

CHAOS, PSEUDOCHAOS, AND QUANTUM CHAOS
IN NON-EQUILIBRIUM STATISTICAL MECHANICS*

J.R. DORFMAN

Institute for Physical Science and Technology
Department of Physics, University of Maryland
College Park, MD, 20742, USA*(Received February 22, 2006)*

The purpose of these lectures is to review some of the recent work devoted to understanding the microscopic foundations of irreversible behavior in fluid systems. We begin by considering the properties of systems whose microscopic dynamics is chaotic. Our goal is to show that, for simple model systems, one can understand the approach of a sufficiently smooth initial phase space distribution to an equilibrium state, or more properly, to a local equilibrium state, without the need to introduce stochastic elements into the description of the system's dynamics. To follow this argument one needs to understand some of the basic ideas of dynamical systems theory as applied to chaotic systems. We first consider the notions of ergodicity and mixing, and discuss the extent to which these ideas really might be applied to systems of large numbers of particles. Then we broaden the discussion to describe the behavior of hyperbolic dynamical systems with exponential separation of infinitesimally close phase space trajectories. These systems are characterized by stable and unstable manifolds, and nonzero Lyapunov exponents. We will briefly touch upon such topics as SRB measures, entropy production and the relations between transport coefficients and properties of the underlying microscopic chaotic behavior of the phase space trajectories of the system. We illustrate these ideas as well as their application to transport theory with several simple models, among them the baker and multi-baker maps. In the second part of these lectures we consider the fact that microscopic chaos is neither necessary nor sufficient for good transport properties. This will lead to a brief discussion of classical systems that are *pseudochaotic*. These are systems with zero Lyapunov exponents, but with some microscopic properties that are similar to those of chaotic systems, including the separation, in time, of nearby phase space trajectories. However for pseudochaotic systems the separation is proportional to some power of time rather than exponential. The third and final part of these lectures is devoted to a consideration of transport in a quantum version of the simple model discussed in the first part, the multi-baker map. The quantum version shows quite different behavior and we conclude the lectures with a brief description of the transition from quantum to classical behavior in the semi-classical limit.

PACS numbers: 05.45.Df, 05.60.-k, 05.70.Ln

* Lectures given at the First Warsaw Summer School on Statistical Physics, Kazimierz-Dolny, June, 2005.

1. Introduction

The study of statistical mechanics has always involved both an examination of its foundations as well as the devising of methods to compute thermodynamic, transport, and related quantities for systems of large numbers of particles. In recent years there has been a great deal of attention focused on the foundations of statistical mechanics prompted by developments in: (i) dynamical systems theory, particularly chaotic dynamics, (ii) the mathematics of Anosov and hard-ball systems, and (iii) the computational physics of systems of particles undergoing non-equilibrium processes of various kinds [1–4]. Moreover, modern developments in quantum physics, particularly those of some relevance for quantum computation have some relation to the foundations of quantum statistical mechanics as well [5, 6]. Here we will review some of the new developments and understandings of the foundations of statistical mechanics, and describe some of the mathematical notions needed to understand them. Our focus will be on the foundations of classical statistical mechanics. The question that will be addressed is to what extent the randomness needed to drive a system to thermodynamic equilibrium is contained in the microscopic dynamics of the constituent particles. We will consider some simple model systems, known as baker maps, multi-baker maps, and cat maps to illustrate some of the answers available for systems with *chaotic* dynamics. However, one can argue that chaotic dynamics is neither necessary nor sufficient for the appearance of good non-equilibrium properties. This leads us into a discussion of systems that are *pseudochaotic* [7, 8]. In the concluding section of the lectures, we will discuss some of the relevant issues for the quantum mechanical versions of classically chaotic systems. These issues can be illustrated using the quantum version of the multi-baker map [9].

The plan of the paper is as follows. In the next section we will discuss the notions of *ergodicity* and of *mixing*, as introduced by Boltzmann and Gibbs, respectively [10–12]. We then assess their importance for the foundations of statistical mechanics and describe the arguments which show that these notions, taken in isolation, are insufficient to provide the necessary foundations for classical statistical mechanics. In Section 3 we will present a more refined picture which may be of greater relevance for statistical mechanics, but which also places strong demands on the underlying microscopic dynamics of the system. In Section 4, we will describe some applications of the theory described in Section 3 to a deeper understanding of transport in non-equilibrium systems and of non-equilibrium stationary states. In Section 5 we will define and discuss pseudochaotic systems and describe some of their features which are relevant for statistical mechanics. In Section 6 we turn our attention to quantum systems and consider the quantum multi-

baker map which shows a nice transition from classical diffusive transport to quantum mechanical ballistic transport as a function of time, in the semi-classical limit, as $\hbar \rightarrow 0$. We conclude with a summary and brief discussion of interesting open problems.

2. Ergodic and mixing systems

2.1. Ergodic systems

As is well known, Boltzmann invented the notion of ergodicity in an attempt to provide a mechanical foundation for the approach of a system composed of many particles to equilibrium. His aim was to reconcile the apparently irreversible approach to thermodynamic equilibrium for many-particle systems with the microscopic reversibility of the underlying equations of motion, which, for Boltzmann, were Newton's laws of mechanics. Boltzmann argued as follows: Consider an isolated system of particles with some total energy E . The dynamics of this system of particles can be represented as a trajectory of a point in a multi-dimensional phase space, Γ , with coordinate axes associated with the canonical position and momenta for each of the degrees of freedom of the system. For an isolated system, the system's trajectory will be confined to an appropriate constant energy surface in Γ . Boltzmann suggested that thermodynamic equilibrium for a mechanical system could be understood purely by mechanical arguments if one can verify an *ergodic hypothesis*: Over a long time interval T , the phase space trajectory of the system spends a fraction of time T in any region of phase space, A , with measure $\mu(A)$ that is equal $\mu(A)$ divided by the total measure of the constant energy surface, assumed to be finite. Here $\mu(A)$ is the standard phase space measure on a constant energy surface given by

$$\mu(A) = \int_A \frac{dS}{|\nabla H|}, \quad (1)$$

where dS is the area of an infinitesimal region of the constant energy surface, and $|\nabla H|$ is the magnitude of the gradient of the Hamiltonian function for the system at the point of integration. Boltzmann's ergodic hypothesis can be stated as

$$\lim_{T \rightarrow \infty} \frac{\tau(A)}{T} = \frac{\mu(A)}{\mu(\mathcal{E})}. \quad (2)$$

Here $\tau(A)$ is the amount of time the system spends in region A during a time interval T , and $\mu(\mathcal{E})$ is the measure of the entire constant energy surface. If one accepts the hypothesis, then one can easily show that the *time average* of any well behaved dynamical quantity approaches its microcanonical ensemble average as the time interval over which the average is taken

approaches infinity [2]. The microcanonical ensemble average is, of course, the equilibrium average that forms the basis of statistical thermodynamics. Boltzmann's hypothesis holds equally well if one considers the time reversed motion of the system, so that it is consistent with the reversibility of the microscopic dynamics.

