This region will contain new macrostates 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 it will with very high “probability” enter the newly available regions of phase space and thus find itself in a succession of new macrostates  $M$  for which  $|\Gamma_M|$  is increasing. This will continue until the system reaches its unconstrained macroscopic equilibrium state,  $M_{eq}$ , that is, until  $X(t)$  reaches  $\Gamma_{M_{eq}}$ , corresponding to approximately half the particles in each half of the box, say within an interval  $(\frac{1}{2} - \epsilon, \frac{1}{2} + \epsilon)$ ,  $\epsilon \ll 1$ , since in fact  $|\Gamma_{M_{eq}}|/|\Sigma_E| \simeq 1$ , where  $|\Sigma_E|$  is the total phase space volume available under the energy constraint. After that time we will see only small fluctuations about the value  $\frac{1}{2}$ , well within the precision  $\epsilon$ , typical fluctuations being of the order of the square root of the number of particles involved.

### Boltzmann’s Entropy

To extend the above observation to more general situations Boltzmann associated with each microscopic state  $X$  of a macroscopic system, be it gas, fluid or solid, a number  $S_B$ , given, up to multiplicative and additive constants (in particular we set Boltzmann’s constant,  $k_B$ , equal to unity), by

$$S_B(X) = \log |\Gamma_{M(X)}|. \quad (1)$$

A crucial observation made by Boltzmann was that when  $X \in M_{eq}$  then  $S_B(X)$  (which following Penrose [2] we shall call the Boltzmann entropy of the macrostate  $M = M(X)$ ) agrees, up to terms negligible in the size of the system, with the thermodynamic entropy of Clausius.  $S_B(X)$  thus provides a microscopic definition of this macroscopically defined, operationally measurable (à la Carnot), extensive property of macroscopic systems in *equilibrium*. Having made this connection Boltzmann found it natural also to use (1) to define the entropy for a macroscopic system not in equilibrium and thus 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<sup>3</sup>, i.e. that  $S_B$  will *typically* increase in a way which *explains* and describes qualitatively the evolution towards equilibrium of macroscopic systems.

Typical, as used here, means that the set of microstates corresponding to a given macrostate  $M$  for which the evolution leads to a macroscopic decrease in the Boltzmann entropy during some fixed time period  $\tau$ , occupies a subset of  $\Gamma_M$  whose Liouville volume is a fraction of  $|\Gamma_M|$  which goes very rapidly (exponentially) to zero as the number of atoms in the system increases.

It is this very large number of degrees of freedom involved in the specification of macroscopic properties which distinguishes macroscopic irreversibility from the weak approach to equilibrium of ensembles for systems with good ergodic properties [1f]. While the former is manifested in a typical evolution of a single macroscopic system, the latter, which is also present in *chaotic* systems with but a few degrees of freedom, e.g. two hard spheres in a box, does not correspond to any appearance of time asymmetry in the evolution of an individual system. On the other hand, because of the exponential increase of the phase space volume, even a system with only a few hundred particles (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.<sup>4</sup> 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 Poincaré recurrence times) in the typical way [3].

Maxwell makes clear the importance of the scale separation when he writes [4]: “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.” We might take as a summary of the discussions in the late part of the last century the statement by Gibbs [5] quoted by Boltzmann (in a German translation) on the cover of his book *Lectures on Gas Theory II*: “In other words, the impossibility of an uncompensated decrease of entropy seems to be reduced to an improbability.”

### The Use of Probabilities

As already noted, typical here refers to a measure which assigns (at least approximately) equal weights to the 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

<sup>3</sup> 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  $S_B$  is more problematical. For a dilute gas in which  $M$  is specified by the density  $f(\mathbf{r}, \mathbf{v})$  of atoms in the six dimensional position and velocity space,  $S_B(X) = - \int f(\mathbf{r}, \mathbf{v}) \log f(\mathbf{r}, \mathbf{v}) d\mathbf{r}d\mathbf{v}$ . This identification is, however, invalid when the potential energy is not negligible; c.f. E. T. Jaynes, *Phys. Rev. A*, **4**, 747 (1971).

<sup>4</sup> 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  $10^{23}$ .

computer simulations.) In fact, any meaningful statement about probable or improbable behavior of a physical system has to refer to some agreed upon measure (probability distribution). It is, however, this use of probabilities (whose justification is beyond the reach of mathematical theorems) and particularly of the notion of typicality for explaining the origin of the apparently deterministic second law which was most difficult for many of Boltzmann's contemporaries, and even for some people today, to accept [1f, g]. This was clearly faced by Boltzmann 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 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."

