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ERGODIC THEORY AND STATISTICAL MECHANICS *

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I. INTRODUCTION

I would like to talk about some of the progress that has been made in recent years in the mathematical theory of measure preserving transformations: ergodic theory. Since the dynamical flow in the phase space, which describes the time evolution of a Hamiltonian system, is an example of such a transformation, this work has, in my opinion, much relevance to statistical mechanics and to the question of irreversibility. While the recent progress in this field is due mostly to the work of mathematicians like von Neumann, Hopf, Kolmogorov, Sinai, Ornstein and others, the origins of the subject go back to the founding fathers of statistical mechanics; Boltzmann, Maxwell, Gibbs and Einstein. These men and their followers invented the concept of ensembles to describe equilibrium and nonequilibrium macroscopic systems. In trying to justify the use of ensembles, and to determine whether the ensembles evolved as expected from nonequilibrium to equilibrium, they introduced further concepts such as "ergodicity" and "coarse graining". The use of these concepts raised mathematical problems that they could not solve, but like the good physicists they were they assumed that everything was or could be made all right mathematically and went on with the physics.

Their mathematical worries, however, became the seeds from which grew a whole beautiful subject called "ergodic theory". Here I will describe some recent (and some not so recent) developments that partially solve some of the problems that worried the Founding Fathers. Although results are not yet well enough developed to answer all the questions in this area that are of interest to physicists, such as the derivation of kinetic equations or the general problem of irreversibility, they do make a start.

Since it has been only in the last few years that physicists have again become deeply involved in this subject, there is a big gap in the statistical mechanics literature concerning the developments in ergodic theory which have occurred in the last forty years. As a recent convert I have preached the gospel of ergodic theory many times in many places. Some of you will therefore have heard some parts of this talk before or you may have read it in some of the reviews of the subject I have written. Indeed these notes contain some (almost) verbatim transcripts of my article with Penrose in Physics Today.

I have also borrowed freely from joint works with Goldstein, Lanford and Aizenman, as well as independent works of these authors. The credit, but certainly not the blame, for what I will present here is therefore a shared one.

A partial list of references, especially suited for physicists, is given at the end.

1.1 Scope of lectures

Ergodic theory is concerned with the time evolution of Gibbs ensembles. It has revealed that there is more to the subject than the simple question of whether a dynamical system is ergodic (which means roughly, whether the system, if left to itself for long enough, will pass close to nearly all the dynamical states compatible with conservation of energy). Instead there is a hierarchy of properties that a dynamical system may have, each property implying the preceding one, and of which ergodicity is only the first (see Table 1). The next one, called "mixing" provides a formulation of the type of irreversible behaviour that people try to obtain by introducing coarse-grained ensembles. At the top of our hierarchy is a condition (the Bernoulli condition) ensuring that in a certain sense the system, though deterministic, may appear to behave as randomly as the numbers produced by a roulette wheel.

Some of the mathematical results we shall be discussing have established the positions of some model physical systems in this hierarchy. Of particular interest to physicists is the work of Ya. Sinai on the hard-sphere system, which shows that this system is both ergodic and mixing. I shall also discuss some work by A.N. Kolmogorov, V.I. Arnold and J. Moser on systems of coupled anharmonic oscillators, which shows that, contrary to a common assumption, these systems may not even reach the "ergodic" rung on the ladder. (G.H. Walker and J. Ford have described this work for physicists).

All the physical systems I shall discuss obey classical mechanics or are models of such systems. I shall consider first systems which have a finite number of degrees of freedom and are confined to a finite region of physical space. Here the concepts, if not the proofs, are basically simple. Later I shall discuss infinite systems, by which I mean the limit of a finite system as its size increases without bound. The concepts involved here are more difficult or at least may be less familiar to you. Also the basic ingredient for the study of the ergodic properties of such systems, the existence of a well-defined

Infinite systems: Ideal gas. Hard rod system, perfect harmonic crystal	Bernoulli system	Equivalent to roulette wheel
Baker's transformation, Geodesic flow on space of negative curvature, Particle moving among fixed convex scatterers		
Infinite system: Lorentz gas	K-system	Essential randomness
Two or more hard spheres moving in two or higher dimensions?		
Simple model system with collisions	Mixing system	Approach to equilibrium
One dimensional harmonic oscillator	Ergodic system	Use of microcanonical ensemble

Table 1. Hierarchy of Systems

The middle column lists the systems that will be discussed in these lectures, with the strongest at the top. Every mixing system is ergodic, every K-system is mixing and every Bernoulli system is a K-system. At the left are examples of the system and at the right physical interpretations or implications.

time evolution, has only very recently been proved by Lanford. My discussion of infinite systems will therefore be even more sketchy than for the finite case. The reason for discussing them at all is that it is only in this limit, usually referred to as the thermodynamic limit, that the distinction between microscopic and macroscopic observables, which appears essential to any complete theory of irreversibility, can be formulated precisely.

My reason for not dealing with quantum systems here is that a finite quantum system can never exhibit any of the properties higher than simple ergodicity in our hierarchy (although, of course, a large quantum system may approximate closely the behaviour characterized by these concepts). This is because the spectrum of a finite quantum

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system is necessarily discrete, whereas for a finite classical system the spectrum (of the Liouville operator) can be continuous. Infinite quantum systems can, and do, exhibit ergodic behaviour similar to classical systems. Some very beautiful work on such systems has just, very recently, been done by Haag, Kastler and Eva Trych-Pohlmeyer, who is here. I hope to elaborate slightly on these remarks about quantum systems during these lectures.

I should point out right here that care must be exercised in drawing analogies between the ergodic properties of finite and infinite systems, as the dependence of these properties on the interactions between the particles, and thus also their physical interpretation, may be very different in the two cases. Thus while a finite ideal gas (classical system of non-interacting point particles) is not even ergodic, the infinite ideal gas has the strongest possible ergodic properties: it is a Bernoulli system, c.f. Table 1.

The explanation of the good ergodic properties of the infinite ideal gas is simple: local disturbances 'fly off' unhindered to infinity where they are no longer observable. This means that the 'approach' or better the return to equilibrium of a large (infinite) system, which is perturbed locally away from equilibrium, may occur even in the absence of a local 'dissipative' mechanism such as is provided by collisions. It can happen simply, as it does in the ideal gas (or the perfect harmonic crystal) by the disturbance disappearing from sight by the free streaming motion of the particles (phonons).

This kind of return to equilibrium is of course not described by a kinetic or hydrodynamic equation and is therefore not the kind of irreversibility which is of interest in real physical systems. It is therefore necessary to introduce additional structure, to that provided by ergodic theory alone, to distinguish between infinite systems of the ideal gas type and more realistic physical systems, such as the Lorentz gas, where there exists a local mechanism, e.g. collisions, for the approach to equilibrium. A start in this direction has been made by S. Goldstein who considered the (generalized) ergodic properties of an infinite system under the joint group consisting of the time evolution and space translations. He showed that these two different kinds of systems can indeed be clearly distinguished with this sharper tool. The work of Haag, Kastler and Pohlmeier, mentioned earlier, also has some bearing on this question and I hope to return to this point later.

II. ERGODICITY AND ENSEMBLE DENSITIES

Before we go on to discuss the new results, we review some mathematical definitions. If our dynamical system has n degrees of freedom, we can think of its possible dynamical states geometrically, as points in a $2n$ -dimensional space (phase space), with n position coordinates and n momentum coordinates. If the energy of the system is E , then its dynamical state $x (= (q_1 \dots q_n, p_1 \dots p_n))$ must lie on the energy surface $H(x) = E$, where H is the Hamiltonian function. We denote the energy surface, which is $(2n - 1)$ -dimensional, by S_E or just S and assume that S is smooth and of finite extent; for example in the case of a system of harmonic oscillators, for which the Hamiltonian is a quadratic form, the energy surfaces are $(2n - 1)$ -dimensional ellipsoids.

The time evolution of the system causes x to move in phase space, but since we are assuming our system to be conservative the point x always stays on the energy surface. If the system is in some state x at some time t_0 then its state at any other time $t_0 + t$ is uniquely determined by x and t (only). Let us call the new state $\phi_t(x)$. This defines a transformation ϕ_t from S onto itself. There is one such function for each value of t .