Boltzmann's hypothesis does not tell us if a given system is ergodic or not. Moreover, even if a system is ergodic, the hypothesis does not tell us how long we will have to wait until the time average is reasonably close to the ensemble average. Moreover, the ergodicity of a system may be more than we actually need to validate the application of statistical mechanics to it. We will return to these issues below, but for the moment let us consider the problems involved in proving that a given system of interest to physicists is ergodic. The kinds of elementary physical systems one studies in physics courses, such as coupled systems of several harmonic oscillators, are generally not ergodic, although some simple systems can be shown to be ergodic. A simple example is the motion of a point particle on the circumference of a circle, where the particle moves a fixed irrational fraction of the length of the circumference at successive time steps. In the long time limit, the circumference is uniformly covered by points visited by the particle [10, 11]. A great deal of mathematical research over the past few decades has been devoted to a study of more complicated ergodic systems. The first dramatic example of a system with ergodic properties, and one that has influenced most of the more recent efforts in this direction is the geodesic motion of a point on a surface of constant negative curvature. This motion was proved to be ergodic by Hopf [13], and the techniques employed remain useful today. Sinai and coworkers, as well as many other workers, have given careful mathematical proofs of ergodic behavior of various systems composed of hard disks or hard spheres, generally referred to as hard-ball systems [14, 15]. However, Turaev and Rom-Kedar [16] have shown that by slightly softening the hard sphere potential one may change an ergodic system into a non-ergodic one. It might very well be that the measure of the "non-ergodic" region of phase space is only a very small fraction of the total measure, and not important physically, but it is clear that there are many mathematical issues yet to be resolved, independent of the utility of ergodic theory for physics.

2.2. *Mixing systems*

Gibbs introduced the stronger notion of a *mixing system* in his efforts to understand why averages, taken over some non-equilibrium ensemble, might be expected to approach equilibrium averages in the course of time. This issue was raised once the founders of statistical mechanics realized that

statistical mechanics could be used to treat even non-equilibrium systems, and to provide a microscopic derivation of the macroscopic equations of fluid dynamics, for example. In considering a non-equilibrium ensemble one has to follow the trajectories of a set of points in phase space, not just a typical trajectory, as in the study of ergodic behavior. Gibbs suggested that the an initial set of points might spread out over the entire available phase space in the course of time, and become finely mixed throughout the phase space. Of course, the measure of phase space occupied by the set of points should remain constant in time, but the set might eventually get uniformly distributed over the constant energy surface. In such a case, a coarse grained observation of the phase space would lead to the conclusion that the set uniformly covers the energy surface, while a fine grained observation would reveal that the coverage consists of a long, thin set of total measure equal to that of the initial set. A nice picture of such behavior is provided by a laboratory demonstration where one follows the motion of a drop of ink in a container of glycerine which is stirred until the ink appears to be uniformly mixed through the bottle of glycerine. If one reverses the stirring mechanism one sees the ink return to the initial drop, and if one then continues the “reversed” stirring, one still sees the ink become uniformly distributed in the glycerine. That is, the mixing takes place both for the forward and the time reversed motion.

The mathematical definition of a mixing system is given by looking at the time development of the initial set of phase points. We denote by A , the initial set of phase points on which the initial ensemble is concentrated, and the set to which this initial set evolves after a time T , by A_T . Then, to examine the mixing of the set in phase space, we consider some arbitrary set of positive measure B and consider the intersection $B \cap A_T$. If the dynamics of the system is mixing, then eventually the fraction of A_T in the set B should approach the fraction of A in the entire phase space, no matter what set of positive measure A and B we consider. That is, a system is mixing if for any sets A and B of positive measure [10–12]

$$\lim_{T \rightarrow \infty} \frac{\mu(A_T \cap B)}{\mu(B)} = \frac{\mu(A)}{\mu(\mathcal{E})}. \quad (3)$$

Here we used the conservation of phase space measure, namely that $\mu(A) = \mu(A_T)$. One can easily prove that a mixing system is also ergodic, but the reverse is not true. A counterexample is provided by the irrational translation of points on the circumference of a circle discussed earlier. If one considers the motion of a set of points on the circle, the set moves rigidly without spreading. Then the limit on the left hand side of Eq. (3) does not exist, and the system is not mixing.

The important physical consequence of the mixing character of a system of particles is that for such systems one can show that non-equilibrium averages of sufficiently smooth functions approach their equilibrium averages in the course of time [2]. Of course this is true of both the forward as well as the time reversed motion, so there is no conflict with the reversibility of the equations of motion. Therefore one might argue that a proof that a system is mixing is equivalent to proving that the methods of non-equilibrium statistical mechanics apply to such systems.

Mathematicians have considered proofs of the mixing property for various systems of interest to physicists. The most important systems studied so far are hard ball systems mentioned above, where the proofs of ergodicity and mixing are consequences of proving a stronger dynamical property, the Bernoulli property of the system, which implies that the system is mixing and therefore ergodic as well [14]. We leave a proper definition of a Bernoulli system to the literature and we will not consider it any further here [10, 12]. Needless to say, the class of systems which can be proved to be mixing is not yet large enough to encompass the typical systems studied in statistical mechanics or in kinetic theory, although considerable progress has been made in this direction over the past several years.

2.3. Are these notions — ergodicity and mixing — relevant for statistical mechanics?

It would appear that with the proof that a system of a large number of particles in a reasonable container is mixing, the foundation for the applications of statistical mechanics to such a system would be secure. That this is not entirely correct may be seen for the following reasons, among others: (1) We have assumed that our systems are isolated from the rest of the universe and not subjected to external forces. This is clearly an idealization, and we know that it is not true of any laboratory system. (2) We have not examined how long it might take for the time average to be reasonably close to the ensemble average for an ergodic system or how long it would take a reasonable initial set to get uniformly mixed over the appropriate phase space, for a mixing system. One can argue that the appropriate times can indeed be very long, typically much longer than the duration of an experiment. (3) We have used classical mechanics as our description of dynamics in natural processes, while we know that nature is fundamentally quantum mechanical. Thus we conclude that the notions of ergodicity and mixing, in the form suggested by Boltzmann and Gibbs, are not directly relevant for physics, although in some modified form they might well be useful.