It should be noted here that an important ingredient in the above analysis is the constancy in time of the Liouville volume of sets in the phase space  $\Gamma$  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. We also note that, in contrast to  $S_B(X)$ , the Gibbs entropy  $S_G(\mu)$ ,

$$S_G(\mu) = - \int \mu \log \mu dX, \quad (2)$$

is defined not for individual microstates but for statistical ensembles or probability distributions  $\mu$ . For equilibrium ensembles  $S_G(\mu_{eq}) \sim \log |\Sigma_E| \sim S_B(X)$ , for  $X \in M_{eq}$ , up to terms negligible in the size of the system. However, unlike  $S_B$ ,  $S_G$  does not change in time even for time dependent ensembles describing (isolated) systems not in equilibrium. Hence the relevant entropy for understanding the time evolution of macroscopic systems is  $S_B$  and not  $S_G$ .

### 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*.

Put another way: why can we use phase space arguments (or time asymmetric diffusion type equations) to predict the macrostate at time  $t$  of an *isolated* system in a nonequilibrium macrostate  $M_b$  at some time  $t_b$ , e.g. a metal bar with a nonuniform temperature, 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 state of the metal bar,  $M_b$ , had its origin in an even more nonuniform macrostate  $M_a$ , prepared by some experimentalist at some earlier time  $t_a < t_b$  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 or she part of the physical universe?

Before trying to answer the last set of “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  $t > t_b$  when the system is isolated for  $t > t_a$ . Note that those microstates in  $\Gamma_{M_b}$  which have come from  $\Gamma_{M_a}$  through the time evolution during the time interval from  $t_a$  to  $t_b$  make up only a very small fraction of the volume of  $\Gamma_{M_b}$ , call it  $\Gamma_{ab}$ . Thus we have to show that the overwhelming majority of points in  $\Gamma_{ab}$  (with respect to Liouville measure on  $\Gamma_{ab}$ , which is the same as Liouville measure on  $\Gamma_{M_a}$ ) have *future* macrostates like those typical of  $\Gamma_b$ —while still being very special and unrepresentative of  $\Gamma_{M_b}$  as far as their *past* macrostates are concerned.<sup>5</sup> This property is explicitly proven by Lanford in his derivation of the Boltzmann equation (for short times) [7], and is part of the derivation of hydrodynamic equations [8]; see also [9].

To see intuitively the origin of this property we note that for systems with realistic interactions the domain  $\Gamma_{ab}$  will be so convoluted as to *appear* uniformly smeared out in  $\Gamma_{M_b}$ . 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, e.g. 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. Our mathematical abilities are, however, equal to this task only in very simple situations, as we shall see below. These results should, however, be enough to convince a ‘reasonable’ person.

The large number of atoms present in a macroscopic system plus the chaotic nature of the dynamics also explains why it is so difficult, essentially impossible (except in some special cases such as experiments of the spin-echo type, and then only for a limited time), for a clever experimentalist to deliberately put such a system in a microstate which will lead it to evolve contrary to the second law. Such microstates certainly exist—just start with a nonuniform temperature, let it evolve for a while, then reverse all velocities. In fact, they are readily created in the computer simulations with no roundoff errors discussed earlier [3]. To quote again from Thomson’s article [1]: “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.” In *addition*, 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 [1f].

<sup>5</sup> We are considering here the case where the macrostate  $M(t)$ , at time  $t$ , determines  $M(t')$  for  $t' > t$ . There are of course situations where  $M(t')$  depends also (weakly or even strongly) on the history of  $M(t)$  in some time interval prior to  $t'$ , e.g. in materials with memory.

Let us return now to the big question posed earlier: what is special about  $t_a$  compared to  $t_b$  in a world with symmetric 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 cosmological considerations and to postulate an initial “macrostate of the universe” having a very small Boltzmann entropy. To again quote Boltzmann [13]: “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 [macro]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”. We do not, however, have to assume a very special initial microstate  $X$ , and this is a very important aspect of our considerations. As Boltzmann further writes: “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.” All that is necessary to assume is a far from equilibrium initial macrostate and this is in accord with all cosmological and other independent evidence.

Feynman clearly agrees with this when he says [11], “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 an understanding of the irreversibility.” More recently the same point was made very clearly by Roger Penrose in connection with the “big bang” cosmology [12]. Penrose, unlike Boltzmann, believes that we should search for a more fundamental theory which will also account for the initial conditions. Meanwhile he takes for the initial macrostate of the universe the smooth energy density state prevalent soon after the big bang. Whether this is the appropriate initial state or not, it captures an essential fact about our universe. Gravity, being purely attractive and long range, is unlike any of the other natural 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.

