THE ERGODIC-HYPOTHESIS

A Complicated Problem in Mathematics and Physics

by Adrian Patrascioiu

There are a few problems in physics that stir deep emotions every time they are discussed. Since physicists are not generally speaking an emotional group of people, the existence of these sensitive issues must be considered a strong indication that something is amiss. One such issue is the interpretation of quantum mechanics. I will take a moment to discuss that problem because it bears directly on the main topic of this article.

In quantum mechanics, if the question asked is a technical one, say how to compute the energy spectrum of a given atom or molecule, there is universal agreement among physicists even though the problem may be analytically intractable. If on the other hand the question asked pertains to the theory of measurement in quantum mechanics, that is, the interpretation of certain experimental observations performed on a microscopic system, it is virtually impossible to find two physicists who agree. What is even more interesting is that usually these controversies are void of any physical predictions and are entirely of an epistemological character. They reflect our difficulty in bridging the gap between the quantum mechanical treatment of the microscopic system being observed and the classical treatment of the macroscopic apparatus with which the measurement is performed. It is usually argued that we, physicists, have difficulty comprehending the formalism of quantum mechanics because our intuition is macroscopic, hence classical, in nature. Now if that were the case, we should have as much difficulty with special relativity, since we are hardly used to speeds comparable to that of light. Yet, strange as it seems at first, I have never heard physicists argue about the "twin paradox," the classic example of an unexpected prediction of Einstein's relativity. So there must be something about quantum mechanics that "rubs us" the wrong way. The question is what?

Perhaps the best way in which the strange predictions of quantum mechanics can be quantified is a certain inequality first formulated by Bell (Bell 1965). For illustration, consider a positronium atom, with total angular momentum zero, that decays into an electron and a positron. Suppose we let the electron and the positron drift apart and then measure their spin components along two axes by passing them through two magnetic fields. Now in quantum mechanics the state of the positronium atom is a linear superposition of spin-up and spin-down states: $(|\uparrow\rangle_+|\downarrow\rangle_- - |\downarrow\rangle_+|\uparrow\rangle_-)/\sqrt{2}$. We could therefore ask ourselves whether in each passage through the apparatus the electron and the positron have a well-defined spin (up or down), albeit unknown to us. Some elementary probabilistic reasoning shows immediately that if that were the case, the probabilities for observing **up** or down spins along given axes would have to obey Bell's inequality. The experimentally measured probabilities violate this inequality, in agreement with the predictions of quantum mechanics. So the uncertainties in quantum mechanics are not due to incomplete knowledge of some local hidden variables. What is even stranger is that in a refinement of the experiment in which the axes of the magnetic fields are changed in an apparently random fashion (Aspect, Grangier, and Roger 1982), the violation of Bell's inequality persists, indicating correlations between space-like events (that is, events that could be causally connected only by signals traveling faster than the speed of light). While in this experiment no information is being transmitted by such superluminal signals, and hence no conflict with special relativity exists, the implication of space-like correlations hardly alleviates the physicist's uneasiness about the correct interpretation of quantum mechanics. Of course this uneasiness is not felt by all physicists. Particle physicists, for instance, take the validity of quantum mechanics for granted. To wit, anybody who reads *Time* knows that they, having "successfully" unified weak, electromagnetic, and strong interactions within the framework of quantum field theory, are presently subduing the last obstacle, quantizing gravity by unifying all interactions into a quantum field theory of strings. And they are doing so in spite of the fact that the existence of classical gravitational radiation, let alone that of the quantized version (gravitons), has not been established experimentally.

An even older controversy, which in the opinion of some physicists has long ceased to be an interesting problem, concerns the ergodic hypothesis, the subject of this discussion. I will try to elaborate on this topic as fully as my knowledge will allow, but, by way of introduction, let me just say that the ergodic hypothesis is an attempt to provide a dynamical basis for statistical mechanics. It states that the time-average value of an observable—which of course is determined by the dynamics—is equivalent to an ensemble average, that is, an average at one time over a large number of systems all of which have identical thermodynamic properties but are not identical on the molecular level. This hypothesis was advanced over one hundred years ago by Boltzmann and Maxwell while they laid the foundations of statistical mechanics (Boltzmann 1868, 1872 and Maxwell 1860, 1867). The general consensus is that the hypothesis, still mathematically unproven, is probably true yet irrelevant for physics. The purpose of this article is to review briefly the status of the ergodic hypothesis from mathematical and physical points of view and to argue that the hypothesis is of interest not only for statistical mechanics but for physics as a whole. Indeed the mystery of quantum mechanics itself may possibly be unraveled by a deeper understanding of the ergodic hypothesis. This last remark should come as no surprise. After all, the birth of quantum mechanics was brought about by the well-known difficulties of classical statistical mechanics in explaining the specific heats of diatomic gases and the blackbody radiation law. I shall elaborate on the possible connection between the ergodic hypothesis and the resolution of these major puzzles in the last part of this article.

The Mathematics of the Ergodic Hypothesis

I shall begin my presentation with the easier part of the problem, the mathematical formulation of the ergodic hypothesis. Consider some physical system with N degrees of freedom and let $q_1, \ldots, q_N$ be its positions and $p_1, \ldots, p_N$ its momenta. We shall assume that the specification of the set of initial positions $\{q_0\}$ and momenta $\{p_0\}$ at time $t = O$ uniquely specifies the state of the system at any other time t via the equations of motion:

$$\frac{\partial q_i(t)}{\partial t} \quad \frac{\partial q_i(\{q(t)\},\{p(t)\})}{\partial t}$$

and

$$\frac{\partial p_i(t)}{\partial t} = \frac{\partial p_i(\{q(t)\},\{p(t)\})}{\partial t}. \tag{1}$$

The time evolution of the system can be represented as a path, or trajectory, through phase space, the region of allowed states in the space defined by the $2N$ independent coordinates $\{q\}$ and $\{p\}$. An observable of this system O is an arbitrary function of $\{q\}$ and $\{p\}$, $O(\{q\},\{p\})$. The time-average value of some observable $O(\{q\},\{p\})$ along the phase-space trajectory starting at $t = 0$ at $\{q_0\},\{p_0\}$ is defined as

$$\overline{O}_T(\{q_0\},\{p_0\}) \equiv \frac{1}{T}\int_0^T dt\, O(\{q(t)\},\{p(t)\}). \tag{2}$$

Obviously the integral in Eq. 2 makes sense only for suitable functions of $\{q\}$ and $\{p\}$, which are the only ones we shall consider. In fact we shall further restrict the class of observables to those for which $\lim_{T\to\infty}\overline{O}_T$ exists. (This is not a severe restriction; for instance, if $O(\{q(t)\},\{p(t)\})$ is bounded along the trajectory, the limit clearly exists.) The notation in Eq. 2 makes clear that, a priori, time-average values depend upon the initial conditions $\{q_0\}$ and $\{p_0\}$.