In the following sections we will address point (2) in some detail, and point (3), briefly. It is important to note, however, that the answers we

shall provide are very incomplete and much more work needs to be done to make these answers believable and secure. Here we consider point (1). It seems clear that external influences on a system of particles should, in general, make the system behave rather more randomly than it might if it were isolated. The question that needs to be asked of any given system is whether the underlying dynamics of the system is capable by itself of providing a mechanism for the approach to equilibrium or whether some source, external to the dynamics itself, is necessary for the achievement of a macroscopic equilibrium state. It is not unreasonable to expect that both the internal microscopic dynamics of a system as well as external “noise” both play a role in driving systems to equilibrium, and it is our job to try to disentangle these different sources of irreversibility. Certainly, external influences on a dynamical system could justify the use of ensembles for describing the average behavior of a system of particles, particularly if these influences are both sufficiently small and random. The success of stochastic theories for describing many physical phenomena suggests that the random nature of the interaction of a system with its environment is an important component of the dynamics of these systems. In these lectures we will take another point of view in order to see if there are aspects of the microscopic dynamics of physical systems that might be used to account for the approach of these systems to an equilibrium state.

3. Anosov and Anosov-like systems

In order to formulate a response to point (2) above, it is helpful to consider some simple model systems that display the kind of irreversible behavior that we would like to be able to describe for more realistic, many particle systems. Two model systems which are useful in this regard are the baker’s map and the Arnold cat map, which itself is an example of more general models called hyperbolic toral automorphisms [12]. We will explain this terminology as we proceed.

The baker’s map is a map from a two dimensional “unit square”, $0 \leq x, y \leq 1$ onto itself, given by (see Fig. 1)

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 2x \\ \frac{y}{2} \end{pmatrix} \quad \text{for } 0 \leq x \leq \frac{1}{2}; \quad \text{and} = \begin{pmatrix} 2x - 1 \\ \frac{(y+1)}{2} \end{pmatrix} \quad \text{for } \frac{1}{2} < x < 1. \quad (4)$$

This map consists of a stretching of the square in the x -direction by a factor of 2, and squeezing in the y -direction by a factor of $1/2$, but the area is preserved. The elongated image of the unit square is then cut in half and the right side is put on top of the left side so that a unit square is reconstructed, after each application of the map [13].

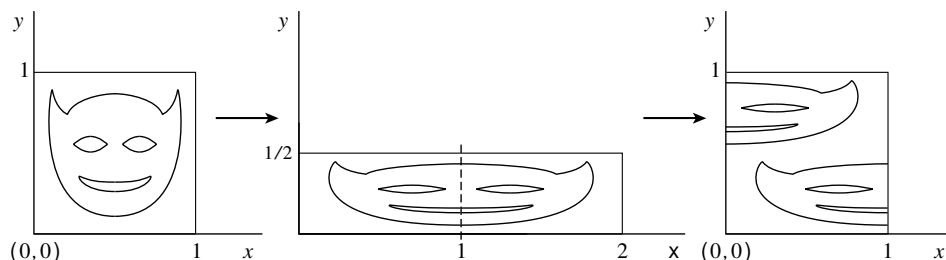


Fig. 1. The baker's transformation.

We now regard the unit square as a “toy” phase space of two dimensions and apply some of the usual techniques of statistical mechanics. The Liouville equation for the motion of any initial distribution of points on this unit square is easily seen to be a simple discretization of the familiar Liouville equation from statistical mechanics, and it takes the form

$$\rho_n(x, y) = \begin{cases} \rho_{n-1}\left(\frac{x}{2}, 2y\right) & \text{for } 0 \leq y \leq \frac{1}{2}, \\ \rho_{n-1}\left(\frac{x+1}{2}, 2y-1\right) & \text{for } \frac{1}{2} < y < 1. \end{cases} \quad (5)$$

Since we are doing statistical mechanics, we can use the fact that we are never interested in the full phase space distribution function, but rather reduced distribution functions of fewer variables. Here there are only two variables, so we consider the reduced distribution function, $W_n(x)$ obtained by integrating $\rho_n(x, y)$ over the y coordinate. Using Eq. (5), we obtain the equation [2, 17]

$$W_n(x) = \frac{1}{2} \left[W_{n-1}\left(\frac{x}{2}\right) + W_{n-1}\left(\frac{x+1}{2}\right) \right]. \quad (6)$$

The remarkable thing about this equation is that if one assumes that the initial value, $W_0(x)$, of the reduced distribution function is a reasonably smooth function of x , then it is easy to show that $W_n(x)$ approaches a constant value as $n \rightarrow \infty$! The simple reason for this is that Eq. (6) says that the reduced distribution at time n at a point x is the average value of the distribution at two points, $x/2$ and $(x+1)/2$ at the previous time, $n-1$. This averaging, if carried on long enough, produces a function which is constant in x . One can readily estimate the time it takes to reach this uniform state in the following way. Suppose that $l < 1$ is some length scale on which $W_0(x)$ varies with x . Then since the baker's map stretches sets of length l into sets of length $2l$ we can estimate the time to reach equilibrium as the time it takes a set of length l to be stretched to a set of length 1, which is $(-\ln l)/(\ln 2)$. This is not an astronomically long time and is certainly

much shorter than the time it takes for the ergodic or mixing properties of the baker's map to make themselves manifest. It is also important to note that if we were to consider the reduced distribution function in the y variable, we would not get a nice equation with a distribution function that approaches equilibrium. Why that is so will be clear in a moment. Finally, it should be realized that we have not introduced any stochastic features into our derivation of Eq. (6), we have only integrated the Liouville equation over one of the variables. Thus we have been able to do for the baker's map what those of us who work on derivations of the Boltzmann equation for simple gases try to do — to start from the Liouville equation, and by introducing nothing but an initial condition and integrating over the appropriate number of unmeasured variables, rigorously obtain the Boltzmann equation and its generalization to higher densities [18].

Now for the baker's map, admittedly a toy model, we have seen that a reduced distribution function approaches equilibrium on a reasonable time scale, and we have not made direct use of any ergodic or mixing property of the baker's map. We did however make strong use of the stretching nature of the map in the x -direction. To shine a stronger light on this stretching feature, we consider another model, the Arnold cat map (see Fig. 2).