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 consequence of) the initial macrostate of the universe. The value of  $S_B$  of the present clumpy macrostate of the universe, consisting of planets, stars, galaxies, and black holes, is much much larger than that in the initial state and also quite far away from its equilibrium value. The ‘natural’ or ‘equilibrium’ state of the universe is, according to Penrose, one with all matter and energy collapsed into one big black hole with a phase space volume some  $10^{10^{120}}$  times that of the initial macrostate. (So we may still have a long way to go.)

### Quantitative Considerations

Let me now describe briefly the very interesting work, still in progress, in which one rigorously derives time asymmetric hydrodynamic equations from reversible microscopic laws [8]. While many qualitative features of irreversible macroscopic behavior depend very little on the positivity of Lyapunov exponents, ergodicity, or mixing properties of the mi-

croscopic dynamics, such properties are important for the quantitative description of the macroscopic evolution, i.e. for the existence of time-asymmetric *autonomous* equations of hydrodynamic type. The existence and form of such equations depend on the instabilities of microscopic trajectories induced by 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.

A simple example in which this can be worked out in detail is the periodic Lorentz gas (or Sinai billiard). 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. The chaotic nature of the microscopic dynamics, which leads 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 profiles of this system [8]. A second example is a system of hard spheres at very low densities for which the Boltzmann equation has been shown to describe the evolution of the density in the six dimensional position and velocity space (at least for short times) [7]. I use these examples, despite their highly idealized nature, because 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, *for essentially all initial microscopic states consistent with a given nonequilibrium macroscopic state*, the latter follows from the former—in complete accord with Boltzmann's ideas. Yet the debate goes on.

### Quantum Mechanics

While the above analysis was done 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  $\psi$ . 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 very large number of degrees of freedom whose irreversibility can be understood using natural extensions of classical ideas [13]. There are however also some genuinely new features in quantum mechanics relevant to our problem.

Let me begin with the similarities. In a surprisingly little quoted part of his famous book on quantum mechanics [14], von Neumann discusses in some detail (but not very clearly) what might be taken to be the quantum analog of the classical Boltzmann entropy  $S_B(X) = \log |\Gamma_{M(X)}|$ . Von Neumann proposes to describe a macrostate  $M$  of an isolated macroscopic quantum system by specifying the values (within some intervals) of a set of “rounded off” commuting macroscopic observables (operators)  $\hat{M}$  representing particle

number, energy, etc. in each of the cells into which the box containing the system is divided to define the macrostate  $M$ . The analog of  $\Gamma_M$  is then taken to be the linear subspace  $\hat{\Gamma}_M$  of the Hilbert space  $\mathcal{H}$  of the system in which the observables  $\hat{M}$  take the values corresponding to  $M$ . Labeling the set of possible macrostates by  $M_\alpha$ ,  $\alpha = 1, \dots, L$ , we will then have, corresponding to the set  $\{M_\alpha\}$ , an orthogonal decomposition  $\{\hat{\Gamma}_\alpha\}$  of  $\mathcal{H}$ . Calling  $E_\alpha$  the projection into  $\hat{\Gamma}_\alpha$ , von Neumann defines the *macroscopic entropy* of a system specified by a wave function  $\psi \in \mathcal{H}$  as

$$\hat{S}_B(\psi) = \sum_{\alpha=1}^L p_\alpha(\psi) \log |\hat{\Gamma}_\alpha| - \sum_{\alpha=1}^L p_\alpha(\psi) \log p_\alpha(\psi) \quad (3)$$

where  $p_\alpha(\psi)$  is the probability of finding the system with wave function  $\psi$  in the macrostate  $M_\alpha$ ,

$$p_\alpha(\psi) = (\psi, E_\alpha \psi), \quad (4)$$

and  $|\hat{\Gamma}_\alpha|$  is the dimension of  $\hat{\Gamma}_\alpha$ .

An entirely analogous definition is made for a system represented by a density matrix  $\hat{\mu}$ : we simply replace  $p_\alpha(\psi)$  in (3) and (4) by  $p_\alpha(\hat{\mu}) = \text{Tr}(E_\alpha \hat{\mu})$ . In fact  $\psi$  just corresponds, as is well known, to a particular *pure* density matrix  $\hat{\mu}_\psi$ . I will therefore from now on use  $\hat{\mu}$  to denote the microstate of a quantum system—always meaning by this the most detailed description possible, within conventional quantum mechanics, of the state of a system (see end of this section).

