March 1994 PHYSICS TODAY was the best to date. I've been reading these roundtables for years, and past participants have inevitably blamed our present problems on (a) Congress, (b) the President, (c) uneducated business executives, (d) lazy graduate students and (e) everyone else except us, the physics community. It was refreshing to read of colleagues who finally realize that *they* (a–e above) are not the problem, but that *we* are, and that until and unless we fix ourselves, things are not going to get any better.

Reading the discussion, two additional thoughts came to mind. First, all the participants seemed to agree that the day of the stereotypical arrogant physicist, who is incapable of interacting with other human beings, is over. So it seems only reasonable that universities start to implement admission standards at both undergraduate and graduate levels that reflect this understanding. Members of admissions committees can start to ask, "Well, candidate X has perfect GRE's and straight A's, but what are his human resources skills?" This approach will go a long way toward creating a pool of physicists for the modern research environment. As Anthony Johnson of AT&T Bell Labs described at the roundtable, in today's industrial teams it doesn't matter how smart you are if you can't work with other people.

Second, it seems that the time has come to establish a political action committee that represents physicists. Whether or not this is done as an APS offshoot needs to be determined. Whatever your feelings about the ethics of PACs, they are a political reality. If every name in the APS directory contributed $1.00 per week, there would be considerable resulting financial clout. (If you think $1.00 per week is too much for job and research funding security, see you at the unemployment office.)

JEFFREY H. HUNT
Chatsworth, California

Is Boltzmann Entropy Time's Arrow's Archer?

Ludwig Boltzmann's ideas on irreversibility are as controversial today as they were at their introduction a hundred years ago. In the article "Boltzmann's Entropy and Time's Arrow" (September 1993, page 32), Joel Lebowitz, by giving a modern exposition of Boltzmann's ideas, tries to assure us that the controversy is unwarranted. Readers left unpersuaded should know that they are not alone. Boltzmann's ideas are indeed controversial, because Boltzmann failed to place them on a firm conceptual foundation. Today a firm foundation can be provided—the key ideas are Claude Shannon's statistical information[1] and Edwin Jaynes's principle of maximum entropy[2]—but Lebowitz's update, instead of providing the necessary clarification, recapitulates the same murky concepts in modern language.

Lebowitz addresses how time-asymmetric behavior of macroscopic variables arises from time-symmetric microscopic equations. He partitions phase space into macrostates, coarse-grained cells M_i (of phase-space volume $|\Gamma_{M_i}|$) defined by the values of the macroscopic variables of interest—for example, the numbers of particles within identical cubes that fill configuration space. To each phase-space point, or microstate, in M_i he assigns the Boltzmann entropy $S_B(M_i) = k \log |\Gamma_{M_i}|$. If the system is initially confined to a small phase-space cell, then when the constraints are released, it will tend to wander into larger cells. Lebowitz quantifies this behavior in terms of the Boltzmann entropy, which tends to increase along a "typical" trajectory.

The problem here is not the story so much as the commentary; for someone outlining an avowedly statistical theory, Lebowitz betrays an odd mistrust of probability concepts. He stresses that he is dealing with the typical behavior of individual systems, not with average behavior within an ensemble. But how can one characterize typical behavior without reference to a probability distribution? Furthermore, he dismisses the Gibbs entropy $S_G = -k \int d\Gamma\, \rho \log \rho$ of a phase-space probability distribution ρ as irrelevant to nonequilibrium phenomena, partly because it remains constant under Hamiltonian evolution, but also because it relies on probabilities. Yet what is the significance of the increase of the Boltzmann entropy when it has an interpretation as a physical quantity only in thermodynamic equilibrium? Indeed, why attribute a Boltzmann entropy to each phase-space point when the Boltzmann entropy is wholly a property of the coarse-graining?

Dealing with these questions entails using probabilities. Lebowitz implies that probabilistic predictions apply only to physical ensembles. To the contrary, when probabilities are sharply peaked, as they are for certain macroscopic variables, they make reliable predictions for *individual* systems. Probabilities provide the *only* way to define typical behavior for individual systems and to assess just how typical it is.