We shall want to integrate dynamical functions (that is, functions of the dynamical state) over S . When doing this it is convenient not to measure $(2n - 1)$ -dimensional "areas" on the surface S in the usual way but to weight the areas in such a way that the natural motion of the system on S carries any region R (after any time t) into a region $\phi_t(R)$ of the same area. This can be accomplished by defining the weighted area of a small surface element near x , dx , to be such that $dx dE$ is the correct Euclidean $2n$ -dimensional volume element of a "pill box" with base dx and height dE . Formally

$$dx = d\sigma_E(x) / |\nabla H(x)|, \quad x \in S_E$$

where $d\sigma_E(x)$ is the 'usual' surface area on S_E and $\nabla H(x)$ is the gradient of the Hamiltonian

$$|\nabla H(x)| = \left\{ \sum_{i=1}^n \left[\left(\frac{\partial H}{\partial q_i} \right)^2 + \left(\frac{\partial H}{\partial p_i} \right)^2 \right] \right\}^{\frac{1}{2}}.$$

By a Gibbs ensemble we mean an infinitely large hypothetical

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collection of systems, all having the same Hamiltonian but not necessarily the same dynamical state. We shall only consider ensembles whose systems all have the same energy, so that their dynamical states are distributed in some way over some energy surface S . It may happen that this distribution can be described by an ensemble density; by this we mean a real-valued function ρ on S such that the fraction of members of the ensemble whose dynamical states lie in any region R on the surface S is

$$\int_R \rho(x) dx$$

with dx the weighted area defined above. The simplest ensemble density on S is given by

$$\rho(x) = C \quad (\text{all } x \text{ in } S)$$

where C is a constant, which can be determined from the normalization condition $\int_S C dx = 1$. This is called the microcanonical ensemble on S .

The systems constituting the ensemble evolve with time, so that the ensemble density will depend on time. The rule connecting the ensemble densities ρ_t describing the same ensemble at different times t is Liouville's theorem, which can be written

$$\rho_t(x) = \rho_0[\phi_{-t}(x)] \quad (\text{all } t, \text{ all } x \text{ in } S)$$

where $\rho_0(x)$ is the ensemble density at time zero. For example, Liouville's theorem shows that the density of the microcanonical ensemble does not change with time: If

$$\rho_0(x) = C$$

for all x in S , then Liouville's theorem gives, for any t ,

$$\rho_t(x) = C$$

for all x in S .

The principal success of ensemble theory has been in its application to equilibrium. To calculate the equilibrium value of any dynamical function we average it over a suitable ensemble. The same ensemble also enables us to estimate the magnitude of the fluctuations of our dynamical function. To ensure that the calculated averages are independent of time, we use an invariant ensemble; that is, one for which the fraction of members of the ensemble in every region R on the energy surface S is independent of time. We already know one invariant ensemble: the microcanonical, whose ensemble density is uniform on S . Before we can use it confidently to calculate equilibrium values, however, we would like to be sure that this is the only invariant ensemble: If other invariant ensembles exist then, in principle, they could do just as well for the calculation of equilibrium properties, and we would have to choose which to use in a particular situation.

There are two questions to settle: the first is whether there are any invariant ensembles on S that do not have an ensemble density. In general there are; for example in the case of a hard-sphere system in a box one could have an invariant ensemble where every particle moves on the same straight line being reflected at each end from a perfectly smooth parallel wall (see fig. 1).

The obviously exceptional character of this motion is reflected mathematically in the fact that this ensemble, though invariant, is confined to a region of zero "area" on S and therefore has no ensemble density. To set up such a motion would presumably be physically impossible because the slightest perturbation would rapidly destroy the perfect alignment. It is therefore natural to rule out such exceptional ensembles by adopting the principle that any ensemble corresponding to a physically realizable situation must have an ensemble density.

There remains the second part of the question: Are there any invariant ensembles on S that do have a density but differ from the microcanonical ensemble? This is equivalent to the ergodic problem in which one compares the time averages of a dynamical function f ,

$$f^*(x) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(\phi_t(x)) dt$$

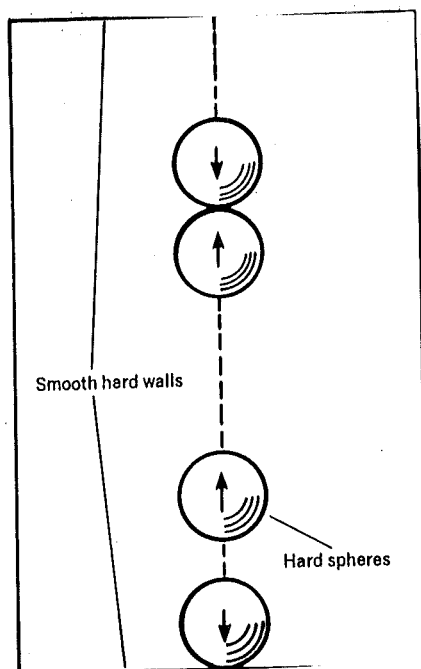


Fig. 1. Ensemble with no ensemble density.

Hard spheres move up and down the dotted line, which meets the perfectly smooth hard walls at right angles. Collisions between particles and collisions with the walls do not deflect the particles from the line if they are perfectly aligned at the start. An ensemble of such systems has no ensemble density because it is concentrated on a region on the energy surface with zero area (just as the area of a line or of a line segment in a plane is zero).

with its microcanonical ensemble average

$$\langle f \rangle = \int_S f(x) dx / \int_S dx .$$

A system is said to be ergodic on its energy surface S if time averages are in general equal to ensemble averages; that is, if for every integrable function f we have

$$f^*(x) = \langle f \rangle \quad (1)$$

for almost all points x on S . "Almost all" means that if M is the set of points x for which eq. 1 is false, we have $\int_M dx = 0$. The answer to our second question is given by a theorem, which

we shall not prove: the microcanonical ensemble density is the only invariant ensemble - that is, the only one satisfying $\rho[\phi_t(x)] = \rho(x)$ for all x in S - if and only if the system is ergodic on S .

The physical importance of ergodicity is that it can be used to justify the use of the microcanonical ensemble for calculating equilibrium values and fluctuations. Suppose f is some macroscopic observable and the system is started at time zero from a dynamical state x , for which $f(x)$ has a value that may be very far from its equilibrium value. As time proceeds, we expect the current value of f , which is $f[\phi_t(x)]$, to approach and mostly stay very close to an equilibrium value with only very rare large fluctuations away from this value. This equilibrium value should therefore be equal to the time average f^* because the initial period during which equilibrium is established contributes only negligibly to the formula defining $f^*(x)$. The theorem tells us that this equilibrium value is almost always equal to $\langle f \rangle$, the average of f in the microcanonical ensemble, provided the system is ergodic.

To justify the use of the microcanonical ensemble in calculating equilibrium fluctuations we proceed in a similar way. For some observable event A (such as the event that the percentage of gas molecules in one half of a container exceeds 51%) let R be the region in phase space consisting of all phase points compatible with the event A ; that is the event A is observed if and only if the phase point is in R at time t . If the system is observed over a long period of time, the fraction of time during which event A will be observed is given by the time average $g^*(x_0)$, where x_0 is the initial dynamical state and g is defined by

$$g(x) = \begin{cases} 1 & \text{if } x \text{ is in } R \\ 0 & \text{if not.} \end{cases}$$

The ergodic theorem tells us that for almost all initial dynamical states this fraction of time is equal to the ensemble average of g , which is

$$\langle g \rangle = \frac{\int_R dx}{\int_S dx}.$$

This is just the "probability" of the event A as calculated in the microcanonical ensemble on S .

Another way of defining ergodicity is to say that any integrable invariant function is constant almost everywhere. That is to say, if

f is an integrable function satisfying the condition that

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$$f[\phi_t(x)] = f(x)$$

for all x in S , then there is a constant c such that $f(x)$ equals c for almost all x : In other words, the set M of points x for which $f(x)$ does not equal c satisfies $\int_M dx = 0$. This has the physical interpretation that for a Hamiltonian system ergodic on S every integrable constant of the motion is constant on S . Furthermore if ergodicity holds on each S_E then there are no integrable constants of the motion other than functions of the energy E . Indeed, if there were other constants of the motion (for example angular momentum if the Hamiltonian had an axis of symmetry) we could construct invariant densities that were not microcanonical by taking $\varphi(x)$ to be a function of one of these other constants of the motion, and so the system would clearly be nonergodic. (When such additional constants of the motion exist they must be taken into account in the statistical mechanics and thermodynamics of the system; the standard methods, based on the microcanonical ensemble, must then be generalized for these systems.)