As time passes, the trajectory of the system winds through the phase space. If the motion takes place in a bounded domain, one might expect that as $T \to \infty$ the average values of most observable settle down to some sort of equilibrium values (time-independent behavior). What would the phase-space trajectory look like if the system approached dynamical equilibrium? One could characterize it by saying that the frequency with which different neighborhoods of the phase space are visited converges to some limiting value $\mu(\{q\},\{p\})$ at each point in phase space. That such limiting frequencies exist under quite general circumstances was shown in 1927 by Birkhoff (see Birkhoff 1966) and constitutes the first step towards bridging the gap between dynamics and statistics. Indeed, Birkhoff's theorem allows one to replace time averages by ensemble averages, defined as follows. Let the state of the system be specified by the sets $\{q\}$ and $\{p\}$, and postulate that the probability for the system to be in the neighborhood of the state $(\{q\}, \{p\})$ is

$$\left(\prod_{i=1}^{N} dq_i\, dp_i\right) \mu(\{q\},\{p\}). \tag{3}$$

That is, the general form of the probability measure is the time-independent frequency μ times the volume element of the phase space. A particular probability measure specifies completely a particular ensemble of representative systems; that is, it gives the fraction of systems in the ensemble that are in the state $(\{q\}, \{p\})$. In keeping with usual probabilistic notions, I shall assume that the probability measure has been normalized so that the integral of the probability measure for all possible states $(\{q\}, \{p\})$ is unity,

$$\int \left(\prod_{i=1}^{N} dp_i\, dq_i\right) \mu(\{q\},\{p\}) = 1 \tag{4}$$

The ensemble average of the observable $O(\{q\},\{p\})$ is defined as

$$\langle O\rangle_\mu \equiv \left(\prod_{i=1}^{N} \int dq_i\, dp_i\right) \mu(\{q\},\{p\})\, O(\{q\},\{p\}). \tag{5}$$

Birkhoff's theorem states that, if the motion is restricted to a bounded domain, then for many initial conditions there exists an ensemble (probability measure) such that the time-average value of the observable equals an ensemble average:

$$\lim_{T\to\infty} \overline{O}_T(\{q_0\},\{p_0\}) = \langle O\rangle_\mu. \tag{6}$$

Please note that Eq. 6 indicates that the time-average value of $O(\{q\}, \{p\})$ becomes independent of the initial conditions $\{q_0\}$ and $\{p_0\}$ as $T \to \infty$. As already mentioned above, this is true for many, but generally not all, initial conditions. If Eq. 6 is true for almost all initial conditions (for all points in the allowed phase space except for a set of measure zero), the flow through phase space described by Eqs. 1 must be fully ergodic; that is, for almost all initial conditions $\{q_0\},\{p_0\}$ and with probability 1, the flow passes arbitrarily close to any point $\{q\}, \{p\}$ in phase space at some later time. The assumption in statistical mechanics that time averages of macroscopic variables can be replaced by ensemble averages (that is, that Eq. 6 holds) is therefore called the ergodic hypothesis.

In general, however, the flow through the phase space defined by the equations of motion may not cover the whole of the allowed phase space for almost all initial conditions. Instead the allowed phase space is divided into several "ergodic" components, that is, subregions Ω_i of the phase space such that if the flow starts in subregion Ω_i, then there exists a time t at which the flow will touch any given neighborhood in the set of neighborhoods covering Ω_i. Moreover the flow remains in Ω_i for all time. Consequently, time-average values do depend on knowing in which "ergodic component" the system was started.

The Ergodic Hypothesis and the Equipartition of Energy. In statistical mechanics the ergodic hypothesis, which proposes a connection between dynamics and statistics, is sometimes regarded as unnecessary, and attention is placed instead on the assumption that all allowed states are equally probable. In this paper I emphasize that when time averaging is relevant to a problem, the assumption of equal a priori probabilities is essentially equivalent to the ergodic hypothesis (Eq. 6). To see this I will restate the general problem and gradually narrow it down to the context of classical statistical mechanics.

In general, given a phase space Ω and a probability density $\mu(\{q\},\{p\})$, one has defined an ensemble. Furthermore one can consider a map of the phase space onto itself. (An example is provided by Eqs. 1, which are really a set of maps indexed by the continuous parameter *t).* A natural question to ask is whether the probability measure

$$\left(\prod_{i=1}^{N} dq_i\, dp_i\right)\mu(\{q\},\{p\})$$

is invariant under this map. As we have said, Birkhoff's theorem states that under many circumstances such invariant measures exist and allow the replacement of time averages by ensemble averages. Thus the existence and construction of all the invariant measures for a certain flow is the first of two mathematical problems related to the ergodic hypothesis.

As stated so far this problem is much more general than the one of interest to Boltzmann and Maxwell in connection with the foundations of statistical mechanics. Indeed, the existence of a probability measure left invariant by a given set of maps can be investigated whether or not the sets {q} and {p} defining the maps are canonically conjugate variables derivable from a Hamiltonian, whether the set of maps is discrete or continuous, etc. At present the construction of such invariant measures is being actively pursued by researchers studying dynamical systems, especially dissipative ones such as those relevant to the investigation of turbulence (for example, systems described by the Navier-Stokes equations). (See the section Geometry, Invariant Measures, and Dynamical Systems in "Probability and Nonlinear Systems.")

Of particular interest in statistical mechanics, especially in connection with the ergodic hypothesis, is the invariant measure appropriate for describing physically isolated systems. The ensemble specified by this measure is traditionally called the microcanonical ensemble. The systems of interest are characterized by nonlinear interactions among the constituents and by a very large number of degrees of freedom. Generically, certain observable of a physically isolated system, such as the total energy and electric charge, are conserved; that is, they remain constant at their initial values. So let $\{I_i(\{q\},\{p\})\}$, $i = 1, \ldots, M$ be the complete set of independent, conserved observable of a system with N degrees of freedom. Obviously $M \leq 2N$. Since the flow in Eqs. 1 obeys all these conservation laws, it is clear that any invariant measure of the flow must be compatible with all the conservation laws. Consequently the probability measure must contain a delta function for each conserved quantity so that the probability is nonzero only when the conservation law is satisfied. (A delta function $\delta(x - x_0)$ can be thought of as having the value $\frac{1}{2\epsilon}$ for x values between $x_0 - \epsilon$ and $x_0 + \epsilon$ for any ϵ, no matter how small, and the value O everywhere else. The integral of a delta function is thus equal to unity.)