The phase-space probability distribution $\rho(t)$ at time t follows from applying the system dynamics to a uniform distribution on the initial cell. The statistics of the macroscopic variables at time t, determined by the probabilities $p_i(t) = \int_{M_i} d\Gamma\, \rho(t)$ to be in cell M_i, are unaffected if $\rho(t)$ is replaced, within each cell M_i, by a uniform distribution containing probability $p_i(t)$. This coarse-grained phase-space distribution can be characterized uniquely as having the maximum Gibbs entropy given the probabilities $p_i(t)$, the maximum being $\bar{S}_G = -k \sum_i p_i \ln p_i + \sum_i p_i S_B(M_i)$.

Lebowitz's insistence on the primacy of Boltzmann entropy over Gibbs entropy is thus stood on its head. The Gibbs entropy $\bar{S}_G$ of the coarse-grained distribution generally increases. Moreover, the increase has a compelling interpretation: Since S_G/k is Shannon's statistical information, the difference between $\bar{S}_G$ and the initial Gibbs entropy is the amount of information discarded when one retains only the statistics of the macroscopic variables. The *average* Boltzmann entropy does contribute to $\bar{S}_G$, but this appearance of the Boltzmann entropies has nothing to do with entropies of individual phase-space points; rather, it is a direct expression of having discarded all information about the details of $\rho(t)$ within the coarse-grained cells.

As Jaynes has emphasized,[2] firm conceptual foundations are required for progress in physics. The shaky foundations provided by Boltzmann and Lebowitz obscure both what has been accomplished and what remains to be done. Boltzmann's ideas can indeed be used to derive time-asymmetric equations for macroscopic variables, once they are supported within the solid framework of Gibbs, Shannon and Jaynes; the Gibbs entropy $\bar{S}_G$ *explains* the time asymmetry as a consequence of discarding microscopic information that is unnecessary for predicting the behavior of the macroscopic variables. Yet this explanation, like all good ones, immediately raises other questions: Why coarse-grain? Why discard information? These questions, the true puzzles of irreversibility, provide the arena for further work.[3]

References

1. C. E. Shannon, W. Weaver, *The Mathematical Theory of Communication*, U. of Illinois P., Urbana (1949).
2. E. T. Jaynes, *Papers on Probability, Statistics and Statistical Physics*, R. D. Rosenkrantz, ed., Kluwer, Dordrecht, The Netherlands (1983).
3. W. H. Zurek, Phys. Rev. A **40**, 4731 (1989). C. M. Caves, Phys. Rev. E **47**, 4010 (1993).

HOWARD BARNUM
CARLTON M. CAVES
CHRISTOPHER FUCHS
RÜDIGER SCHACK
University of New Mexico
Albuquerque, New Mexico

Joel L. Lebowitz's article "Boltzmann's Entropy and Time's Arrow" purports that consideration of the Boltzmann entropy gives a complete resolution of the apparent irreconcilability of the observed irreversible behavior of systems in nature with the time-reversible dynamical laws governing the evolution of trajectories. Lebowitz is correct in pointing out that the Gibbs entropy is constant in all processes and so is not appropriate as a nonequilibrium entropy. However, consideration of the Boltzmann entropy does not give a complete explanation of the problem of irreversibility.

The main virtue of the Boltzmann entropy that is touted in the article is that it "captures the separation between microscopic and macroscopic scales." If the scale-separation argument were the whole story, then irreversibility would be due to our approximate observation or limited knowledge of the system. This is difficult to reconcile with the constructive role of irreversible processes.[1] Furthermore, where the scale separation takes place is not well defined. When the Boltzmann entropy apparently works, as in a gas, it describes only the approach to equilibrium of the velocity distribution for certain initial conditions and does not describe the appearance of correlations.[2]

For these reasons the Brussels–Austin group of which I am a member has for some years proceeded in a different direction. Irreversibility is not to be found on the level of trajectories or wavefunctions but is instead manifest on the level of probability distributions. Both classical and quantum mechanics therefore have to be formulated on the level of probabilities for the classes of dynamical systems where irreversibility takes place. This led to the theory of subdynamics, which allowed the treatment of irreversible processes in terms of both the velocity distribution and correlations.[3] The aim has been to obtain a formulation of the laws of nature in terms of a complex spectral representation of the time-evolution operator for probability densities that is not implementable for trajectories or wavefunctions. This aim has now been fulfilled for classes of chaotic systems[4] and so-called large Poincaré systems[5] by extending the Liouville(–von Neumann) operator to generalized functional spaces. The meaning of entropy becomes clear in this new, extended formulation of dynamics, where the original reversible group splits into two distinct semigroups; as a result, broken time symmetry appears already at the microscopic level.