These relationships between ergodicity and constants of the motion are a consequence of Birkhoff's theorem that ergodicity, as defined by the equality of the time average to the ensemble average, eq. 1, is equivalent to the energy surface being "metrically transitive". Stated precisely this means that a system is ergodic on S if and only if all the regions R on S left invariant by the time evolution, $\phi_t(R) = R$, either have zero area or have an area equal to the area of S .

The difficult part of Birkhoff's Theorem is to show that $f^*(x)$, which involves taking the time average over infinite times, actually exists for almost all x when $f(x)$ is an integrable function. It is then relatively easy to show that $f^*(x)$ is time invariant; that is, $f^*[\phi_t(x)] = f^*(x)$, and that ergodicity is equivalent to S being metrically intransitive.

2.2 Brief history of ergodic theory

The "ergodic hypothesis" was introduced by Boltzmann in 1871. To quote Maxwell "... (it) is that the system, if left to itself in its actual state of motion, will, sooner or later, pass through every phase which is consistent with the equation of energy." In our

notation "phase" means dynamical state and the original ergodic hypothesis means that if y and x are any two points on the energy surface S_E , then $y = \phi_t(x)$ for some t . The ergodic hypothesis thus stated was proven to be false, whenever S_E has dimensionality greater than one, by A. Rosenthal and M. Plancherel in 1913. S.G. Brush gives a nice account of the early work on this problem.

The definition of an ergodic system given in eq. 1 can be shown to imply what is sometimes called the "quasi-ergodic" hypothesis, which replaces "every phase" in Maxwell's statement by "every region R on S_E of finite area", with the further qualification that this is true for "almost all" dynamical states. Indeed as was pointed out, the fraction of time that the system will spend in R is equal, for an ergodic system, to the fraction of the area of S_E that is occupied by R .

III. SYSTEMS OF OSCILLATORS AND THE KAM THEOREM

We shall now consider some examples of ergodic and non-ergodic systems. The simplest example of an ergodic system is the simple harmonic oscillator whose Hamiltonian (in some suitable units) is

$$H(q,p) = \frac{1}{2} \omega (p^2 + q^2)$$

where ω is the angular frequency. The transformation ϕ_t for this system is a rotation through angle ωt in the (q,p) plane. The trajectories, which here coincide with the energy surfaces S_E , are circles of radius $(2E)^{1/2}$. (The surface element dx is here proportional to the ordinary length of an arc segment.) To be invariant under the transformation ϕ_t an ensemble density on S must be unaffected by rotations and is therefore a constant. It follows, then, that the only invariant density is the microcanonical density and so the simple harmonic oscillator is ergodic.

Almost as simple is the multiple harmonic oscillator (physically, say, an ideal crystal), that is, a system with two or more degrees of freedom whose potential energy is a quadratic form in the position coordinates. Unlike the simple harmonic oscillator it cannot be ergodic, because it has constants of the motion (the energies of the individual normal modes) that are not constant on the energy surfaces (the surfaces of constant total energy).

It used to be thought that this lack of ergodicity was an

accident and that any small anharmonicity (such as would inevitably be present in a real system) must make the system ergodic by permitting transfer of energy from one mode to another. In 1954, however, Kolmogorov announced results that contradicted this belief. In 1955, Enrico Fermi, J. Pasta and S.W. Ulam carried out a computer simulation of such a system. Initially, they excited one mode only, and instead of the equipartition of the energy between all modes predicted by the microcanonical ensemble they found that most of it appeared to remain concentrated in a few modes; this indicated that anharmonic oscillator systems may not be ergodic.

The lack of ergodicity was proved rigorously by Kolmogorov, Arnold and Moser. They found that if the frequencies of the unperturbed oscillators are not "rationally connected" (that is, if no rational linear combination of them is zero) then, in general, adding to the Hamiltonian an anharmonic perturbation sufficiently small compared to the total energy does not make the system ergodic. The unperturbed trajectories (possible paths of the phase point) all lie on n -dimensional surfaces in S (which has $2n-1$ dimensions) called "invariant tori", and "KAM" prove that under a weak perturbation most trajectories continue to lie within smooth n -dimensional tori, so that the perturbed system is also non-ergodic. The trajectories that do not lie on the new invariant tori are, on the other hand, very erratic and may fill some $(2n - 1)$ -dimensional region densely. One consequence of this very complicated behaviour is that even though the system is not ergodic the motion can no longer be decomposed into independent normal modes.

Similar results probably hold also for rationally connected frequencies (which cannot be treated rigorously, although they are of more physical interest); thus Michael Hénon and Carl Heiles carried out computer calculations for the Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + (q_1^2 q_2 - \frac{1}{3} q_2^3) \quad (3.1)$$

whose unperturbed frequencies $\omega_1 = 1$, $\omega_2 = 1$, are rationally connected since $1 \cdot \omega_1 - 1 \cdot \omega_2 = 0$. They found that the energy surfaces with E equal to $1/12$, $1/8$ and probably also $1/6$ are not ergodic (see figure 2). As seen in the diagrams the fraction of the area corresponding to smooth curves (which are responsible for the non-ergodic behaviour) decreases as the energy increases.

For a general system of anharmonic oscillators, such as a real crystal, we expect similar behaviour, with the fraction of S_E corresponding to non-ergodic behaviour decreasing as E increases, and

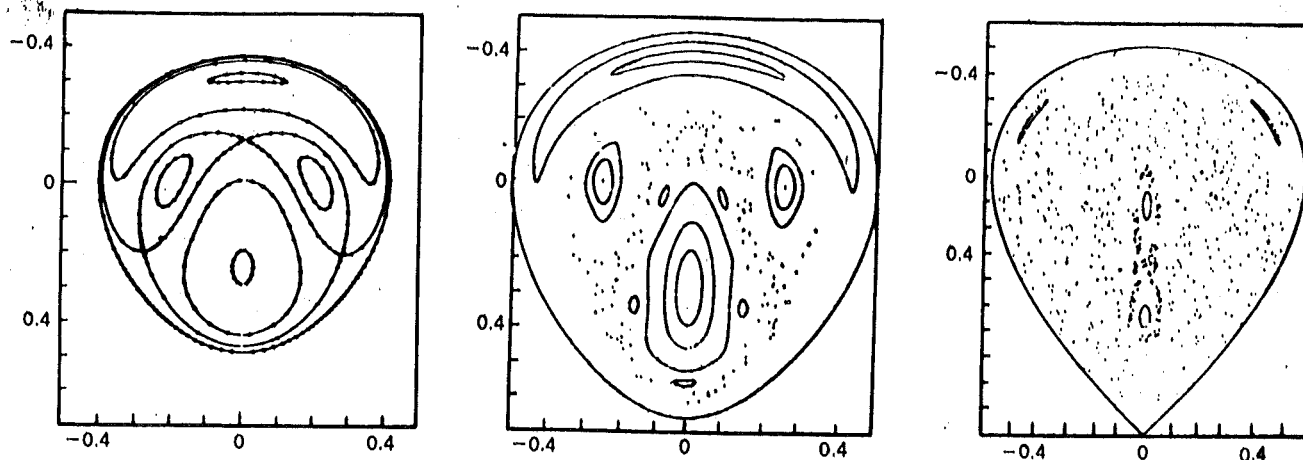


Fig. 2. Nonergodicity of an anharmonic oscillator system with rationally connected frequencies.

The Hamiltonian for this system is given in eq. (3.1). Michael Hénon and Carl Heiles did computer calculations for this system and found that energy surfaces S_E with E equal to $1/12$, $1/8$ and probably $1/6$ are not ergodic. The planes shown here are intersections of the surface q_1 equal to zero with S_E for E equal to $1/12$ (a), $1/8$ (b) and $1/6$ (c), and the points are the intersections of a trajectory with this plane. When the trajectory lies on a smooth two-dimensional invariant torus, the intersection points form a smooth curve, but the intersections of an "erratic" trajectory (one that does not lie on a smooth curve) are more or less random. Note that the fraction of area corresponding to smooth curves (which are responsible for the nonergodic behaviour) decreases with increasing energy.

probably disappearing altogether at some critical energy, above which the system would be ergodic and perhaps also show the stronger properties that we shall discuss. At present very little is known about the magnitude of this critical energy in a system with many degrees of freedom.