The fundamental hypothesis in statistical mechanics is that for isolated systems of physical interest (complicated nonlinear systems with many degrees of freedom), the measure

$$\left(\prod_{i=1}^{N} dq_i\, dp_i\right) \prod_{j=1}^{M} \delta\left(I_j(\{q\},\{p\}) - I_j(\{q_0\},\{p_0\})\right) \tag{7}$$

is left invariant by the equations of motion and is the only such measure. In other words, the hypothesis states that the microcanonical ensemble is defined by the measure in Eq. 7. Note that the probability density in Eq. 7 is flat; that is, all regions of phase space consistent with the conservation laws are equally probable.

To understand why this assumption of equal a priori probabilities is, in effect, a restatement of the ergodic hypothesis, one must realize that the only systems under consideration in classical statistical mechanics are Hamiltonian systems (systems for which the equations of motion can be derived from a Hamiltonian principle). The existence of a Hamiltonian function $H(\{q\}, \{p\})$ means that the equations describing the flow through phase space, Eqs. 1, can be written in the form

$$\dot{q}_i = [q_i, H]$$

and

$$\dot{p}_i = [p_i, H] \tag{8}$$

Here $[f, g]$ denotes the Poisson bracket:

$$[f, g] = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} \right). \tag{9}$$

The existence of a simplectic structure (the Poisson bracket) is a very restrictive condition on the flow, much more so than the mere conservation of the energy. Indeed, through Liouville's theorem, it guarantees the conservation of the phase-space volume element

$$\left(\prod_{i=1}^{N} dq_i\, dp_i\right), \tag{10}$$

and thus it proves that the measure in Eq. 7 is invariant under Hamiltonian flows. Thus the first mathematical problem of constructing an invariant measure is solved for Hamiltonian systems. Consequently the ergodic hypothesis (Eq. 6) is automatically satisfied *provided that the flow is fully ergodic.* Proving that the flow is fully ergodic is the second mathematical problem related to the ergodic hypothesis and is the one that remains to be solved for Hamiltonian systems. If in fact the flow is not ergodic, then the assumption of equal a priori probabilities would not describe the time-average behavior of the system, at least not for all possible observable.

Note that if the flow is fully ergodic and all allowed states are equally probable, then we have an equipartition of energy; that is, the energy of the system is divided equally among the N degrees of freedom. Indeed, let us consider for simplicity the case of a Hamiltonian system in which only the total energy is conserved. The microcanonical measure then is simply

$$\left(\prod_{i=1}^{N} dq_i\, dp_i\right) \delta\big(H(\{q\},\{p\}) - E\big). \tag{11}$$

Quite often the Hamiltonian has the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(\{q\}), \tag{12}$$

where the m_i's are the particle masses. Because of the symmetry of the measure defined by Eqs. 11 and 12 under the interchange of the p_i's, one can easily show that the average kinetic energy $\langle p_i^2/2m_i\rangle$ is independent of i. Usually one uses that fact to define a temperature T via $\langle p^2/2m\rangle = kT/2$ (where k is the Boltzmann constant). Such considerations can be extended to the normal modes of a lattice, which will be discussed later, and are generically referred to as the equipartition of energy.

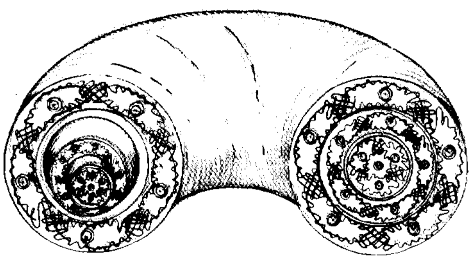
Mathematical Results. Having formulated the mathematical problem, it may be of interest to state briefly what rigorous results have been obtained so far about the circumstances under which a flow is fully ergodic.

i) Oxtoby and Ulam proved in 1941 that in a bounded phase space the continuous ergodic transformations are everywhere dense in the space of all continuous measure-preserving transformations. In other words, a topology can be chosen such that ergodic transformations form the "bulk" of the whole space of continuous measure-preserving maps. This theorem says nothing about the measure of the ergodic transformations, which may even be vanishing. (See page 110 in "Learning from Ulam.") A corresponding theorem stating an analogous property of a real dynamical system with a finite number of degrees of freedom does not exist, and in fact the KAM theorem proves the contrary (see below). It is also known that Hamiltonian flows are quite rare among measure-preserving maps, and therefore the Oxtoby and Ulam result guarantees nothing about the density of ergodic Hamiltonian flows in the space of all Hamiltonian flows.

ii) For finite N the Kolmogorov-Arnold-Moser (KAM) theorem (see Arnold and Avez 1968) guarantees that the ergodic hypothesis is violated for a certain class of systems. The theorem considers a completely integrable system (M = N in Eq. 7) and its response to an arbitrary, weak nonlinear perturbation. By a canonical transformation one can show that a completely integrable system with N degrees of freedom is equivalent to N decoupled harmonic oscillators; hence it is a linear system, and its motion in phase space occurs on hypertori rather than on the whole phase space. The KAM theorem states that in the phase space of a weakly nonintegrable (weakly nonlinear) Hamiltonian, some motions still are restricted to tori, and these tori occupy a nonzero measure of the phase space. (Figure 1 shows a typical structure of the

PHASE SPACE OF A WEAKLY NONINTEGRABLE HAMILTONIAN SYSTEM

Fig. 1. The system has four degrees of freedom, but conservation of energy allows us to display the phase space in three dimensions, which represent the variables x, y, and $\frac{\partial y}{\partial t}$. The phase space contains nested invariant tori on which motion is quasiperiodic so that a single orbit covers a torus densely. The gaps between the tori are chaotic regions in which the orbits appear as random as the toss of a coin. Since the nested tori have a finite measure in the phase space, this Hamiltonian system violates the ergodic hypothesis.



phase space for a weakly nonintegrable Hamiltonian.) Thus these systems have several ergodic components.

iii) In 1963 Sinai proved the ergodic hypothesis for certain billiard systems (Hamiltonian systems in which hard spheres bounce elastically off each other and the container walls). The geometry of the boundary turns out to be a crucial factor in proving that the flow is ergodic.

iv) It has not been possible to prove the ergodic hypothesis even for a gas of hard spheres, although it is generally believed to be true in this case.

v) For a long time the general belief was that the KAM theorem poses no problem for the ergodic hypothesis once the thermodynamic limit (the limit as $N \to \infty$ at fixed density) is taken. Counterexamples to this claim have recently been constructed (Bellissard and Vittot 1985), but it is premature to judge their generality.

vi) There exists no satisfactory formulation of the ergodic hypothesis for continuous media (field theory), since it is not known how to generalize the microcanonical measure to systems with an infinite number of degrees of freedom, especially when the total energy of the system is finite. It is interesting that while appropriate ensemble averages have not been defined, the existence of global solutions (in time), and therefore the existence of time averages, for several interesting field theories (such as classical electrodynamics and Yang-Mills theories) has been established (Eardley and Moncrief 1982).