Also, a crucial point that is neglected in Lebowitz's article is that irreversible processes are well observed in systems with few degrees of freedom, such as the baker and multibaker transformations.[1,4] Hence, many degrees of freedom is not a necessary condition for irreversible behavior. It is the chaotic dynamics, associated with positive Lyapunov exponents or Poincaré resonances, that causes the system to behave irreversibly.

In conclusion, the arrow of time is not due to some phenomenological approximations but is an intrinsic property of classes of unstable dynamical systems. For these systems the dynamical laws may be formulated in extended functional spaces to include the arrow of time. In this formulation probability appears in an irreducible way. This is of special interest for quantum mechanics, as it leads to a unified formulation avoiding the collapse of the wavefunction (since the basic laws are now given on the level of density matrices).

However, dynamics cannot answer why all semigroups in nature are oriented in the same way. The orientation must be mutually compatible, though, because all systems "communicate"; that is, there are no truly isolated systems in nature. The common orientation of the semigroups expresses the unity of nature.

References

1. I. Prigogine, *From Being to Becoming*, Freeman, San Francisco (1980).
2. D. J. Driebe, T. Y. Petrosky, J. Stat. Phys. **67**, 369 (1992). E. T. Jaynes, Phys. Rev. A **4**, 747 (1971).
3. I. Prigogine, C. George, F. Henin, L. Rosenfeld, Chem. Scripta **45**, 5 (1973). I. Prigogine, T. Petrosky, H. Hasegawa, S. Tasaki, Chaos, Solitons and Fractals **1**, 3 (1991). I. Antoniou, S. Tasaki, Int. J. Quantum Chem. **46**, 425 (1993).
4. H. H. Hasegawa, W. C. Saphir, Phys. Rev. A **46**, 7401 (1992). P. Gaspard, J. Phys. A **25**, L483 (1992). I. Antoniou, S. Tasaki, J. Phys. A **26**, 73 (1992); Physica A **190**, 303 (1992). H. H. Hasegawa, D. J. Driebe, Phys. Lett. A **168**, 18 (1992); **176**, 193 (1993); Phys. Rev. E, to appear (1994).
5. T. Petrosky, I. Prigogine, S. Tasaki, Physica A **173**, 175 (1991). I. Antoniou, I. Prigogine, Physica A **192**, 443 (1993). T. Petrosky, I. Prigogine, Physica A **175**, 146 (1991); Proc. Natl. Acad. Sci. USA **90**, 9393 (1993); Chaos, Solitons and Fractals **4**, 311 (1994).

DEAN J. DRIEBE
International Solvay Institutes for Physics and Chemistry
Brussels, Belgium
and University of Texas, Austin

Joel Lebowitz's accurate and entertaining account of Boltzmann's classic explanation of macroscopic irreversibility emphasizes *isolated* systems. Gibbs's ensembles made it possible to widen this explanation to include microscopic systems interacting with thermal reservoirs. And in 1984 Shuichi Nosé discovered a reversible dynamics[1] describing Gibbs's thermostatted systems and leading to a new and seminal view of microscopic irreversibility.