In the case of gases, the situation is somewhat different. If there were no interaction at all between the molecules then the energy of each molecule would be an invariant of the motion, so that the system (an ideal gas) would be nonergodic. The KAM theorem would therefore lead us to expect nonergodicity to persist in the event of a sufficiently weak interaction between the particles. The actual interactions, however, are not weak because two molecules very close together repel each other strongly; consequently the theorem does not apply. A simple model of this type is the hard-sphere gas enclosed in a cube with perfectly reflecting walls or periodic boundary conditions. Sinai has outlined a proof that this system is ergodic; he has published a detailed proof, based on the same ideas, for a

particle moving in a periodic box containing any number of rigid convex elastic scatterers. We shall refer again to this important result.

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IV. MIXING

We have seen how to formulate a condition to ensure that the equilibrium properties of a dynamical system are determined by its energy alone and can be calculated from a microcanonical ensemble. This ergodicity condition does not, however, ensure that if we start from a non-equilibrium ensemble the expectation values of dynamical functions will approach their equilibrium values as time proceeds. An illustrative example is given by the harmonic oscillator. For the harmonic-oscillator system, Liouville's theorem shows that the ensemble density repeats itself regularly at time intervals of $2\pi/\omega$; therefore all ensemble averages also have this periodicity, and so cannot irreversibly approach their equilibrium values.

To ensure that our ensembles approach equilibrium in the way we would expect of ensembles composed of real systems, we need a stronger condition than ergodicity. To see what is required, let us start at $t = 0$ with some ensemble density $\rho_0(x)$ on S , which is supposed to represent the initial non-equilibrium state. At a later time t the ensemble density is, by Liouville's theorem, $\rho_0[\phi_{-t}(x)]$. The expectation value of any dynamical variable f at time t is therefore

$$\int_S f(x) \rho_0[\phi_{-t}(x)] dx \quad (4.1)$$

As t becomes large we would like this integral to approach the equilibrium value of f , which is (for an ergodic system)

$\int_S f(x) dx / \int_S dx$. A sufficient condition for this is that the system should satisfy the condition called mixing which is that for every pair of functions f and g whose squares are integrable on S , we require

$$\lim_{t \rightarrow \pm \infty} \int_S f(x) g(\phi_{-t}(x)) dx = \frac{\int_S f(x) dx \int_S g(x) dx}{\int_S dx} \quad (4.2)$$

The special case where g is ρ_0 shows that integral (4.1) will approach the equilibrium value of f for large t when the system

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is mixing. Another way of looking at this condition is that it requires every equilibrium time-dependent correlation function such as $\langle f(x)g[\phi_t(x)] \rangle$ to approach a limit $\langle f \rangle \langle g \rangle$ as t approaches $\pm \infty$.

The condition of mixing can be shown to be equivalent to the following requirement: if Q and R are arbitrary regions in S , and an ensemble is initially distributed uniformly over Q , then the fraction of members of the ensemble with phase points in R at time t will approach a limit as t approaches ∞ ; this limit equals the fraction of the area of S occupied by R .

This condition can be stated formally as follows: Let $\mu(A)$ denote the normalized area of a set A on the energy surface S , i.e. the probability in the microcanonical ensemble of finding the system in A ,

$$\mu(A) = \int_A dx / \int_S dx .$$

(For simplicity we shall set $\int_S dx = 1$ from now on.)

A system is mixing iff for any sets A and B

$$\mu(A_t \cap B) \xrightarrow[t \rightarrow \pm \infty]{} \mu(A)\mu(B) , \quad A_t = \phi_t(A) . \quad (4.3)$$

We can interpret this to mean that if we start with an ensemble at $t = 0$ such that all the systems are in region A ,

$$\rho_0(x) = \begin{cases} [\mu(A)]^{-1} & \text{if } x \in A \\ 0 & \text{otherwise} \end{cases} ,$$

then the fraction of systems in this ensemble that will be in region B at time t will approach $\mu(B)$, see figure 3.

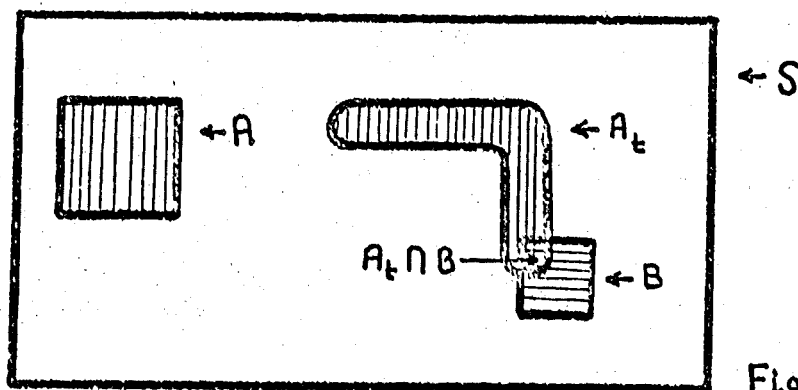


Figure 3.

Mixing is a stronger condition than ergodicity: it can easily be shown to imply ergodicity but is not implied by it, as we have seen

in the case of a simple harmonic oscillator.

The proof is simple. Suppose that A is an invariant set, $A_t = A$. Then if the system is mixing we must have,

$$\mu(A_t \cap A) = \mu(A) = [\mu(A)]^2$$

so that $\mu(A) = 0$ or $\mu(A) = 1$ which, since it holds for all invariant sets, implies ergodicity as was noted earlier.

The mathematical definition of mixing was introduced by John von Neumann in 1932 and developed by E. Hopf, but goes back to J. Willard Gibbs, who discusses it by means of an analogy: "... the effect of stirring an incompressible liquid Let us suppose the liquid to contain a certain amount of colouring matter which does not affect its hydrodynamic properties ... (and) that the colouring matter is distributed with variable density. If we give the liquid any motion whatever ... the density of the colouring matter at any same point of the liquid will be unchanged ... Yet... stirring tends to bring a liquid to a state of uniform mixture."

Gibbs saw clearly that the ensemble density ϱ_t of a mixing system does not approach its limit in the usual "fine-grained" or "pointwise" sense of $\varrho_t(x)$ approaching a limit as $t \rightarrow \infty$ for each fixed x . Rather, it is a "coarse-grained" or "weak" limit, in which the average of $\varrho_t(x)$ over a region R in S approaches a limit as $t \rightarrow \infty$ for each fixed R . (A similar distinction applies in defining the entropy. The fine-grained entropy $-k \int \varrho_t(x) \log \varrho_t(x) dx$, where k is Boltzmann's constant, retains its initial value forever, but the coarse-grained entropy $-k \int \bar{\varrho}_t(x) [\log \bar{\varrho}_t(x)] dx$, where $\bar{\varrho}_t(x)$ is a coarse-grained ensemble density obtained by averaging $\varrho_t(x)$ over cells in phase space, does change for a non-equilibrium ensemble, and approaches as its limit the equilibrium entropy value $k \log \int_S dx$).

It is sometimes argued that one cannot have a proper approach to equilibrium for any finite mechanical system because of a theorem, due to Poincaré, that every such system eventually returns arbitrarily close to its initial state. (The time involved, however, will be enormously large for a macroscopic system. Boltzmann, for example, estimated a typical Poincaré period for 100 cm^3 of gas to be enormously long compared to 10 raised to the power 10 raised to the power 10 years.) Here, however, we are considering ensembles, not individual systems, and the mixing condition guarantees that the ensemble density eventually becomes indistinguishable from the microcanonical density

and remains so forever after. It is true that individual systems in the ensemble will return to their initial dynamical states, as required by Poincaré's theorem, but this will happen at different times for different systems, so that at any particular time only a very small fraction of the systems in the ensemble are close to their initial dynamical states.