In conclusion, from a mathematical point of view, the ergodic hypothesis has proved to be one of the most difficult problems in the last hundred years or so. Only two flows, both billiards, have been proven to be ergodic. Perhaps today's computers will speed up the rate of analytical progress by helping our intuition about the nature of the flow.

The Physics of the Ergodic Hypothesis

Next I wish to analyze the ergodic hypothesis from a physical point of view. Undoubtedly, a dynamical approach to a physical system with many degrees of freedom, such as a gas, is impossible, and a statistical one must be developed. In doing so one must endeavor to capture the right physics. If the attempt has been really successful, the theory will withstand experimental scrutiny. But what should be done if the predictions go astray, as did the predictions of classical statistical mechanics for blackbody radiation? A sensible approach is to go back and examine what fundamental assumptions were made, which is what I shall do now.

The first question that must be settled is what should be considered "the system." Indeed the instruction in statistical mechanics is to integrate over all canonical positions and momenta with a certain measure. However, one must decide which degrees of freedom to include. For instance, take the case of the diatomic gas. Each molecule has two atoms, each atom has its own electrons and nucleus, and the latter in turn is made of quarks and gluons, say. Moreover, since the constituents are charged, they are coupled to the electromagnetic field inside the container (and also to the gravitational field). Probably most readers will think that this is not a serious question: at a certain temperature only certain degrees of freedom are excited, and these are the only ones to be integrated over. Hidden within this superficially sensible-sounding answer is one of two extremely important assumptions:

i) The ergodic hypothesis is strictly false, so that certain degrees of freedom, although dynamically coupled, never get excited and act as spectators to the thermal equilibrium that sets in for the remaining degrees of freedom.

ii) Or, the system dynamically develops largely different time scales, and the number of degrees of freedom that are more or less in equilibrium keeps increasing with time.

In either case the use of statistical mechanics becomes more subtle, since only by gaining a good grasp of the underlying dynamics can one decide what degrees of freedom are relevant in certain circumstances. In particular, there is no a priori reason to believe that the contributions to the specific heat of the vibrations and the rotations of a diatomic gas ought to be equal at all temperatures and during a typical time of observation, as was assumed in the classical predictions of statistical mechanics. Neither is there any reason to predict the Rayleigh-Jeans distribution (Fig. 2) for black-body radiation (which assumes the equipartition of energy between all modes of the electromagnetic field), since some modes of the cavity may be effectively decoupled (case i above) or so weakly coupled that they haven't had time to thermalize (case ii). Thus the standard examples for the breakdown of classical statistical mechanics may reflect an inappropriate application of the ergodic hypothesis rather than a need for quantization, as is usually argued in physics textbooks.

The second important question that must be addressed in deciding the relevance of the ergodic hypothesis for physics is why we are using a statistical description in a given physical situation. Consider, for instance, the measurement of the specific heat of a diatomic gas. Typically one lets the gas "reach equilibrium" with a reservoir at a given temperature and then makes a certain macroscopic measurement during a certain time interval. To obtain reasonable statistics, the measurement is repeated several times. Clearly the process just described involves three types of averaging at the molecular dynamics level:

i) over initial conditions (each repetition of the measurement involves a different set of initial conditions);

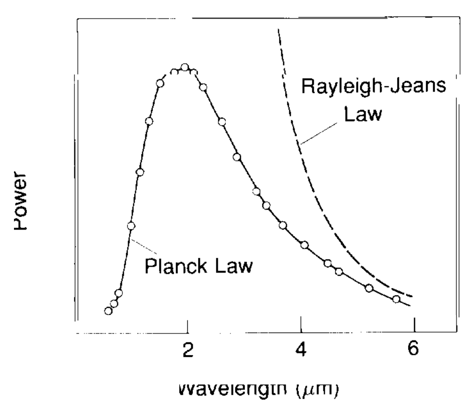
ii) over time (each measurement extends over a certain time, during which the gas evolves as a dynamical system); and

iii) over microscopic degrees of freedom (this type of averaging is inherent in the measurement of macroscopic variables).

Before analyzing in detail the likely statistical relevance of each of these averaging operations, let me hasten to say that clearly only the averaging over time has anything to do with the ergodic hypothesis. Those physicists who believe that the ergodic hypothesis is not important for the foundations of statistical mechanics dismiss the

BLACKBODY RADIATION AT 1600 K

Fig. 2. Theoretical predictions and experimental data for the power radiated by a blackbody at 1600 K. The classical Rayleigh-Jeans law, $u(\nu, T) = (8\pi/c^{-})\nu^{-}kT$, is based on equipartition of energy among all the modes of an electromagnetic field. The total (kinetic plus potential) energy in each mode is kT, and the number of modes in the frequency interval $(\nu, \nu+d\nu)$ is $8\pi\nu^{-}/c^{-}$, which is proportional to A^{-2}. The quantum Planck law, in agreement with experiment, yields a peaked distribution that decreases rapidly with wavelength. The Planck law is based on the assumption that the energy in each mode is quantized; that is E = *nhν*, where *n* is an integer and *h* is Planck's constant.



The FPU Problem

Excerpts from "Studies of Nonlinear Problems" by Fermi, Pasta, and Ulam

This report is intended to be the first one of a series dealing with the behavior of certain nonlinear physical systems where the nonlinearity is introduced as a perturbation to a primarily linear problem. The behavior of the systems is to be studied for times which are long compared to the characteristic periods of the corresponding linear problems.