Von Neumann then notes (as we did earlier for classical systems) that unlike  $\hat{S}_G(\hat{\mu}) \equiv -\text{Tr}(\hat{\mu} \log \hat{\mu})$ ,  $\hat{S}_B(\hat{\mu})$  will change in time for an isolated quantum system not in equilibrium. He also gives a rather lengthy proof of the fact (which is by now well known and easy to prove) that  $\hat{S}_B(\hat{\mu}) \geq \hat{S}_G(\hat{\mu})$ . Thus if we start the system at  $t = t_0$  with a density matrix  $\hat{\mu}_0 = \sum p_\alpha E_\alpha / |\hat{\Gamma}_\alpha|$  so that at  $t_0$   $\hat{S}_B$  and  $\hat{S}_G$  are equal then, for  $t > t_0$ ,  $\hat{S}_B(\hat{\mu}) \geq \hat{S}_G(\hat{\mu}_t) = \hat{S}_G(\hat{\mu}_0) = \hat{S}_B(\hat{\mu}_0)$ . Unfortunately the fact that  $\hat{S}_B(\hat{\mu}_t) \geq \hat{S}_B(\hat{\mu}_0)$ , which is of course true also in the classical case, doesn't tell us much (if anything) about the actual evolution of the system. (If it did, the second law would be trivially true and we wouldn't need this article.)

On the other hand one can give arguments for expecting  $\hat{S}_B(\hat{\mu}_t)$  to increase with  $t$  after a constraint is lifted in a macroscopic system until the system reaches the macrostate  $M_{eq}$ . These arguments are on the heuristic conceptual level analogous to those given above for classical systems [15], 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: see [16] for some interesting work in that direction.) In fact, with the correspondence between linear dimension,  $|\hat{\Gamma}_M|$ , and phase space volume,  $|\Gamma_M|$ , the first term on the right side of equation (3) 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  $p_\alpha$ , about its temperature (i.e. energy density) profile. (The second term in (3) 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.)

We come now to the differences between the classical and quantum pictures. While in the classical case the  $p_\alpha$  are just an expression of our ignorance, the actual state of

the system being definitely in one of the macrostates  $M_\alpha$ , this is not so for the quantum system—at least with the conventional Copenhagen interpretation of quantum mechanics [17, 18]. In fact, even when the system is in a definite macrostate at time  $t_0$ , say  $p_\alpha = \delta_{\alpha,k}$ , only the classical system will remain in a unique macrostate for times  $t > t_0$ . The quantum system may evolve to a superposition of different macrostates, as happens in the well known Schrödinger cat paradigm or paradox where a wave functions  $\psi$  defining a particular macrostate evolves into a linear combination of wave functions associated with very different macrostates, one corresponding to a live and one to a dead cat.

The possibility of superposition of wave functions 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  $\Gamma_M$  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 the recent articles by S. Goldstein and references there for a careful analysis of these problems [18b].

Another related difference between classical and quantum mechanics is that quantum correlations between separated systems arising from wave function entanglements preclude, in general, our assigning a wave function to a subsystem  $\mathcal{S}_1$  of a system  $\mathcal{S}$  in a definite state  $\psi$ , even at a time when there is no direct interaction between  $\mathcal{S}_1$  and the rest of  $\mathcal{S}$ . This makes the standard idealization of physics — an isolated system — much more problematical in quantum mechanics than in classical theory. One might in fact argue that any real system, considered as a subsystem of the universe described by some wave function  $\Psi$ , will in general not be described by a wave function but by a density matrix. For ways of giving meaning to the wave function of a subsystem see [18b] and papers by Dürr et al. and by Gell-Mann and Hartle [19].

### Final Remarks

As I stated in the beginning, I have completely ignored relativity here, special or general. The phenomenon we wish to explain, namely the time-asymmetric behavior of spatially localized macroscopic objects, has certainly many aspects which are the same in the relativistic (real) universe as in a (model) non-relativistic one. In fact the only way I see relativity modifying the discussion is in the nature of the appropriate initial cosmological state and in the light it may shed on the interpretation of quantum mechanics; see [11]. This assessment is based on 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, all the essential ingredients for understanding this phenomena in real systems.

Abandoning Boltzmann's insights would, as Schrödinger says<sup>6</sup>, be a most serious scientific regression. I have yet to see any good reason to doubt Schrödinger's assessment.

### Acknowledgments

Very extensive and very useful discussions with my colleagues Sheldon Goldstein and Eugene Speer are gratefully acknowledged. Research supported in part by NSF Grant 95-23266, and AFOSR Grant F49620-98-1-0207.

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<sup>6</sup> Schrödinger writes [20], “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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