The reason for the irrelevance of Poincaré recurrences in mixing systems is that the motion of the phase point is very unstable. Dynamical states that start very close to each other in phase space

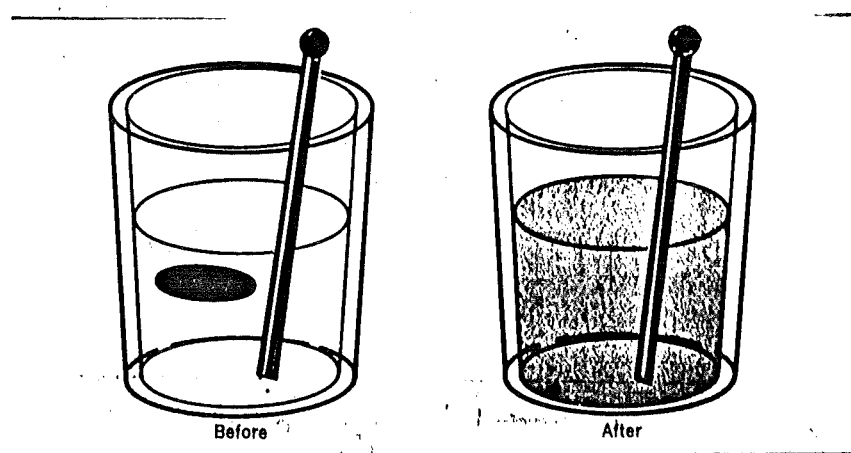


Fig. 4. A familiar example of "mixing".

According to V.I. Arnold and A. Avez, the two liquids are rum (twenty percent) and cola (eighty per cent), with the result of the mixing process known as a "Cuba libre".

become widely separated as time progresses, so that the recurrence time depends extremely sensitively on the initial conditions of the motion. (The importance of this instability in statistical mechanics was first recognized by N.S. Krylov, a Russian physicist who died in his twenties in 1947.) This type of instability appears to be characteristic of real physical systems, and leads to one sort of irreversibility: even if we could reverse the velocities of every particle in a real system that has been evolving towards equilibrium, the system would not necessarily return or even come close to its initial dynamical state with the velocities reversed because the unavoidable small external perturbations would be magnified. This instability is noticeable in molecular-dynamics calculations with hard-sphere systems:

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if we numerically integrate the equations of motion from time 0 to time t and then try to recover the initial state by integrating backwards from time t to time 0, we obtain instead a completely new state. This is because the numerical integration is unstable to small rounding-off errors made during the computation, which play the same role as external perturbations in a real system.

Only a few physical systems have been proven so far to be mixing. The most important is the hard-sphere gas, mentioned above. Sinai's proof that this system is ergodic also gives the stronger result that it is mixing. Roughly, Sinai's method of proving mixing is to show that the hard-sphere system is unstable in the sense discussed above. Physically this instability comes from the fact that a slight change in direction of motion of any particle is magnified at each collision with the convex surface of another particle. The full proof for the simplest case of a "single" particle moving among fixed convex scatterers is already quite complicated and the proof for moving hard sphere has not yet appeared. That is why I put a question mark next to this system in Table 1. I have some private information however (from G. Gallavotti) that Sinai is in the process of writing up the proof and has already finished a hundred pages of manuscript. As indicated in Table 1 the proof will actually be that this system is a K-system.

A very simple model system with 'collisions' which is mixing was considered by Goldstein, Lanford and Lebowitz. This will be described in the Appendix.

4.1 Time correlations and transport coefficients

As indicated by all the speakers here, the study of time correlation functions of the form $\langle g(t)f \rangle$ plays a central role in the statistical mechanical theory of non-equilibrium phenomena. When a system is mixing then these functions will certainly approach their uncorrelated values as $|t| \rightarrow \infty$, provided that g and f are square integrable, $\langle g^2 \rangle < \infty$, $\langle f^2 \rangle < \infty$, i.e.

$$\langle g(t)f \rangle - \langle g \rangle \langle f \rangle \longrightarrow 0 \quad \text{as} \quad |t| \rightarrow \infty. \quad (4.4)$$

A system is said to be weakly mixing if, under the same conditions on square integrability

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\langle g(t)f \rangle - \langle g \rangle \langle f \rangle| dt \rightarrow 0 \text{ as } T \rightarrow \pm \infty \quad (4.5)$$

This is clearly a weaker requirement than (4.4). It is however still stronger than ergodicity which can be shown to be equivalent to the requirement that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T [\langle g(t)f \rangle - \langle g \rangle \langle f \rangle] dt \rightarrow 0 \text{ as } T \rightarrow \pm \infty \quad (4.6)$$

In many cases one is interested in the time integrals of these correlations. This stems from the fact, pointed out by many of the lecturers here (indeed Professor Kubo is the modern father of this subject) that linear transport coefficients, such as heat conductivity, viscosity etc., may be expressed as integrals over time (from $t = 0$ to $t = \infty$) of the time correlation of appropriate dynamical functions (Einstein-Green-Kubo). These functions represent the 'fluxes' associated with the transport processes in question. A well known example of such a 'formula' is the Einstein relation between the self-diffusion constant D and the integral of the velocity auto-correlation function of a specified particle, say particle one,

$$\langle v_1(t) v_1 \rangle, (\langle v_1 \rangle = 0).$$

It might appear that for mixing systems these transport coefficients could be defined meaningfully, without going to the thermodynamic limit of an infinite size system, as long as $[\langle g(t)f \rangle - \langle g \rangle \langle f \rangle]$ approached zero sufficiently rapidly to be integrable. Such is, however, not the case, as indeed it should not be on physical grounds. Formally this occurs because the flux functions whose time correlations are of interest for transport coefficients can generally be written as Poisson brackets with the Hamiltonian H , i.e. $f = (F, H)$, $g = (G, H)$, and for mixing systems it can be shown that when f, g, F, G are all square integrable, then

$$\lim_{T \rightarrow \infty} \int_0^T \langle f(t)g \rangle dt = \langle (F, H)G \rangle,$$

$$\lim_{T \rightarrow \infty} \int_0^T \langle f(t)f \rangle dt = 0$$

Thus for a finite mixing system confined by a wall,

$$\lim_{T \rightarrow \infty} \int_0^T \langle v_1(t)v_1 \rangle dt = \lim_{T \rightarrow \infty} \langle q_1(T)v_1 \rangle = 0 \quad (4.7)$$

since

$$v_1 = (q_1, H) \quad \text{and} \quad \int v_1^2 dx < \infty, \quad \int q_1^2 dx < \infty.$$

Note that when q_1 is an angle variable, e.g., in the case of periodic boundary conditions, then $v_1 \neq (q_1, H)$ and (4.7) need not hold. We would still have, however, $\langle v_1(t)v_1 \rangle \rightarrow 0$ if the system is mixing.

When the system is not mixing, the limit $T \rightarrow \infty$ in the above integrals need not exist. It is still true however that for any finite system

$$\lim_{T \rightarrow \infty} \int \langle f(t)f \rangle dt = \lim_{T \rightarrow \infty} \left[-\frac{d}{dT} \langle F(T)F \rangle \right] = 0, \quad \text{if it exists.}$$

This is so since,

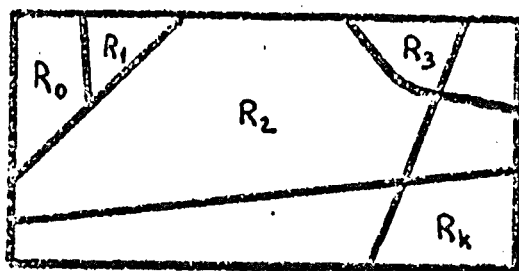
$$\langle F(T)F \rangle \leq \langle F(T)F(T) \rangle^{\frac{1}{2}} \langle F^2 \rangle^{\frac{1}{2}} = \langle F^2 \rangle,$$

so that when F is square integrable $d/dt \langle F(T)F \rangle$ can either oscillate or approach zero.

These time correlation integrals will therefore, if they exist, at all, be equal to zero in any finite system. (The interesting fact is that they do exist for mixing systems). The Einstein-Kubo type formulae for transport coefficients can therefore be mathematically meaningful only in the thermodynamic limit. It is of course possible, and even likely, that for macroscopic systems there exists values of T for which the integral in (4.7) is 'close' to the diffusion constant.

V. K- AND BERNOUILLI SYSTEMS

In order to give a physical definition of these systems we define a finite partition of the energy surface S of our dynamical system as any finite collection of n non-overlapping regions R_0, \dots, R_k which together cover the whole of S (see Fig. 5).



$$\sum \mu(R_i) = 1, \quad \mu(R_i \cap R_j) = 0.$$

Figure 5.