The problems in question do not seem to admit of analytic solutions in closed form, and heuristic work was performed numerically on a fast electronic computing machine (MANIAC I at Los Alamos). * The ergodic behavior of such systems was studied with the primary aim of establishing, experimentally, the rate of approach to the equipartition of energy among the various degrees of freedom of the system. Several problems will be considered in order of increasing complexity. This paper is devoted to the first one only.

We imagine a one-dimensional continuum with the ends kept fixed and with forces acting on the elements of this string. In addition to the usual linear term expressing the dependence of the force on the displacement of the element, this force contains higher order terms. For the purposes of numerical work this continuum is replaced by a finite number of points (at most 64 in our actual computation) so that the partial differential equation defining the motion of this string is replaced by a finite number of total differential equations. . . .

The solution to the corresponding linear problem is a periodic vibration of the string. If the initial position of the string is, say, a single sine wave, the string will oscillate in this mode indefinitely. Starting with the string in a simple configuration, for example in the first mode (or in other problems, starting with a combination of a few low modes), the purpose of our computations was to see how, due to nonlinear forces perturbing the periodic linear solution, the string would assume more and more complicated shapes, and, for t tending to infinity, would get into states where all the Fourier modes acquire increasing importance. In order to see this, the shape of the string, that is to say . . . [its displacement,] and the kinetic energy . . . were analyzed periodically in Fourier series. . . .

Let us say here that the results of our computations show features which were, from the beginning, surprising to us. Instead of a gradual, continuous flow of energy from the first mode to the higher modes, all of the problems show an entirely different behavior. Starting in one problem with a quadratic force and a pure sine wave as the initial position of the sting, we indeed observe initially [see figures on next page] a gradual increase of energy in the higher modes as predicted (e.g., by Rayleigh in an infinitesimal analysis). Mode 2 starts increasing first, followed by mode 3, and so on. Later on, however, this gradual sharing of energy among successive modes ceases. Instead, it is one or the other mode that predominates. For example, mode 2 decides, as it were, to increase rather rapidly at the cost of all other modes and becomes predominant. At one time, it has more energy than all the others put together! Then mode 3 undertakes this role. It is only the first few modes which exchange energy among themselves and they do this in a rather regular fashion. Finally, at a later time mode 1 comes back to within one per cent of its initial value so that the system seems to be almost periodic. All our problems have at least this one feature in common. Instead of gradual increase of all the higher modes, the energy is exchanged, essentially, among only a certain few. It is, therefore, very hard to observe the rate of "thermalization" or mixing in our problem, and this was the initial purpose of the calculation.

If one should look at the problem from the point of view of statistical mechanics, the situation could be described as follows: the phase space of a point representing our entire system has a great number of dimensions. Only a very small part of its volume is represented by the regions where only one or a few out of all possible Fourier modes have divided among themselves almost all the available energy. If our system with nonlinear forces acting between the neighboring points should serve as a good example of a transformation of the phase space which is ergodic or metrically transitive, then the trajectory of almost every point should be everywhere dense in the whole phase space. With overwhelming probability this should also be true of the point which at time $t = 0$ represents our initial configuration, and this point should spend most of its time in regions corresponding to the equipartition of energy among various degrees of freedom. As will be seen from the results this seems hardly the case. . . .

In a linear problem the tendency of the system to approach a fixed "state" amounts, mathematically, to convergence of iterates of a transformation in accordance with an algebraic theorem due to Frobenius and Perron. . . . Such behavior is in a sense diametrically opposite to an ergodic motion and is due to a very special character, linearity of the transformations of the phase space. The results of our calculation on the nonlinear vibrating string suggest that in the case of transformations which are approximately linear, differing from linear ones by terms which are very simple in the algebraic sense (quadratic or cubic in our case), something analogous to the convergence to eigenstates may obtain. . . . ■

Editor's note: The interpretation of the unexpected recurrences is now different. See David Campbell's discussion on page 244.

*We thank Miss Mary Tsingou for efficient coding of the problems and for ruining the computations on the Los Alamos MANIAC machine.

statistical relevance of time averaging for macroscopic observable.

The averaging over initial conditions should not be of much consequence statistically. Indeed, even if one assumes that the gas is simply a collection of hard spheres (with no internal structure), the gas still constitutes a dynamical system with somewhere on the order of 10^{23} degrees of freedom. Unless the initial state is very special or the time of observation very short, repeating an experiment ten or a hundred times should not have important consequences. In fact, a typical measurement lasts at least a few minutes; during such a time interval each molecule undergoes, at room temperature and normal pressure, about 107 collisions. Hence the number of states through which the gas passes dynamically (in time) is much larger than that due to the repetition of the experiment. Of course, as one lowers the temperature or the pressure, the collisions become more rare, so the time of observation must be increased to avoid large fluctuations in individual measurements.

Perhaps the most important averaging is the "coarse graining" involved in obtaining macroscopic variables. Two large numbers are involved in a typical measurement: the total number of degrees of freedom of the system and the number of degrees of freedom that are averaged together to obtain a macroscopic variable. The second number appears naturally in a system containing a large number of indistinguishable constituents. For instance, in determining the local density in a gas, one does not care about the trajectory of any single particle but rather about the average number of trajectories crossing a macroscopic volume at any time. Use of the laws of large numbers (see "A Tutorial on Probability, Measure, and the Laws of Large Numbers") in this context guarantees that, in spite of the fact that the underlying dynamics may be time-reversal invariant, macroscopic variables (almost) always tend to relax to their equilibrium values. In other words, because of the large numbers involved in specifying macroscopic variables, the microscopically specified state of the system has overwhelming probability to evolve towards the equilibrium state, even if the microscopic dynamics is time-reversal invariant. Hence, an arrow of time exists at the macroscopic level even if it does not at the microscopic level. This frequently stated paradox of statistical mechanics is a straightforward consequence of the laws of large numbers.

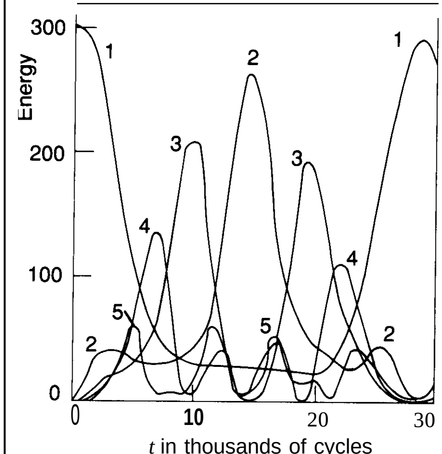
Confronting the Ergodic Hypothesis with Experiment

Having discussed the types of averaging involved in a real experiment, let us reconsider the experimental circumstances under which classical statistical mechanics could be expected to work. Historically, statistical mechanics appeared in connection with the endeavors to study, for example, very nearly ideal gases. (In an ideal gas the molecules are free except for occasional elastic collisions with each other or with the walls of the container.) Its foundations were statistical (predictions were based on considering an ensemble of systems, primarily the microcanonical or the canonical ensemble), in spite of the efforts of Boltzmann and Maxwell to give it a dynamical basis by invoking the ergodic hypothesis.