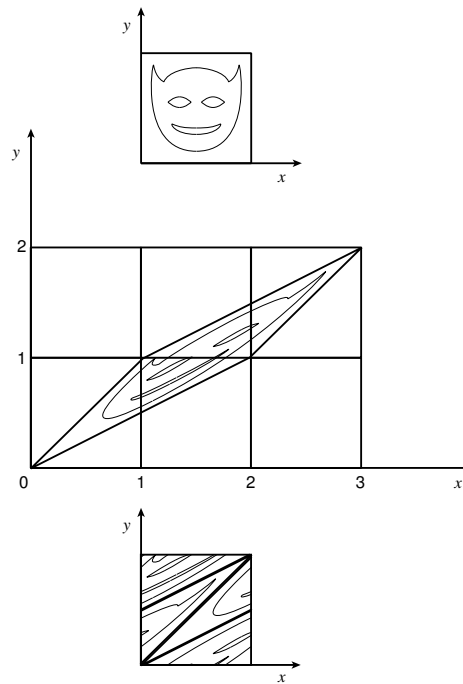


Fig. 2. The Arnold cat map.

Here we regard the unit square as representing a torus, with opposite sides identified. Then the map takes the unit square continuously (that is, there is no cutting and moving of any section as there is in the baker's map) into its image which is also a unit square. The map is given as a 2×2 matrix with unit determinant and integer elements. These conditions are needed for the map to be measure preserving and for the torus to be mapped smoothly onto itself, hence the designation as a *toral automorphism*. We will also suppose that the map has the *hyperbolic* property, namely, that one of its eigenvalues is greater than unity. It follows from the fact that the determinant is unity, that the other eigenvalue is less than 1, and the product of the two is 1. A standard version of the map, called the Arnold cat map is given by [10]

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \mathbf{T} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix}, \text{ modulo } 1. \quad (7)$$

The eigenvalues of $\mathbf{T}$ are easily seen to be given by $(3 \pm \sqrt{5})/2$ and the eigendirections are perpendicular to each other, and both make non-zero angles with the x and y axes. There is a stretching direction which corresponds to the direction of the larger eigenvalue, and a contracting direction which corresponds to the smaller eigenvalue. While the equation for the projection of the "phase space" distribution function onto the x or y directions is not as simple as that for $W_n(x)$ given above, it is not difficult to write a computer program which shows the values of these projections after a few time steps, starting with a simple initial distribution on the unit torus. Here the initial distribution is taken to be uniform on a small square with area 10^{-2} .

Figures 3 and 4 show the behavior of the projected distribution functions, $W(x, n)$ and $G(y, n)$, onto the x and y directions, respectively, for an initial set of points that is uniform over the region $0 \leq x, y \leq 0.1$ and zero everywhere else. One readily sees that both these distribution functions become uniform after three or four time steps. In figures 5, 6, and 7, we show what is going on at the same time in the full phase space. One can easily see that after three iterations of the map, the phase space distribution is hardly uniform, but the projections onto the x and y directions are quite uniform by this time.

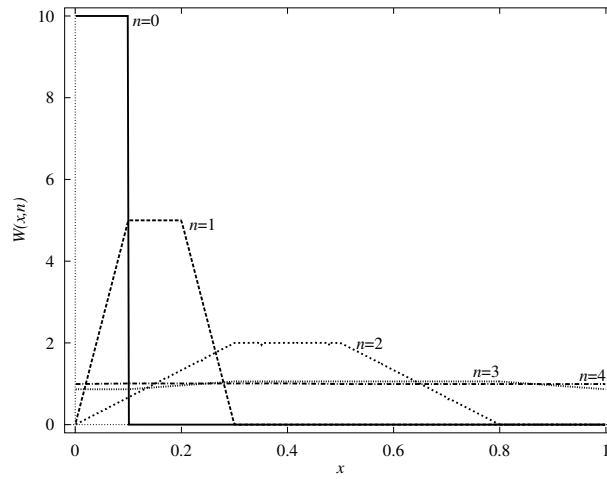


Fig. 3. The projection, $W(x, n)$, onto the x -coordinate, of the phase-space distribution function for the Arnold cat map. The initial conditions are those illustrated in Fig. 5.

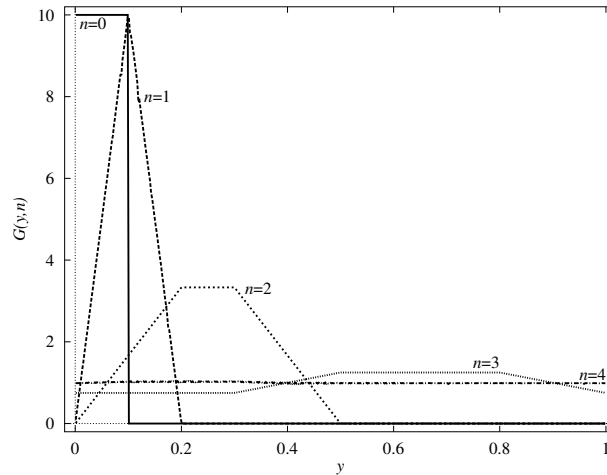


Fig. 4. The projection, $G(y, n)$, onto the y -coordinate, of the phase-space distribution function for the Arnold cat map, for the same initial conditions as in Fig. 3.

The special feature that both the baker's map and the cat map described above have in common is that they are both area preserving maps with a stretching direction, called an *unstable* direction, and a contracting direction, called a *stable* direction. These directions are associated with *stretching* and *contracting* eigenvalues, respectively, whose logarithms are called

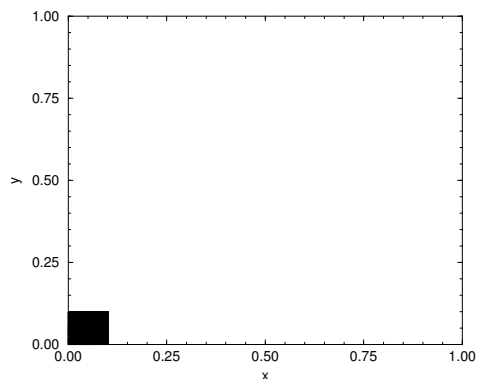


Fig. 5. Initial configuration for the Arnold cat map.

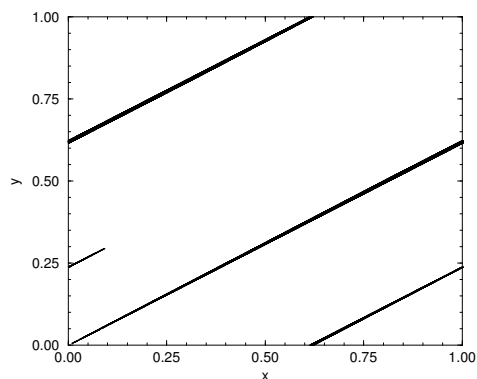


Fig. 6. Evolution of the initial configuration after three iterations of the Arnold cat map.