Nosé's dynamics makes it possible to generate *non*equilibrium ensembles, characterizing nonequilibrium steady states. Strain rate and heat flux can be specified, as well as composition, energy and volume. Generally, these nonequilibrium ensembles occupy fractal (fractional dimensional) portions of Gibbs's equilibrium phase space. The nonequilibrium phase volume is completely negligible relative to the phase volume of the corresponding Gibbs's equilibrium ensemble—that with the same number of particles, same energy and same volume, but without the nonequilibrium fluxes.[2]

The negligible phase volume of the nonequilibrium states results from the multiplicity of constraints implicit in a "steady state." In a system undergoing steady shear at the strain rate ε, for instance, not only $d\varepsilon/dt$ but also all the higher derivatives ($d^2\varepsilon/dt^2$, $d^3\varepsilon/dt^3$, . . .) must vanish. It is remarkable that Nosé's thermostatted equations of motion are strictly *time reversible*. And their time behavior on velocity reversal is exactly that described by Lebowitz for isolated systems: The time-reversed flow is less stable with time reversal than is the forward-in-time evolution. This difference in (Lyapunov) stability has recently been rigorously quantified for a restricted set of homogeneously thermostatted nonequilibrium systems.[3] Our own very recent numerical investigations suggest strongly that this asymmetry between the two time directions in steady-state nonequilibrium ensembles can only increase as the homogeneity restriction is relaxed.[4]

References

1. S. Nosé, Prog. Theor. Phys. **103**, 1 (1991).

continued on page 115

continued from page 15

2. B. L. Holian, W. G. Hoover, H. A. Posch, Phys. Rev. Lett. **59**, 10 (1987).
3. S. Sarman, D. J. Evans, G. P. Morriss, Phys. Rev. A **45**, 2233 (1992).
4. W. G. Hoover, H. A. Posch, Phys. Rev. E **49**, 1913 (1994).

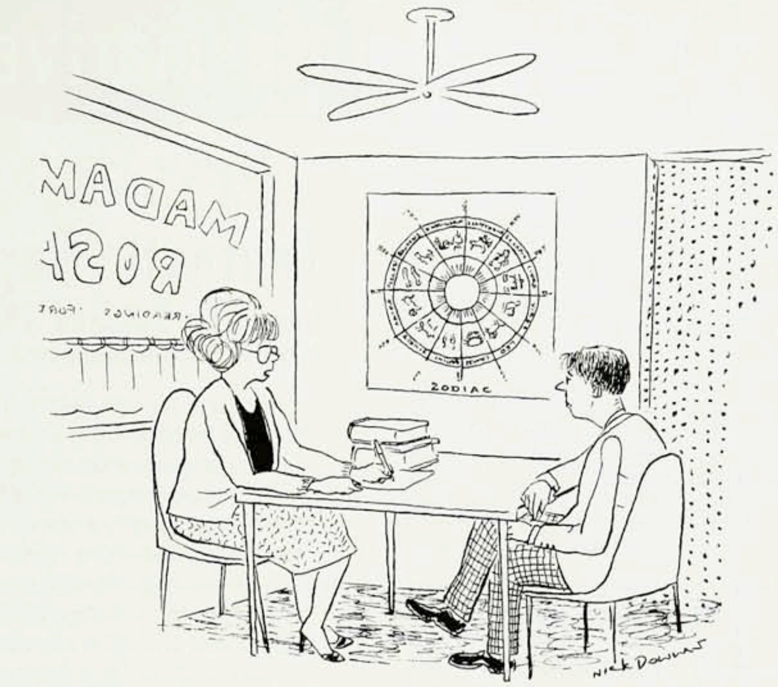
WILLIAM G. HOOVER
University of California, Davis
HARALD POSCH
University of Vienna
Vienna, Austria
BRAD LEE HOLIAN
Los Alamos National Laboratory
Los Alamos, New Mexico

In his interesting article "Boltzmann's Entropy and Time's Arrow" Joel Lebowitz claims, following Boltzmann, that macroscopic irreversibility is explained by the large number of degrees of freedom involved. This view is incomplete. A set of time-symmetric equations evidently cannot lead uniquely to a time-asymmetric solution. There must be another cause.

This cause rests in the fact that we are always concerned with initial, not with terminal, conditions. The mechanical problems we are solving are of the form that at some initial time, say $t = 0$, some macroscopic parameters are given and other variables are random. We then follow the development for $t > 0$. Following the solution for negative times, the entropy would also be larger than at $t = 0$; in other words it decreases with time.

The extension to negative times is, however, not of practical interest, because it does not describe a possible situation. In the laboratory this is due to the fact that we can remember the past and make plans for the future, but not vice versa. As regards the world around us, it is no doubt due to the fact that it all started from the Big Bang. Here lies the real reason for the asymmetry.