Suppose now that an experiment is made that will determine which of these regions the phase point is in at any time, but gives no information whatever about which part of the region it is in. That is, every time we use this measuring device we obtain an outcome that is a positive integer - the label of the region the phase point of the system is in at that time. As an example we may consider a system of k particles in a box and the experiment consists of measuring the number of particles in one half of the box.

Suppose we use the device repeatedly at intervals of, say, τ seconds. Its outcome will be a sequence of positive integers from the set $\{0, \dots, k\}$, which can be extended indefinitely. In general, we would expect these integers to be correlated; that is, the microcanonical probability for each new observation depends on what has been observed before (as in a Markov process, for example). This correlation comes about because the dynamical states of the system at different times are deterministically related, through the equations of motion. Indeed, it may be possible to choose the partition and the time intervals between measurements in such a way that the outcome of later measurements is completely determined by the outcome of the earlier ones. That this is possible even in the case of ergodic systems may be seen easily by considering the simple harmonic oscillator considered earlier and making the interval between measurements equal to the period τ . The oscillator will then be found each time in the same set R_i , since $\phi_\tau R_j = R_j$ for a system with period τ .

It should be clear however from our earlier discussion that such a deterministic behaviour of successive measurements is impossible

for a mixing system. For in a mixing system each set R_i will eventually become uniformly spread out over the whole energy surface, i.e.

$$\lim_{n \rightarrow \infty} \mu[(\phi_{nz}(R_i) \cap R_j)] = \mu(R_i)\mu(R_j),$$

for every value of z . It might still be possible however that successive measurements provide more and more information so that eventually one really knows what the result of the next measurement will be. Somewhat more formally we may let $\epsilon(n)$ be the uncertainty in the outcome of the n -th measurement (given the results of the first $n-1$ measurements). A K-system is then a system for which $\epsilon(n) \geq \epsilon > 0$ no matter how large n is and no matter what the partition, or z , is. For a system which is only mixing there will be partitions for which $\epsilon(n) \rightarrow 0$ as $n \rightarrow \infty$. It is, in this sense, that K-systems have an essential randomness in them.

This will be made more precise in the next section when we discuss the Kolmogorov-Sinai entropy of a flow. First however I shall discuss the last and highest member of our hierarchy: the Bernoulli system. This will also give me the opportunity to introduce to you the paradigm of Bernoulli systems; the baker's transformation.

A Bernoulli system is one for which it is possible to choose the regions R_0, \dots, R_{n-1} in such a way that the observations made at different times are completely uncorrelated, just like the numbers shown at different times by a roulette wheel. At the same time, the regions so chosen give enough information to discriminate between dynamical states: if two systems have different dynamical states at some time, then the observations made on them cannot yield identical results for the observations at every time. Such a partition is called a generating partition. When such regions can be chosen, we call the system a Bernoulli system, i.e. a Bernoulli system permits the construction of an independent generating partition. There is of course no requirement, and indeed no possibility, that all partitions be of this type. Since however a Bernoulli system is also a K-system, every partition will have the inherent randomness associated with K-systems which we discussed earlier.

Recently Gallavotti and Ornstein showed that a point particle moving (in two or higher dimensions) among fixed convex scatterers (in a box with rigid walls or on a torus; periodic boundary conditions) is a Bernoulli system. (More precisely a Bernoulli flow, which means that there exists an independent generating partition

for every $\tau > 0$). The proof of Gallavotti and Ornstein utilizes the results of Sinai that this system is a K-system as well as the techniques developed by Ornstein and Weiss who showed that the geodesic flow on a space of constant negative curvature is Bernoulli.

5.1 The baker's transformation

As an illustration of a simple Bernoulli system, consider a system whose phase space is the square $0 < p \leq 1$, $0 < q \leq 1$ shown in Figure 6, and whose (non-Hamiltonian) law of motion is given by a mapping known as the baker's transformation because it recalls the kneading of a piece of dough.

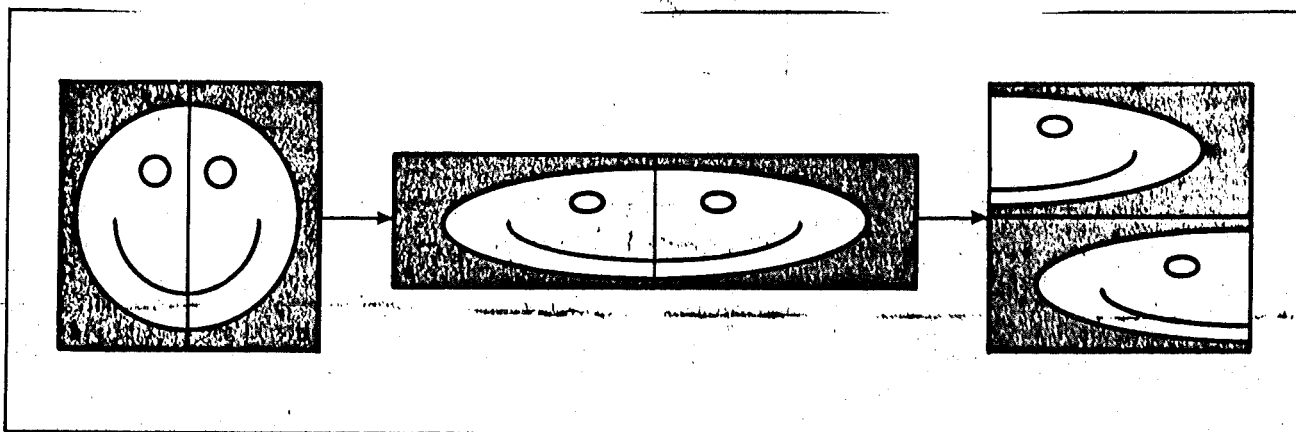


Fig. 6. The baker's transformation recalls the kneading of a piece of dough.

We first squash the square to half its original height and twice its original width, and then cut the resulting rectangle in half and move the right half of the rectangle above the left.

If the phase point is (p, q) at time t , then at time $t + 1$ it is at the point obtained by squashing the square to a $(1/2 \times 2)$ rectangle, then cutting and reassembling to form a new square as shown in the diagram. The formula for this transformation is

$$\phi(p, q) = \begin{cases} (2p, q/2) & \text{if } 0 \leq p \leq 1/2 \\ [2p - 1, q/2 + 1/2] & \text{if } 1/2 < p \leq 1. \end{cases} \quad (5.1)$$

If p and q are written in binary notation ($1/8$ in binary notation is $0.00100 \dots$, $1/4$ is 0.01000 , and so on), the transformation removes the first digit after the binary point from p and attaches it to q , so that

$$\phi(0.p_1p_2 \dots, 0.q_1q_2 \dots) = (0.p_2p_3 \dots, 0.p_1q_1q_2 \dots)$$

where the p_i and q_i take on the values 0 and 1. This transformation is invertible and from it we can define ϕ_{-1} as the inverse of ϕ and $\phi_{\pm t}$ as the t -th iteration of $\phi_{\pm 1}$. (Only integer values of the time are used here, rather than all real values, as in our discussion of dynamics earlier in this talk, but we do not regard this distinction as important.) Moreover, the transformation preserves geometrical area, and so the analog of the microcanonical distribution is just a uniform density.

To see how this completely deterministic system can at the same time behave like a roulette wheel, we take the regions R_0 and R_1 to be the two rectangles $0 \leq p < 1/2$, $1/2 \leq p < 1$ as shown in Fig. 7.

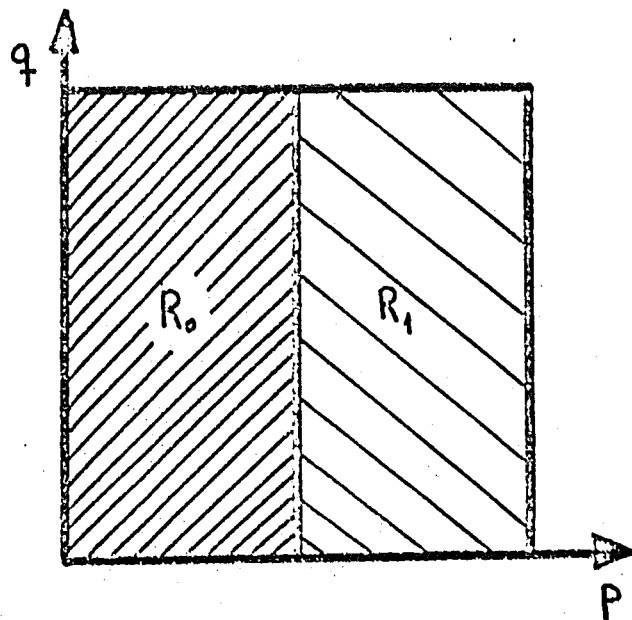


Fig. 7. Definition of the regions R_0 and R_1 used to show that the baker's transformation is a Bernoulli system.