Lyapunov exponents. For the baker's map the two Lyapunov exponents are $\lambda_{\pm} = \pm \ln 2$, and for the cat map above, the two Lyapunov exponents are $\lambda_{\pm} = \ln[(3 \pm \sqrt{5})/2]$. In order to get a reduced distribution function that approaches an equilibrium distribution for long enough times, one clearly must project the Liouville distribution onto directions that are not orthogonal to the unstable directions. In such a case, the expanding property of the underlying microscopic dynamics will smooth out any non-uniformities in the initial distribution, provided they are not too singular, and cause the reduced distribution function to approach an equilibrium value.

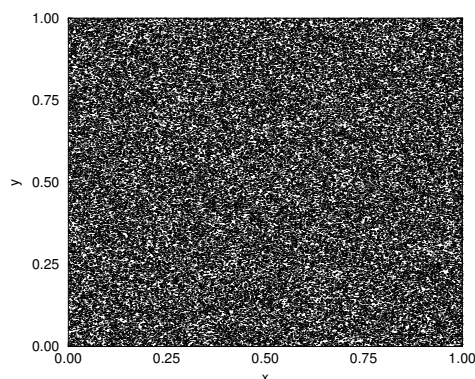


Fig. 7. Evolution of the initial configuration after ten iterations of the Arnold cat map.

General dynamical systems that have properties similar to the cat map or the baker's map are called Anosov or Anosov-like systems, respectively. Anosov systems are continuous dynamical systems such that at every point in phase space there are stable and unstable directions, with positive and negative Lyapunov exponents, respectively [12,19]. There may also be some *neutral* directions with zero Lyapunov exponents, but there must be at least one positive Lyapunov exponent. The presence of positive Lyapunov exponents defines a hyperbolic system. Furthermore there must be at least one trajectory in phase space that is dense, a requirement which is called *transitivity*. Of course for a multi-dimensional Anosov system, there may be many stable and unstable directions, but they are never tangent to one another. Instead all stable and unstable directions intersect transversally. If the dynamical system is measure preserving, the sum of *all* of the Lyapunov exponents must be zero. Systems with some positive Lyapunov exponents are commonly referred to as being *chaotic*, although there is no universally agreed upon requirement that must be satisfied for a system to be called chaotic.

The simple examples of the baker's map and the cat map give us some reason to believe that reduced distribution functions will approach equilibrium values, or more realistically, local equilibrium values (see below), on reasonable time scales, even if the full phase space distribution function is not uniform by the time the reduced functions have reached almost uniform values. This conclusion depends, of course, on the assumption that the underlying microscopic dynamics is of the Anosov or Anosov-like variety. This assumption has been made a central feature of work by Gallavotti and Co-

hen [20], who have called it the *chaotic hypothesis*, and used it to obtain a fluctuation theorem that applies to non-equilibrium stationary states for systems with dissipation¹. It should also be clear that if an Anosov-like system were subject to small, random external perturbations, then the approach to equilibrium of the system would not be greatly effected, since the dynamics is already capable of making the reduced distribution functions reach local equilibrium values. However, if a system were to have no positive Lyapunov exponents and no unstable directions in phase space, then externally introduced randomness of some sort would appear to be essential for the system's reaching an equilibrium state. Actually, this randomness can be quite mild, as we will see when considering pseudochaotic systems.

The approach to equilibrium described above for the baker and cat maps should properly be seen as simple models for the approach of a macroscopic system to *local equilibrium*. That is, if one thinks of the extent of the coordinate part of phase space for these models as standing in for some mesoscopic length in a real, physical system, then one can plausibly argue that what the maps illustrate is an approach to equilibrium on the mesoscopic length scale. It would take a much longer time for a system to reach total equilibrium on a macroscopic length scale. A typical mesoscopic length scale would be, for example, a distance of a few mean free paths in a dilute gas, where the collisions between particles play the role of the elementary steps in the maps. Thus, one might expect a local equilibrium to be established on the time scale of a few mean free times, but the relaxation of some local equilibrium distribution might take a much longer time, determined by the physical size of the system and the boundary conditions imposed upon it. This picture is, in fact, the standard description of the approach to equilibrium of some non-equilibrium disturbance in a fluid, described in some detail by Bogoliubov [18,21], many years ago, but understood previously by those using the Boltzmann equation to describe hydrodynamic flows in dilute gases. The basic description is that there are three, well separated time scales: The shortest time is the duration of a collision τ_d , then a kinetic time scale, τ_k which is on the order of the time between collisions during which time a local equilibrium state can be established, followed by a hydrodynamic time scale, τ_h , which is determined by the macroscopic size of the system and gives the time scale on which a local equilibrium state relaxes to total equilibrium. This picture makes sense and is physically plausible provided

$$\tau_d \ll \tau_k \ll \tau_h. \quad (8)$$

¹ We will discuss the Gallavotti-Cohen fluctuation theorem briefly in the next section.

4. Some applications

In addition to providing some insights into the approach to local equilibrium for large systems, the dynamical systems approach gives us results of a more practical sort. Among these results are: *(i)* relations between transport coefficients and dynamical quantities, such as Lyapunov exponents and Kolmogorov–Sinai entropies [22, 23], to be defined below; *(ii)* a theory of entropy production in non-equilibrium steady states and in the approach of a system to equilibrium [24, 25]; and *(iii)* fluctuation theorems, such as the Gallavotti–Cohen theorem — which describe the fluctuations in entropy production, or related quantities, of dissipative systems in non-equilibrium steady states [20, 26, 27]. Here we will summarize these results so that the reader gets some of their flavor, but we refer the reader to the literature for a more complete discussion of these and related topics.

4.1. Microscopic dynamical quantities and macroscopic transport coefficients

Among the many reasons dynamical systems theory attracted the attention of workers in non-equilibrium statistical mechanics are the connections between macroscopic transport coefficients of a system of particles and quantities that characterize the system’s chaotic behavior discovered by Gaspard and Nicolis, for Hamiltonian systems [22], and by Evans, Hoover, and coworkers for dissipative systems with Gaussian thermostats [3, 4]. We discuss each case separately.