The fundamental assumption of statistical mechanics for an isolated system is the equal a priori probability on the hypersurface (in phase space) determined by all the conservation laws (Eq. 7). This probability measure defines the microcanonical ensemble. If the underlying dynamics is derivable from a Hamiltonian, by Liouville's

FIGURES FROM THE FERMI-PASTA-ULAM PAPER

Fig. 1. The quantity plotted is the energy (kinetic and potential in each of the first five modes). The units for energy are arbitrary. N [the number of parts into which the string is divided] = 32; α [the coefficient of the quadratic term in the force equation] = $\frac{1}{4}$; $\delta t^2 = \frac{1}{8}$ [δt is the length of the computational cycle]. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.



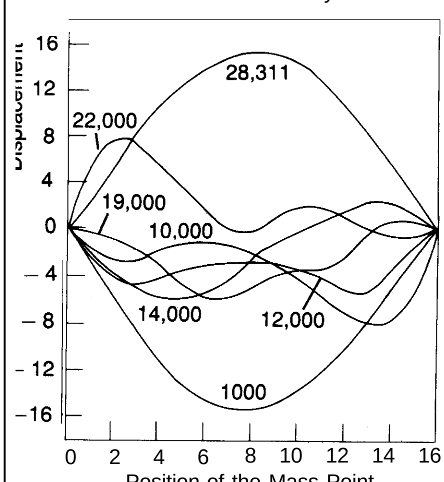


Fig. 8. This drawing shows not the energy but the actual shapes, i.e., the displacement of the string at various times (in cycles) indicated on each curve. The problem is that of Fig. 1.

theorem such a probability measure is invariant in time. Thus the only reason time averages could be different from ensemble averages would be a lack of ergodicity in the flow. In the case of a system consisting of only one species of indistinguishable particles, this potential difficulty is suppressed first by averaging over many initial conditions (so that even if the flow is not ergodic, the starting points may fall in different "ergodic" subregions) and second by measuring time-average values of macroscopic, not microscopic, variables. The chances that under these circumstances one would observe a difference between the predictions of statistical mechanics and experiment are very slim (recall the laws of large numbers), and indeed under these experimental conditions the predictions of classical statistical mechanics enjoyed great success. This explains the utter confidence of most physicists in the predictive power of statistical mechanics and their dismissal of the ergodic hypothesis as a technical, probably irrelevant detail.

On the other hand, suppose one uses the theory to make predictions about a diatomic gas, which even under the most simplifying assumptions has at least two species of indistinguishable degrees of freedom, say vibrations and translations. Without invoking the ergodic hypothesis, I can think of no a priori reason for the contributions to the specific heat of these two types of motions being found equal in typical measurements. In fact, even if the ergodic hypothesis is true, it is possible that the coupling of these two types of motions is so weak that during typical times of observation they do not reach equilibrium with each other. Yet it was the assumption that the two types of motion are in equilibrium that led to the discrepancy between classical statistical mechanics and experiment. Therefore I feel that it is unjustified to rely upon the many successes of statistical mechanics to dismiss questions regarding its foundations. On the contrary, an understanding of the ergodic hypothesis and especially of the times involved for exciting certain degrees of freedom should be equally challenging for the mathematician and the physicist.

Quantum Mechanics: A Case of Mistaken Identity? I would like to close this brief review of these complicated and long-standing problems with some speculations about a possible connection between the ergodic hypothesis and the necessity of using quantum mechanics at the microscopic level. First a few words about the blackbody radiation law. I have tried to emphasize the importance of measuring macroscopic averages, as well as that of particle indistinguishability, in obtaining agreement between the predictions of statistical mechanics and experiment. I think the case of the blackbody falls outside this realm. Consider a cubic lattice in D dimensions. At each site let there be a particle sitting in some enharmonic potential, attached through harmonic springs to its $2D$ nearest neighbors. If the boundary conditions are periodic, the system consists of identical yet distinguishable (by site coordinates) particles. We could form macroscopic quantities by averaging over the positions or velocities of all the particles in a cube of macroscopic size and expect reasonable agreement with the predictions of statistical mechanics. Alternatively we could describe the system in terms of its normal modes and attempt to verify the classical prediction, namely, the Rayleigh-Jeans energy distribution shown in Fig. 2 (that is, the equipartition of the energy among all the normal modes). Many such studies have been performed numerically, the first being the celebrated 1955 work of Fermi, Pasta, and Ulam (see "The Femi-Pasta-Ulam Problem"). It is always found that at sufficiently low energy density, the distribution of energy among the modes of the lattice differs drastically from the statistical prediction and in fact depends upon the initial conditions. Obviously either these systems are not ergodic, or at least the times of thermalizing the different modes are much longer than a typical time of numerical integration. And no macroscopic averaging is available to save the day! It is also known that leaving the energy density fixed and refining the lattice (taking the continuum limit) increases the discrepancy (Patrascioiu, Seiler, and Stamatescu 1985). Although such results have been accumulating for over thirty years now, they are not yet understood. Some say the systems are so close to being integrable that KAM tori or very slow diffusion rates occur in the phase space. Others claim that statistical mechanics should hold only in the thermodynamic limit (which is clearly not attainable numerically). Most physicists dismiss the whole story, since they "know" that statistical mechanics works in real life. I think this is a very narrow point of view: the problem being discussed is very much like that of the blackbody radiation law, and that was one of the failures of classical statistical mechanics. Is there a good theoretical (dynamical) basis for predicting the Rayleigh-Jeans distribution in classical physics, as the standard textbooks claim? Or are we pushing the statistical predictions in a domain for which there is no reason to expect them to hold? In "Does Equipartition of Energy Occur in Nonlinear Continuous Systems?" I describe some numerical experiments I have performed to test the validity of the statistical-mechanics predictions for a one-dimensional version of the blackbody problem and for the specific heats of systems with more than one species of degrees of freedom. Notably I found that, over the times of observation available in computer experiments, the systems failed to fulfill the ordinary expectations of an equipartition of energy. The same discrepancy has been found in many other numerical experiments.