Suppose the phase point at time 0 is

$$(p, q) = (0.p_1p_2 \dots, 0.q_1q_2 \dots)$$

If p_1 is zero, the system at time 0 is in R_0 ; if p_1 is one, the system at time 0 is in R_1 . At time 1 the phase point is

$$(0.p_2p_3 \dots, 0.p_1q_1q_2 \dots)$$

and so we observe the phase point in region R_{p_2} . At time 2 it is in R_{p_3} and so on. Likewise, at time -1 it is in R_{q_2} , at time -2 in R_{q_1} , and so on. Each observation is determined by a different digit in the binary representation of the number pair (p,q) .

Since the analog of the microcanonical ensemble for this system has a uniform density in the square it is not difficult to see that the microcanonical probability of each of these digits in the binary expression for (p,q) is $1/2$, and is uncorrelated with all the other digits. The observations made at different times t ($=$ integer) are therefore uncorrelated, and so the baker's transformation model is a Bernoulli system.

The baker's transformation is an example of a Bernoulli shift. Let ξ denote a point in the space of doubly infinite sequences $\xi_i \in (0, 1)$, with i an integer (positive, negative or zero). We set $\xi_i = p_{i+1}$ for $i \geq 0$, and $\xi_i = q_{-i}$ for $i < 0$. The ξ specifies a point in the unit square

$$\xi = (\dots \xi_{-1}, \xi_0, \xi_1, \dots)$$

and the baker's transformation is simply the shift

$$(\theta \xi)_i = \xi_{i+1}$$

Possibly one should not read too much physical meaning into this type of result, for with a more complicated dynamical system the regions $R_0, R_1, R_2, \dots, R_n$ would probably be exceedingly complicated sets in phase space, but from a "philosophical" point of view it is very interesting to see how the same dynamical system can show perfect determinism on the microscopic level and at the same time perfect randomness on a "macroscopic" level.

It is the interplay of these two apparently incompatible levels of description that give the foundations of statistical mechanics their fascination.

5.2 The Kolmogorov-Sinai entropy

We consider as before a partition of the energy surface S into k disjoint cells A_i , $i = 1, \dots, k$. (This is a slight

change in notation). This collection of sets $\{A_i\}$ is called a partition \mathcal{A} , $\mathcal{A} = \{A_i\}$; the A_i are the 'atoms' of \mathcal{A} . Since $\mu(A_i)$ is the probability (in the microcanonical ensemble) of finding the system in A_i , Kolmogorov defined the 'entropy' (not to be confused with the thermodynamic entropy) of this partition $h(\mathcal{A})$, in analogy with information theory entropy, as

$$h(\mathcal{A}) = -\sum \mu_0(A_i) \ln \mu_0(A_i) ,$$

Clearly, $h(\mathcal{A}) \geq 0$, with the equality holding if and only if $\mu_0(A_j) = 1$, for some j , i.e., there is complete certainty that $x \in A_j$. (We shall generally ignore sets of measure zero, setting $\mu_0(C) \ln \mu_0(C) = 0$ if $\mu_0(C) = 0$, and writing $A_j = S_E$ when $\mu_0(A_j) = 1$.) The maximum value which $h(\mathcal{A})$ can take is $\ln k$ corresponding to $\mu_0(A_i) = k^{-1}$ for all $i = 1, \dots, k$.

Given two partitions $\mathcal{A} = \{A_i\}$, $i = 1, \dots, k$ and $\mathcal{B} = \{B_j\}$, $j = 1, \dots, m$, we denote the 'sum' of the partitions \mathcal{A} and \mathcal{B} by $\mathcal{A} \vee \mathcal{B}$; $\mathcal{A} \vee \mathcal{B}$ is the partition whose atoms are all (non-zero measure) sets $A_i \cap B_j$. The entropy of $\mathcal{A} \vee \mathcal{B}$ is,

$$h(\mathcal{A} \vee \mathcal{B}) = \sum_{i,j} \mu(A_i \cap B_j) \ln \mu(A_i \cap B_j) .$$

The 'conditional entropy' of a partition \mathcal{A} , relative to a partition \mathcal{B} is defined as

$$h(\mathcal{A}/\mathcal{B}) = \sum_j \mu(B_j) \left\{ \sum_i \mu(A_i/B_j) \ln \mu(A_i/B_j) \right\} ,$$

where

$$\mu(A_i/B_j) \equiv \mu(A_i \cap B_j) / \mu(B_j) .$$

For a given flow operator ϕ_t , and some fixed time interval τ , we construct the sets $\phi_1 A_i, \phi_2 A_i, \dots$ and define $\phi_\tau \mathcal{A}$ as the partition whose atoms are the sets $\{\phi_\tau A_i\}$. Kolmogorov then sets

$$h(\mathcal{A}, \phi_\tau) = \lim_{n \rightarrow \infty} \frac{1}{n} h\left(\bigvee_{j=0}^{n-1} \phi_{j\tau} \mathcal{A}\right) .$$

It can be shown that $h(\mathcal{A}, \phi_{j\tau}) = jh(\mathcal{A}, \phi_\tau)$. The K-S entropy of the flow ϕ_τ is defined as (S for Sinai)

$$h(\phi_\tau) = \sup_{\mathcal{A}} h(\mathcal{A}, \phi_\tau) = h\tau ,$$

where h is now an intrinsic property of the flow. It was shown by Sinai that a system is a K-system iff $h(\Lambda, \phi_\tau) > 0$ for all non-trivial partitions Λ , i.e., for partitions whose atoms are not all of measure zero or one.

We can now specify the precise sense in which K-systems are 'random' even when the flow is entirely deterministic. As indicated earlier the atoms of the partition Λ , $\{A_i\}$, $i = 1, \dots, k$, correspond to different possible outcomes of the measurement of some dynamical function $f(x)$, i.e. if $x \in A_i$ then the result of the measurement will be α_i , etc. (Since the set of outcomes of the measurement is finite, being equal to k , $k < \infty$, the measurement is a 'gross' one. It need now however be restricted to measuring just one property of the system; we can replace $f(x)$ by a finite set of functions.) The probability (in the microcanonical ensemble) of an outcome α_i is $\mu_0(A_i) \equiv p(\alpha_i)$. Now if these dynamical functions were measured first at $t = -\tau$, and then at $t = 0$, the joint probability that the result of the first measurement is α_j and the result of the second is α_i , is equal to the probability that the dynamical state of the system x at the time of the present measurement $t = 0$ is in the set $A_i \cap \phi_\tau A_j$, i.e., $p(\alpha_i, \alpha_j) = \mu_0(A_i \cap \phi_\tau A_j)$. The conditional probability of finding the value α_i , if the result of the previous measurement was α_j , is $p(\alpha_i/\alpha_j) = \mu(A_i \cap \phi_\tau A_j) / \mu(\phi_\tau A_j) = \mu(A_i \cap \phi_\tau A_j) / \mu(A_j)$. In a similar way the probability of finding the result α_i at $t=0$, given that the results of the previous measurements at times $-\tau, -2\tau, \dots, -n\tau$ were $\alpha_{i_1}, \alpha_{i_2}, \dots, \alpha_{i_n}$,

$$p(\alpha_i/\alpha_{i_1}, \dots, \alpha_{i_n}) = [\mu(A_i \cap \phi_{\tau} A_{i_1} \dots \cap \phi_{n\tau} A_{i_n}) / \mu_0(\phi_{\tau} A_{i_1} \cap \phi_{\tau} A_{i_2} \dots \cap \phi_{n\tau} A_{i_n})].$$

It can be readily shown that

$$h(\Lambda, \phi_\tau) = \lim_{n \rightarrow \infty} h(\Lambda / \bigvee_{k=1}^n \phi_{k\tau} \Lambda) = \lim_{n \rightarrow \infty} \left\{ -\sum p(\alpha_{i_1}, \alpha_{i_2}, \dots, \alpha_{i_n}) \times \left[\sum_{i=1}^k p(\alpha_i/\alpha_{i_1}, \dots, \alpha_{i_n}) \ln p(\alpha_i/\alpha_{i_1}, \dots, \alpha_{i_n}) \right] \right\}.$$

Hence $h(\Lambda, \phi_\tau) > 0$ for all non-trivial partitions implies

that no matter how many measurements of the values of $f(x)$ we make on a system at times, $-\tau, \dots, -n\tau$, the outcome of the next measurement is still uncertain. (N.B. the measurements are 'coarse' since $\mu(A_i) > 0$).