4.1.1. The escape-rate formulae for transport coefficients

Let us imagine that we have some system of fixed particles in which another set of moving particles are located. To simplify matters, we will suppose that the moving particles do not interact with each other, but that they do interact with the fixed scatterers. This model is usually called a Lorentz gas. Assuming that the fixed particles are not arranged in such a way as to form traps for the moving ones, and assuming also that the free path length of any moving particle between collisions with the fixed scatterers is finite, then we can suppose that macroscopically the moving particles undergo a diffusion among the fixed scatterers. That is, the number density, $n(\vec{r}, t)$, of moving particles in a macroscopic region of space with scatterers should satisfy the diffusion equation

$$\frac{\partial}{\partial t} n(\vec{r}, t) = D \nabla^2 n(\vec{r}, t), \quad (9)$$

where D is the diffusion coefficient for the moving particles among the scatterers. Suppose further that the macroscopic region in which this system is

located is surrounded by an absorbing wall, such that particles reaching the wall are removed from the system. In such a case, the diffusion equation, Eq. (9), can be solved with the boundary condition, $n(\vec{r}, t) = 0$ for $\vec{r}$ on the boundary. With this boundary condition, the number of particles in the system at any time $t > 0$, $N(t)$ decays exponentially as

$$N(t) = N(0)e^{[-aDt/L^2]}. \quad (10)$$

Here $N(0)$ is the number of moving particles initially in the system, L is a length that characterizes the dimension of the system, and a is a numerical constant of order unity whose precise value depends of the geometry of the region occupied by the system. We can therefore characterize the decay of particles in the system by a macroscopic escape-rate, γ_{mac} given by

$$\gamma_{\text{mac}} = \frac{aD}{L^2}. \quad (11)$$

It is remarkable that there is also a dynamical systems theory result for the escape-rate of the particles from the system, obtained under the assumption that the dynamics of the moving particles in the presence of the scatterers is Anosov-like [28–30]. This microscopic *escape-rate formula* for the escape-rate, γ_{mic} is

$$\gamma_{\text{mic}} = \sum_i \lambda_i^+(\mathcal{R}) - h_{\text{KS}}(\mathcal{R}). \quad (12)$$

All of the terms on the right hand side of Eq. (12) require some explanation. To get some insight into this formula, imagine that there is a set of initial conditions for the moving particle in the arrangement of scatterers that will never lead to the particle escaping. One can imagine, for example, trajectories where the moving particle bounces forever among a few scatterers. However, a slight displacement of the moving particle from this bouncing trajectory will eventually lead to the particle's escape. The set of initial conditions which lead to the particle's remaining in the system forever is called a *repeller* and denoted by $\mathcal{R}$. It is typically a fractal set of points, usually of measure zero in the set of all possible trajectories, but with a non-zero fractal, that is Hausdorff, dimension, and as mentioned above, a highly unstable set since an arbitrarily small displacement of the initial phase of the particle from a point in $\mathcal{R}$ will lead to escape.

In order to get some feeling for the dynamical origin of the escape rate formula, Eq. (12), we use the notion that hyperbolic dynamics generates information about the phase space region where the initial positions and momenta of the particles of the system are located, when confined to the repeller: Suppose that we know that initially the phase point is located in

a region in Γ -space of order ϵ on a side, where ϵ sets the scale of distances that we can use to distinguish two points in phase space. That is we can distinguish between points separated by ϵ or greater, but not smaller. Next, because of the hyperbolic dynamics, the points in this region separate in phase space in the course of time, and as time goes on the separation of points in the unstable directions grow exponentially. This allows us to make distinctions between points at time t , even if we cannot make them initially. Thus we have more information about the initial locations of the phase points at time t than we did initially. This rate of information growth is characterized by the sum of the positive Lyapunov exponents, each of which is denoted by $\lambda_i^+(\mathcal{R})$ in Eq. (12). However, the rate of information growth is reduced by the fact that particles escape. When that happens, we lost track of them altogether. Thus the escape rate reduces the rate of information growth. If we call the net rate of information growth an entropy, called in the literature, the Kolmogorov–Sinai entropy, $h_{\text{KS}}(\mathcal{R})$, the net rate of information growth, including the exponential separation of trajectories that produce information and the escape of particles which reduce it, is given by

$$h_{\text{KS}}(\mathcal{R}) = \sum_i \lambda_i^+(\mathcal{R}) - \gamma_{\text{mic}}. \quad (13)$$

This is just the escape rate formula, expressed in another way.

In any case we now have two expressions for the same escape-rate for a hyperbolic system, and by equating them, we obtain an expression for the diffusion coefficient, D , in terms of microscopic dynamical quantities, as

$$D = \lim_{L \rightarrow \infty} \frac{L^2}{a} \left[\sum_i \lambda_i^+(\mathcal{R}) - h_{\text{KS}}(\mathcal{R}) \right]. \quad (14)$$

We have taken the large system limit to remove any possible dependence of the right hand side of Eq. (14) on the shape of the boundaries or on the size of the system. This result is due to Gaspard and Nicolis [22]. It has since been generalized to other transport coefficients [23], and applied to determine transport coefficients for simple models of diffusion and of viscous flow [31, 32].

The escape-rate formulae for transport coefficients are among the very intriguing results of transport theory for systems with microscopic chaos, in that it makes a direct connection between the macroscopic and microscopic descriptions of transport. The drawback of the escape-rate method is that there are as yet very few methods to compute the Kolmogorov–Sinai entropy for the repeller, while both the diffusion coefficient, and, it turns out, the sum of the positive Lyapunov exponents on the repeller are amenable

to treatment by the usual methods of statistical mechanics and kinetic theory [33]. At the moment, this escape-rate formula is most simply used to determine the KS entropy of trajectories on the fractal repeller. However, as noted above, Gaspard and co-workers have been able to independently determine the KS entropy for some interesting models of transport, and thereby obtain numerical results for the corresponding transport coefficients that compare very well with more established methods based on Green–Kubo formulae [31, 32].

4.1.2. Deterministic random walk on the real line: the multi-baker map

In order to illustrate the escape-rate method and to introduce a useful model of transport in chaotic systems, we consider a generalization of the baker map, called the *multi-baker map* [1]. This map lifts the baker map from the unit square to a strip of height one in the y -direction and to an arbitrary number of units, possibly infinite, in the x -direction. We write the dynamic equations for the multi-baker map in terms of three variables n, x, y where x, y satisfy $0 \leq x, y < 1$, and n denotes the unit interval along the x -axis where the phase point $\Gamma = (n + x, y)$ is located. The dynamics is specified as follows:

$$\begin{aligned}\Gamma' = (n' + x', y') &= \left(n + 1, 2x, \frac{y}{2}\right) \quad \text{for } x \leq \frac{1}{2}, \\ &= \left(n - 1, 2x - 1, \frac{y + 1}{2}\right) \quad \text{for } \frac{1}{2} < x < 1.\end{aligned}\quad (15)$$

Of course, this is a chaotic, measure preserving transformation with Lyapunov exponents $\pm \ln 2$. Apart from the fact that the time variable is discrete, a distribution function defined on the strip, obeys a standard Liouville equation, called the Frobenius–Perron equation in this context, which is

$$\begin{aligned}\rho(n, x, y, t) &= \rho\left(n - 1, \frac{x}{2}, 2y, t - 1\right) \quad \text{for } y \leq \frac{1}{2}, \\ &= \rho\left(n + 1, \frac{(x + 1)}{2}, 2y - 1, t - 1\right) \quad \text{for } \frac{1}{2} < y < 1.\end{aligned}\quad (16)$$