This is reflected in Boltzmann's *Stosszahlansatz*. This *Ansatz* is based on the seemingly innocuous assumption that the number density of molecules moving in a certain direction in a volume element from which they will in a given time collide with a scattering center is the same as in any other volume element, because "they do not know they are going to collide." However, the molecules that have just collided (which, in the time-reversed situation, would be the ones about to collide) have a different distribution, because they have been scattered. Thus the "arrow of time" is included in Boltzmann's treatment, and it is not surprising that it is reflected in the solution.



"You have little understanding of probability, causation and coincidence."

Lebowitz's discussion demonstrates that our preference for following evolution forward in time is so strongly ingrained that we do not always realize that this is a choice not forced upon us by the equations of mechanics.

I have discussed these arguments in detail.[1] Similar arguments were given by Feynman.[2] The intention is not to detract from Boltzmann's merit for having clarified so much of the problem but to point out that an extra step is needed for a complete account of the situation.

References

1. R. Peierls, *Surprises in Theoretical Physics*, Princeton U. P., Princeton, N. J. (1979), sec. 3.8.
2. R. P. Feynman, *The Character of Physical Law*, BBC Publications, London (1965).

RUDOLF PEIERLS
Oxford, England

LEBOWITZ REPLIES: Let me deal first with Rudolf Peierls's letter. (I was not aware of his very nice article when I wrote mine.) I agree entirely with him about the importance of initial conditions and I believe that this is stated clearly in my article; see the section "Initial conditions." I also believe that he will agree that Boltzmann said it very elegantly in one of his responses:[1]

> From the fact that the differential equations of mechanics are left unchanged by reversing the sign of time without anything else, Herr [Wilhelm] Ostwald concludes that the mechanical view of the world cannot explain why natural processes always run preferentially in a definite direction. But such a view appears to me to overlook that mechanical events are determined not only by differential equations, but also by initial conditions. In direct contrast to Herr Ostwald I have called it one of the most brilliant confirmations of the mechanical view of Nature that it provides an extraordinarily good picture of the dissipation of energy, as long as one assumes that the world began in an initial state satisfying certain conditions. I have called this state an improbable state.

The other three letters (a subset of those received) unfortunately illustrate how much confusion still exists about the problem of macroscopic irreversibility. Each of these letters offers a different solution. According to Howard Barnum and his colleagues the solution lies in information theory; Dean J. Driebe believes that we must reformulate the laws of nature using the mathematics of subdynamics; and according to William G. Hoover and coworkers it is Nosé dynamics that saves the day.

In my opinion information theory, subdynamics and Nosé dynamics all contain interesting and useful ideas and can be illuminating when properly applied. I believe, however, that they are neither needed for nor really relevant to the problem of the asymmetry of observed macroscopic behavior. Boltzmann's ideas adequately explain these observations without requiring reliance on ignorance or modification of the laws of nature. Of course such modifications may come about for other reasons—relativity and quantum mechanics are such modifications that came after Boltzmann's work—but this is not the issue discussed in the article or in the letters.

What Driebe and Barnum and coworkers (and some other writers) have in common is their refusal to accept what to me seems an obvious fact: that irreversible behavior is observed in the evolution of a single macroscopic system that can be adequately described as isolated during the relevant period, be it a jar of fluid or the solar system. Thus when we pour some blue ink into a glass of red ink (of the same density) and seal up the glass tightly (making it an "isolated" system) we *always* see it becoming a uniform color. We don't need to repeat the experiment many times to get an ensemble or a probability distribution, nor do we need to refer to ignorance about the exact microscopic state of the system—any more than we would have needed such considerations to predict the fate of Comet Shoemaker–Levy after it hit Jupiter. Both events are described by deterministic, time-asymmetric macroscopic laws.

In deriving such time-asymmetric laws one of course has to use probability theory to characterize the typicality of the initial microstate of the system with respect to the initial macrostate discussed earlier. One shows (or proves) then that the results for macroscopic observations are so highly peaked that for large macro-to-micro ratios they amount to certainties. In this way probabilities or ensembles are convenient tools for describing "typically" observed phenomena. This is discussed in my article and in the references there; see in particular the section "Notions of probability."