It is well known that the resolution of the above-mentioned experimental difficulties of statistical mechanics (specific heats and blackbody radiation) was found in abandoning the classical approach to physics in favor of the quantum one. As mentioned in the introduction, this revolution has had an unqualified experimental success, although it has raised serious epistemological questions, which continue to haunt us more than sixty years after the advent of the quantum theory. I would like to give a brief outline of a heresy that I have advocated for a few years now (Patrascioiu 1983), one directly connected to the ergodic hypothesis. As I mentioned earlier, if one contemplates a dynamical basis for statistical mechanics, one is faced with a real dilemma. The accepted formulation of the electromagnetic and the gravitational interactions demands that, in essence, everything in the universe interact with everything else. (This is so because of the long-range nature of these interactions.) In fact, the notion of an isolated object (or even system) is clearly an abstraction without any a priori physical basis, since ultimately everything is coupled to everything else through the electromagnetic and gravitational fields. All we can hope is either that the ergodic hypothesis is strictly false or that the times needed to excite certain degrees of freedom are so large that we can ignore them under some circumstances. In either case certain prejudices that have been passed from generation to generation should be abandoned and their bases be opened for investigation. For instance, in the absence of a dynamical calculation, there is no basis to claim that Planck's distribution for blackbody radiation is irreconcilable with classical electromagnetism. (In fact, the distribution found numerically and shown in Fig. 2 of the sidebar very much resembles Planck's law.)

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Does Equipartition of Energy Occur in Nonlinear Continuous Systems?

The celebrated work of Fermi, Pasta, and Ulam was the first of numerous attempts to study the distribution of energy in nonlinear continuous media. These attempts have all been indirect in that the systems are simulated by lattices of particles interacting through nonlinear potentials. The results have consistently failed to support the classical point of view regarding equipartition of energy—and yet they have stirred little excitement in the physics community. Perhaps this is so for two reasons: (i) the systems analyzed may be subject to an infinite number of conservation laws (and thus may be effectively linear), so that the individual degrees of freedom are not coupled and equipartition of energy cannot occur; (ii) the results may simply be artifacts of the lattice simulations.

Here I present some results from two of my own studies, the first of a one-dimensional model of the blackbody problem (Adrian Patrascioiu, *Physical Review Letters 50(1983): 1879)* and the second of a three-dimensional system that may give insight into the specific heats of systems with two species of degrees of freedom, such as the rotations and vibrations of diatomic molecules (K. R. S. Devi and A. Patrascioiu, *Physica D 11(1984): 359).*

In the case of blackbody radiation, the continuous medium (the electromagnetic field) is linear. Nonlinearity is introduced into the problem through the interaction of the field with the atoms in the walls of the cavity. Let us investigate a one-dimensional version of this problem, two nonlinear oscillators (particles and nonlinear springs) interacting through a linear string (Fig. 1). The string represents the electromagnetic field, and the oscillators represent the atoms. This model has the advantage that the string can be treated exactly so that no spatial lattice is needed.

The string and the particles move in the z direction only. The equation of motion for the string is

$$\frac{\partial^2 z(x,t)}{\partial t^2} - \frac{\partial^2 z(x,t)}{\partial x^2} = 0, \quad \text{for } x \neq \pm 1, \tag{1}$$

and the equations of motion for the particles on the left and right, respectively, are

$$m\frac{\partial^2 z(x,t)}{\partial t^2}\bigg|_{x=-1} = \mu \frac{\partial z(x,t)}{\partial x}\bigg|_{x=-1} + F\big(z(-1,t)\big) \tag{2}$$

and

$$m\frac{\partial^2 z(x,t)}{\partial t^2}\bigg|_{x=1} = -\mu \frac{\partial z(x,t)}{\partial x}\bigg|_{x=1} + F\big(z(1,t)\big). \tag{3}$$

Here m is the mass of each particle, μ is the string tension, and the nonlinear spring force F'(z) is defined by

$$F(z) = -\frac{dV}{dz},$$

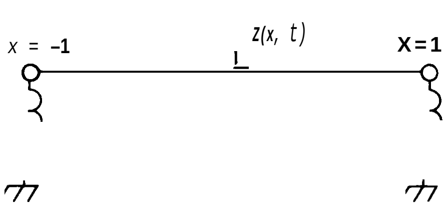
where

$$V = k\frac{z^2}{2} + \lambda\frac{z^4}{4} + c\,|z|.$$

These equations are written in units such that the length of the string is 2 and the speed of sound is 1. The most general form for the solution of Eq. 1 is $z(x,t) = f(t+x) + g(t-x)$. Substituting this general solution into Eqs. 2 and **3** yields a system

A ONE-DIMENSIONAL MODEL OF THE BLACKBODY PROBLEM

Fig. 1. The blackbody problem was modeled as the interaction of a linear string (which represents the electromagnetic field) and two nonlinear oscillators (which represent atoms in the walls of the cavity). Motion of both the string and the oscillators is restricted to the z direction and is described by the function *z(x, t)*.



of two coupled ordinary differential equations for the functions f and g.

The excitation of the string at $t = 0$ was specified by setting $f(x) = a \sin(\omega x + \pi/2)$ and $g(x)$ = O. The differential equations were integrated numerically, and conservation of energy was used to verify the accuracy of the calculations.

I would like to emphasize what outcome one would predict by following the same line of thought used to derive the Rayleigh-Jeans formula. The system, being nonlinear and (probably?) sufficiently complicated, will wander with equal probability throughout its phase space of given total energy. Let us choose initial conditions such that the total energy is finite. If ensemble averages and time averages are equal for this microcanonical ensemble, that is, if

$$\langle A\rangle_\mu = \lim_{T\to\infty} \frac{1}{T} \int dt\, A(t),$$

then the time-average kinetic energy of either particle should tend to zero for any initial conditions since the number of degrees of freedom is infinite. Over my times of observation, this did not seem to be the case! Under the assumption that the times of observation were sufficiently long, this result indicates that the microcanonial measure (Eq. 7 in the main text) is not applicable. We are left with two possibilities: (i) the motion of the system is quasiperiodic, or (ii) the phase space is broken into an infinite number of ergodic cells of finite size.