In order to see how the escape-rate formalism can be used to calculate the KS-entropy on the repeller, let us imagine that the system is confined to L unit cells, where L is an integer. We start with an initial distribution that is uniform in each cell, but differs from cell to cell. We further suppose that the cells $n = 0, L + 1$ are absorbing. That is, the distribution function is set equal to zero for cells $0, L + 1$ for all times t . By looking at the projected distribution function, $W(n, x, t)$ obtained in a similar way as done for the

baker map, we find that W obeys the equation

$$W(n, x, t) = \frac{1}{2} \left[W\left(n-1, \frac{x}{2}, t-1\right) + W\left(n+1, \frac{(x+1)}{2}, t-1\right) \right]. \quad (17)$$

For the above initial conditions, the solution of Eq. (17), that satisfies the boundary conditions, depends only on the cell index n , and not on the internal x value. This solution is given by

$$W(n, t) = \sum_k A_k (\cos k)^t \sin kn, \quad (18)$$

where the allowed values of the wave number k are

$$k = \frac{j\pi}{L+1} \text{ for } j = 1, \dots, L. \quad (19)$$

For large times, the smallest wave number dominates the sum and the escape-rate, γ , is easily found to be

$$\gamma = -\ln \cos \left(\frac{\pi}{L+1} \right) \approx \frac{\pi^2}{2(L+1)^2}. \quad (20)$$

From this result we can immediately identify the diffusion coefficient as the coefficient of the square of the wave number, namely, $D = 1/2$. Using this result and the escape-rate formula Eq. (13), we find that

$$h_{\text{KS}}(\mathcal{R}) = \ln 2 - \frac{\pi^2}{2(L+1)^2}. \quad (21)$$

Using various formulae from dynamical systems theory, such as Young's dimension formula [34], one can use the values of the Lyapunov exponent and the KS entropy given above to calculate the fractal dimension of the repeller. We leave that as a simple exercise for the reader.

4.2. Fractal forms in the multi-baker map

The chaotic nature of particle dynamics in a fluid has interesting consequences for the fine details of transport processes, details that are generally inaccessible using the mesoscopic descriptions of transport processes. To illustrate some of these consequences, we consider the case of diffusion of a particle undergoing a deterministic random walk as described by the multi-baker map. The main idea that we illustrate here is the fact that the displacement of the particle is a very sensitive function of its initial position in a unit square. The effects of this sensitive dependence can be captured by considering a quantity which we call a *partial van Hove function* [1, 35, 36].

The van Hove function appears in a natural way in the description of diffusion of a tagged particle in a many particle system. It is relatively straightforward to show, using standard statistical mechanical arguments, that the probability, $P(\mathbf{r}, t)$, to find a diffusing particle at a point $\mathbf{r}$ at time t is given by [2]

$$P(\mathbf{r}, t) = \int \frac{d\mathbf{k}}{(2\pi)^d} P_{\mathbf{k}} F(\mathbf{k}, t), \quad (22)$$

where $P_{\mathbf{k}}$ is the Fourier transform of the initial probability distribution $P(\mathbf{r}, t = 0)$, and $F(\mathbf{k}, t)$ is the van Hove function, given in general by

$$F(\mathbf{k}, t) = \left\langle e^{i\mathbf{k} \cdot (\mathbf{r}(t) - \mathbf{r}(0))} \right\rangle. \quad (23)$$

The angular brackets denote an equilibrium ensemble average. The important quantity in the van Hove function is the displacement, $(\mathbf{r}(t) - \mathbf{r}(0))$ of the diffusing particle, which is, for chaotic systems, a very sensitive function of the initial phase point of the system of particles. The van Hove function itself, for a system undergoing normal diffusion, and for times long compared to some microscopic time, has the form

$$F(\mathbf{k}, t) = e^{s(\mathbf{k})t}, \quad (24)$$

where the function $s(\mathbf{k})$ describes the decay of a density fluctuation with wave number $\mathbf{k}$ and is given by

$$s(\mathbf{k}) = -D\mathbf{k}^2 + O(k^4). \quad (25)$$

In order to illustrate the effects of chaotic dynamics that are hidden in the equilibrium average, we turn again to the multi-baker map, and consider the analog of the van Hove function, defined by

$$F(k, t) = \int_0^1 dx \int_0^1 dy e^{ik(n(x_t, y_t) - n(x, y))}, \quad (26)$$

where we measure displacement in terms of the change over time t of the unit interval in which the particle is located. We have used the fact that the equilibrium distribution is uniform for a (closed) multi-baker system. Due to the periodicity of the system, the displacement of the particle depends upon the initial starting point, (x, y) , within a unit cell but not on the location of the initial unit cell. Note that the integration is over the coordinates, (x, y) of the initial point. Here the complete integration hides the chaotic nature

of the displacement and to reveal it, we consider the normalized, partial van Hove function, $I_k(x, y, t)$ given by

$$I_k(x, y, t) = e^{-s(k)t} \int_0^x dx' \int_0^y dy' e^{ik(n(x'_t, y'_t) - n(x', y'))}. \quad (27)$$

The quantity $s(k) = \ln \cos k$ has been found earlier. Using the multi-baker transformation, Eq. (15), we easily obtain the recursion relation for $I_k(x, y, t)$, which is

$$\begin{aligned} I_k(x, y, t) &= e^{(-s(k)+ik)t} I_k\left(2x, \frac{y}{2}, t-1\right) \text{ for } x < \frac{1}{2} \\ &= e^{(-s(k)+ik)t} I_k\left(1, \frac{y}{2}, t-1\right) + e^{(-s(k)-ik)t} \\ &\quad \times \left[I_k\left(2x-1, \frac{(y+1)}{2}, t-1\right) - I_k\left(2x-1, \frac{1}{2}\right) \right] \text{ for } x > \frac{1}{2}. \end{aligned} \quad (28)$$

Considered as a mathematical object, this recursion relation may have many solutions. However its structure suggests the simple structure $I_k(x, y, t) = yH_k(x, t)$, with the normalization $H_k(1, t) = 1$. This substitution leads to the recursion relation

$$\begin{aligned} H_k(x, t) &= \frac{1}{2} e^{(-s(k)+ik)t} H_k(2x, t-1) \text{ for } x < \frac{1}{2} \\ &= \frac{1}{2} e^{(-s(k)+ik)t} + \frac{1}{2} e^{(-s(k)-ik)t} H_k(2x-1, t-1) \text{ for } x > \frac{1}{2}. \end{aligned} \quad (29)$$

The recursion equation, Eq. (29) can be solved numerically by starting with the initial value, $H_k(x, t=0) = x$ and then solving recursively. The result rapidly approaches the asymptotic form obtained by looking for solutions that are independent of time. In figure 8 we illustrate this function for small wave numbers by plotting the real and imaginary parts of the function along the horizontal and vertical axes, respectively.