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VI. ERGODIC PROPERTIES AND SPECTRUM OF THE INDUCED UNITARY TRANSFORMATION

It is possible, and for many purposes useful, to consider the Hilbert space L^2 of square integrable functions on the energy surface S (Koopman). The integration here is again with respect to the microcanonical ensemble density dx ; $\psi(x) \in L^2$ is a complex valued function of $x \in S$, such that

$$\int_S |\psi|^2 dx < \infty.$$

The time evolution ϕ_t then induces a transformation U_t in L^2 ,

$$U_t \psi(x) = \psi[\phi_t(x)]$$

which is unitary.

$$\int |U_t \psi|^2 dx = \int |\psi|^2 dx.$$

We may therefore write $U_t = \exp[itL]$ where iL is the generator of U_t . For a Hamiltonian flow with $H = H(q_1, \dots, q_n, p_1, \dots, p_n)$ iL is the Liouville operator or Poisson bracket

$$iL f = (f, H) = \sum_i \left[\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right].$$

There is an intimate connection between the ergodic properties of the flow and the spectrum of U_t which is of the form $\exp(it\lambda)$, with λ in the spectrum of L . Clearly $\lambda = 0$ is always a discrete eigenvalue of L corresponding to the eigenfunction $\psi = \text{const.}$

The following equivalences and implications can be shown to hold:
 K-property \Rightarrow absolute continuity of the spectrum of L with respect to Lebesgue measure (on the space orthogonal to the constants) \Rightarrow mixing \Rightarrow continuity of the spectrum \Leftrightarrow weak mixing \Rightarrow

ergodicity $\Leftrightarrow \lambda = 0$ is a simple eigenvalue.

This may be a good place to note that, due to the discrete nature of the energy spectrum for finite quantum systems confined to a bounded domain V , there will be no mixing (decay of correlations) in such a system. For such quantum systems we do not therefore gain anything from the use of ensembles and we are forced to look at the infinite volume limit for signs of long time irreversibility. The remarkable thing about Sinai's result for hard spheres is that it shows that finite classical systems can and do have purely continuous spectra. (Note that when Planck's constant $h \rightarrow 0$ the number of energy levels between some fixed E and $E + \Delta E$ becomes infinite.)

VII. INFINITE SYSTEMS

Since the number of particles contained in a typical macroscopic system is very large ($\sim 10^{26}$) there is great interest from the point of view of statistical mechanics in the ergodic properties of infinite systems (corresponding to the thermodynamic limit in equilibrium statistical mechanics). As I indicated in the introduction, there are still some serious conceptual problems about the nature of the ingredients, in addition to ergodic theory, which are necessary to get the right physics. I shall therefore be extremely brief here.

The natural setting for this discussion is the more abstract form of ergodic theory. This theory deals typically with the triplet (X, μ, ϕ_t) , X is a space equipped with a measure μ which is left invariant by ϕ_t . (I have left out explicit mention of Σ the collection of measurable sets). ϕ_t is a flow if t is a real variable and a discrete transformation if t is an integer (in which case $\phi_n = \phi^n$ and we can write the triplet as (X, μ, ϕ)). The triplet (X, μ, ϕ_t) is usually referred to as the dynamical system.

In our discussion of finite Hamiltonian systems we had $X = S_E$, μ = microcanonical measure (ensemble), and ϕ_t the time evolution given by the solution of the Hamiltonian equations of motion. All our analysis can be easily translated to the more general setting. Thus we say that the dynamical system (X, μ, ϕ_t) is ergodic if for any set $A \subset X$, which is left invariant by ϕ_t , $\mu(A) = 0$ or $\mu(A) = 1$. Equivalently (X, μ, ϕ_t) is ergodic if there does not exist another measure μ' , which is absolutely continuous with respect to μ , and is also invariant under ϕ_t .

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We say that μ' is absolutely continuous with respect to μ if $\mu(A) = 0 \Rightarrow \mu'(A) = 0$. When μ' is absolutely continuous with respect to μ we can write $d\mu' = \rho(x)d\mu$, i.e. μ' has an 'ensemble density' with respect to $d\mu$.

It should now be clear what is involved in the ergodic theory of infinite systems: X will be the space of infinite configurations (locally finite), μ will be some stationary measure under the time evolution ϕ_t assuming this can be suitably defined. It may now be much more difficult to justify a priori the use of the Gibbs measure (at a given temperature and chemical potential) and those absolutely continuous with respect to it as the only physically suitable measures (assuming there are also other stationary measures available) than it was to argue in the finite system for the use of ensembles with ensemble densities. I will leave the discussion of this to Professor Haag and only refer you now to Table 1 for some of the results known for infinite systems.

Acknowledgements

As already indicated, parts of these lecture notes come from my article with O. Penrose in Physics Today.

Appendix: Ergodic properties of simple model system with collisions

We are interested in the ergodic properties of dilute gas systems. These may be thought of as Hamiltonian dynamical systems in which the particles move freely except during binary "collisions". In a collision the velocities of the colliding particles undergo a transformation with "good" mixing properties (cf. Sinai's study of the billiard problem). To gain an understanding of such systems we have studied the following simple discrete time model: The system consists of a single particle with coordinate $\underline{r} = (x, y)$ in a two-dimensional torus with sides of length (L_x, L_y) , and "velocity" $\underline{v} = (v_x, v_y)$, in the unit square $v_x \in [0, 1]$, $v_y \in [0, 1]$. The phase space Γ is thus a direct product of the torus and the unit square. The transformation T which takes the system from a dynamical state $(\underline{r}, \underline{v})$ at "time" j to a new dynamical state $T(\underline{r}, \underline{v})$ at time $j+1$ may be pictured as resulting from the particle moving freely during the unit time interval between j and $j+1$ and then

*From paper by S. Goldstein, O.E. Landford III and J.L. Lebowitz.

undergoing a "collision" in which its velocity changes according to the baker's transformation, i.e.

$$T(\underline{r}, \underline{v}) = (\underline{r} + \underline{v}, B\underline{v})$$

with B the baker's transformation defined in Section 5,

$$B(v_x, v_y) = \begin{cases} (2v_x, \frac{1}{2}v_y), & 0 \leq v_x \leq \frac{1}{2} \\ (2v_x - 1, \frac{1}{2}v_y + \frac{1}{2}), & \frac{1}{2} < v_x \leq 1. \end{cases}$$

The normalized Lebesgue measure $d\mu = dx dy dv_x dv_y / L_x L_y = d\underline{r} d\underline{v} / L_x L_y$ in Γ is left invariant by T . We call U_T the unitary transformation induced by T on $L^2(d\mu)$, $U_T \phi = \phi \circ T$. Our interest lies then in the ergodic properties of T and in the spectrum of U_T .

We note first that the transformation B on the velocities is, when taken by itself as a transformation of the unit square with measure $d\underline{v}$, well known to be isomorphic to a Bernoulli shift. It therefore has very good mixing properties.

The ergodic properties of our system which combines B with free motion turn out to depend on whether L_x^{-1} and L_y^{-1} satisfy the independence condition (I),

$$n_x L_x^{-1} + n_y L_y^{-1} \notin \mathbb{Z} \text{ for } n_x \text{ and } n_y \text{ integers} \\ \text{unless } n_x = n_y = 0. \quad (I)$$

Theorem 1: When (I) holds, the spectrum of U_T , on the complement of the one-dimensional subspace generated by the constants, is absolutely continuous with respect to Lebesgue measure and has infinite multiplicity.

It follows from Theorem 1 that when (I) holds the dynamical system (Γ, T, μ) is at least mixing. We do not know at present whether it is also a Bernoulli shift or at least a K system.

Theorem 2: When (I) does not hold the system (Γ, T, μ) is not ergodic.

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