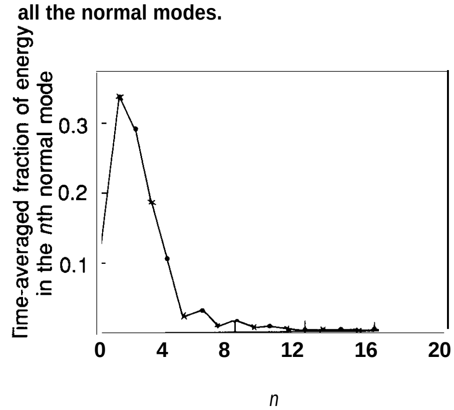
I also investigated the distribution of energy among the normal modes of the string. Figure 2 shows typical results for the time-average values of the fraction of the string energy in the *nth* normal mode. In all the runs performed the distribution of energy of the string among its normal modes is highly peaked (like the Planck distribution) and shows no tendency to become flat. Its shape does depend on the values of the various parameters in the problem and on the initial conditions. If all the parameters are kept fixed and the total energy is increased, the peak broadens. The shape of the distribution also varies with the frequency chosen for the initial excitation of the string, remaining constant over some range of ω and then jumping to a new shape.

The results of this study raised naturally several questions: (i) Was the observed unequal partition of energy among the normal modes of the string (the continuous medium) related to the one-dimensional nature of the medium? (ii) The unequal partition of energy reflected in the specific heats of diatomic gases results from motions of particles (rather than motions of a field, as in the case of blackbody radiation). Can this phenomenon be reproduced in a classical dynamical system?

To help answer these questions, Devi and I performed a study of a three-dimensional version of the system shown in Fig. 1. This system included four particles and six strings (Fig. 3). Our results exhibited several notable features over the times of observation: (i) time averages of, for example, total energies of particles and strings seemed to reach their asymptotic values; (ii) unequal partition of energy among the normal modes of the strings persisted, and the distributions obtained were reminiscent of that given by Planck's law; and (iii) for a variety of initial conditions, the four particles did not achieve the same average kinetic energy, a situation similar to the unequal partition of energy between the vibrational and the rotational degrees of freedom of diatomic gases. The fact that we obtained these types of results using several nonlinear (spring) potentials suggests their generality. ■

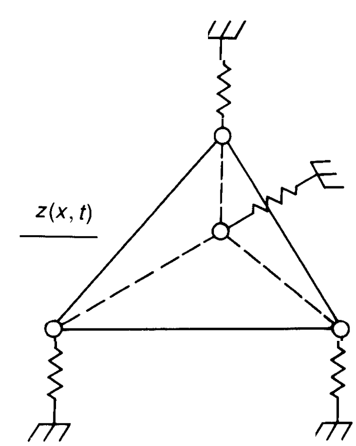
UNEQUAL PARTITION OF ENERGY

Fig. 2. Typical results for the distribution of energy among the normal modes of the string in the one-dimensional model of the blackbody problem (see Fig. 1). The exact shape of the energy distribution depends on the values assigned to various parameters, but in all cases the distribution was similar to a Planck distribution (see Fig. 2 of the main text) and was never flat, as it would be if the energy were partitioned equally among all the normal modes.



A THREE-DIMENSIONAL LATTICE

Fig. 3. The lattice below was used to investigate the dynamical behavior of a three-dimensional nonlinear system of particles and fields. Each of the four particles at the vertices of the regular tetrahedron is coupled to a nonlinear spring, and the particles are coupled to each other through linear strings.



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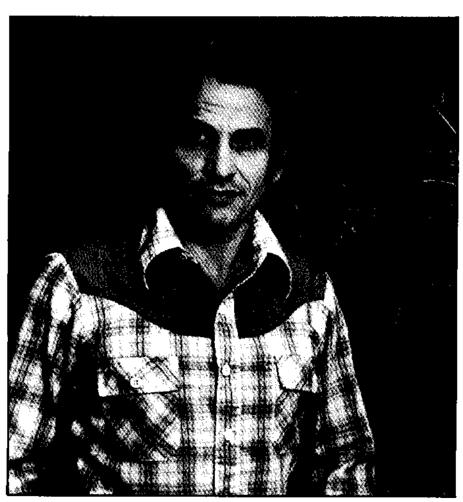
Nor is there any basis to the claim that the classical atom is inevitably unstable because of the "ultraviolet catastrophe" (escape of all of the energy into the ultraviolet modes of the electromagnetic field, as required by the equipartition-of-energy principle of classical statistical mechanics). After all, maybe classical electromagnetism leads to a nonergodic flow (if the notion of ergodicity makes sense at all for a continuous medium) or maybe the diffusion of energy to the high modes is so slow that it has not occurred appreciably in the twelve to eighteen billion years since the big bang. That such slow diffusion is not a far-fetched supposition follows from some results obtained in the last few years. Since point charges have infinite self-energies, let us spread them by introducing a charged scalar (zero-spin) field. It has been shown rigorously that, in a certain gauge (axial), the system of coupled nonlinear equations describing the interaction of the classical electromagnetic field with this classical charged field has finite-energy-density solutions for all times. Moreover, these solutions retain their initial smoothness (number of derivatives). Using this latter property one can show that after an arbitrarily long time of evolution, an infinite number of normal modes of these fields are arbitrarily close to their initial energies (Patrascioiu 1984). Whereas there is no guarantee that this model captures the true physics in the universe, it seems hard to imagine a field whose modes thermalize in a finite amount of time.

So perhaps quantum mechanics is nothing more than classical statistical mechanics done the right way in a universe filled with particles interacting primarily via electromagnetic and gravitational forces. If so, its mysteries should be understandable once the complicated Brownian process produced by particles constantly absorbing and emitting radiation is mastered. While this scenario may seem far-fetched to many, I think it arises inescapably from contemplating the foundations of statistical mechanics. It does not contradict the experimentally observed violation of Bell's inequality unless the latter persists for truly space-like settings of the magnets. It has epistemological value and would, for example, allow the computation of the fine-structure constant and its variation with temperature (Patrascioiu 198 I).

In conclusion, I think neither physicists nor mathematicians should close the book on the venerable problem of the ergodic hypothesis, and I guess some big surprises may be in store once the problem is better understood. ■



Adrian Patrascioiu, a native of Rumania, received his Ph.D. in theoretical physics from the Massachusetts Institute of Technology in 1973. He then spent two years as a member of the Institute for Advanced Study and two more years as a research associate at the University of California, San Diego. Since 1978 he has been a member of the Physics Department at the University of Arizona, where he is now a Professor. His honors include a Sloan Fellowship and a Los Alamos National Laboratory Stanislaw M. Ulam Scholarship.

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