This excessive obsession with probabilities is the source of Driebe's contention that irreversibility is observed in a system whose microscopic state is specified by a point X in the unit square evolving under the baker's dynamics—a paradigm of the confusion surrounding the subject. The macroscopic state of such a system (specified, say, by which half of the square the point X is in) will keep on changing back and forth with time as its microscopic state X jumps all over the square. No observations on such a system will produce anything that looks time asymmetric, just because the system does not have many degrees of freedom. As put by Maxwell, "The second law 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."[2]

Turning now to Nosé dynamics and its various generalizations, these are useful for computer simulations and exhibit interesting analytic behavior. But as I have said in other places[3] there is no reason to believe that they have anything to do with the actual laws governing the dynamics of the microscopic constituents of our actual world. So while it is interesting to speculate on what the world would look like with such dynamics, I believe it is confusing to bring them into the discussion of the conceptual problem of macroscopic irreversibility.

References

1. Quoted in E. Broda, *Ludwig Boltzmann, Man–Physicist–Philosopher*, Ox Box Press, Woodbridge, Conn. (1983), p. 74.
2. G. Eyink, J. Lebowitz, in *Microscopic Simulations of Complex Hydrodynamic Phenomena*, Proc. NATO Adv. Study Inst., M. Mareschal, B. L. Holian, eds., Plenum, New York (1992), p. 323.
3. J. C. Maxwell, Nature **17**, 257 (1878).

JOEL L. LEBOWITZ
Rutgers University
New Brunswick, New Jersey

Working Retirements Can Open Up Jobs

We need to create more openings in physics research and physics teaching, both for the benefit of those young people who have the vocation and for the health of our physics enterprise and institutions. Older physicists who regret the dearth of employment opportunities for young scientists at universities and national laboratories can help by voluntarily retiring around the traditional age of 65 and continuing to work unpaid if that is what they want to do. Many physicists have done that, and I speculate that many more would follow them if their institutions made the working conditions attractive. It can be done, and financial incentives are not necessarily the decisive issue.

In the physics division at Argonne National Laboratory, six of us have retired but continue to work unpaid, making it possible for a similar number of young people to join the division. (For comparison, we have about 40 regular scientific staff.)

The following perceptions and opinions are my personal ones. I describe the Argonne physics division experience because I know it. Ours is by no means the only institution where working retirement is practiced, although we may have a stronger tradition than others.

There is no financial incentive to retire at Argonne. Voluntary retirement works well in the physics division because the retirees are treated the same as others. The consumption of facilities and other resources by retirees has to be justified by productivity, just as it does for other staff, although the standards can be relaxed significantly because the cost is so much less. No Argonne policy is involved. We serve at the pleasure of the division director. However, no division director is likely to discourage a practice that benefits the laboratory and the profession.

In fact it also benefits the retirees by permitting us to work less hard or less steadily if we so choose, although that benefit is severely limited. A person cannot justify occupying facilities or even space idly. Besides, people who are active in research can't really reduce their momentum very much without losing it.

Financial fears appear not to be a major deterrent for most people. The TIAA–CREF retirement system, which we share with many universities and laboratories, works well. The retirees I have asked at Argonne and at a few universities all say the money is adequate. Of course there are individuals whose financial needs or responsibilities are much greater than those of the majority, and such a person cannot reasonably be expected to retire voluntarily. There are institutions where unusually low salaries systematically put people in that category. There are also persons whose work situations are incompatible with retirement, especially leaders of projects whose funding will collapse if they retire. I believe the great majority do not fall into any of those categories.

From conversations with colleagues at universities, I have the impression that voluntary retirement around age 65 is relatively uncommon in most places and that the primary deterrent is most often anticipated lack of respect, not financial concerns or insensitivity to the ethical advantages. Amenities ranging from office space to secretarial service may be withheld from or offered grudgingly to a retiree, or the individual may simply be made to feel unwelcome. A retiree may receive less departmental support for research and professional costs than a paid colleague doing equally valued work.