The function so obtained is a fractal, with a Hausdorff dimension, D_H that satisfies the rather remarkable relation

$$D_H = 1 + \frac{D}{\lambda} k^2 + O(k^4). \quad (30)$$

Here D is the diffusion coefficient of the moving particle, and λ is the positive Lyapunov exponent for the map. This equation is interesting because it shows that both a macroscopic quantity, D , and a microscopic quantity, λ are encoded in the fractal structure of the partial van Hove function [35, 36].

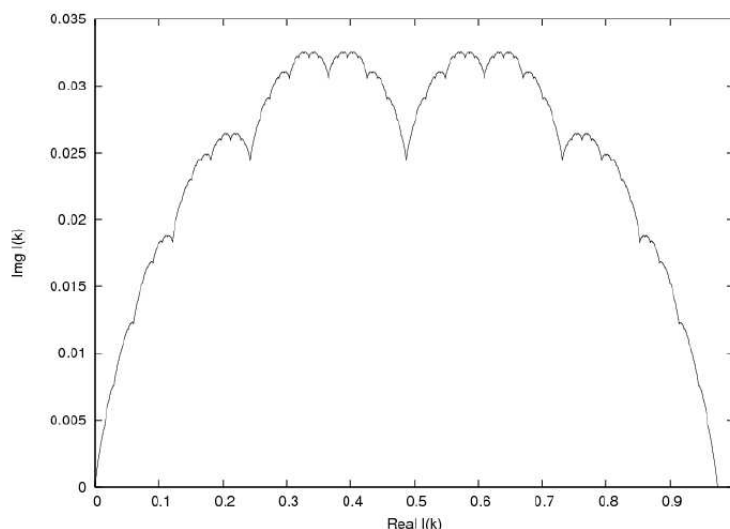


Fig. 8. The fractal van Hove function for the multi-baker map. The real part of this function is plotted on the horizontal axis and the imaginary part is plotted along the vertical axis. The value of the wave number is $k = 0.05$ in units where the size of a unit cell is unity.

It has been possible to derive Eq. (30) for diffusive systems which are chaotic, measure preserving, and have one conjugate pair of Lyapunov exponents whose sum is zero [36]. It has been verified numerically for two dimensional, periodic Lorentz gases, with either hard disk or attractive Yukawa potentials between the moving particle and the scatterers. We refer to the literature for more details. Here we only mention that Eq. (30) is one of a number of similar formulas, including the escape rate formula, Eq. (14), that relate fractal properties of some kind to both transport coefficients and quantities that characterize the chaotic nature of the system.

4.2.1. Transport coefficients and phase-space contraction in Gaussian thermostatted systems

An alternative method for relating macroscopic transport coefficients to Lyapunov exponents was developed by Evans, Hoover, Posch and co-workers in their work on developing computer algorithms to simulate non-equilibrium flows in many-particle systems [3,4,37]. A problem arose in these simulations because the systems tended to heat up considerably due to the presence of viscous friction or, for charged particle systems, ohmic heating. To counteract this heating, these workers introduce a fictitious thermostat which maintains a constant value for either the total energy or the total kinetic

energy of the system. The thermostat is introduced by a modification of the equations of motion in such a way the Hamiltonian nature of the system, in the usual coordinate, momentum, and time variables, was lost. As a result, the phase space volumes of these thermostatted systems do not remain constant in time, but rather, the phase space volume of a set decreases with time, and the system's trajectories concentrate on an attractor. The rate of decrease of the phase space volume is characterized by a negative value of the sum of all of the Lyapunov exponents of the system. Moreover, the decrease of the phase space volume can be related to the entropy production in the system+thermostat, and this entropy production can also be related to the transport coefficients via the usual macroscopic laws. Thus one has a way to relate transport coefficients to the sum of the Lyapunov exponents for these thermostatted systems. For a variety of reasons, this method has found more numerical applications than the escape-rate method discussed above. The non-equilibrium stationary state on the attractor can be characterized by a special type of measure, called a Sinai–Ruelle–Bowen (SRB) measure, which can be used to provide a physically useful measure of different sets on the repeller. The SRB measure is characterized by the fact that it is smooth in the unstable directions in phase space but may be fractal in the stable directions [38]. Simple examples of this type of measure can be found in the literature [39].

To make this discussion more concrete, we consider an example. Again we consider the Lorentz gas, a collection of non-interacting moving particles in an array of fixed, hard scatterers. We assume that the moving particles have a bounded free path between collisions with the fixed scatterers, and that the scatterers do not form traps for the moving particles. We suppose the moving particles carry a charge, q , (but still do not interact with each other) and are placed in a constant, external electric field, $\vec{E}$. Ordinarily, the field will accelerate the moving particles in such a way that their energy increases over time. To avoid this we add a frictional force to the equations of motion of the moving particle, and adjust the frictional force so as to keep the kinetic energy of the moving particle constant in time. The equations of motion for the position, $\vec{r}$ and velocity, $\vec{v}$, of the moving particle between collisions with scatterers are

$$\dot{\vec{r}} = \vec{v}, \quad (31)$$

$$\dot{\vec{v}} = q\vec{E} - \alpha\vec{v}, \quad (32)$$

where α is a dynamical variable defined by the constant energy condition, $\vec{v} \cdot \vec{v} = 0$. Thus we find that

$$\alpha = \frac{q\vec{v} \cdot \vec{E}}{v^2}. \quad (33)$$

The equations of motion given above for the moving particle must be supplemented by the equations describing the collisions of the moving particles with the scatterers. To simplify matters, we will suppose that the particles make instantaneous, elastic, and specular collisions with the scatterers.

It is relatively easy to show that the conservation equation for the phase space distribution function, $\rho(\vec{r}, \vec{v}, t)$, for the moving particles is now modified to

$$\frac{d}{dt}\rho(\vec{r}, \vec{v}, t) = \alpha\rho(\vec{r}, \vec{v}, t). \quad (34)$$

In order to relate this distribution function to entropy production, we define the Gibbs entropy for this system by

$$S_G(t) = -k_B \int d\vec{r} \int d\vec{v} \rho(\vec{r}, \vec{v}, t) [\ln \rho(\vec{r}, \vec{v}, t) - 1], \quad (35)$$

where k_B is Boltzmann's constant. By taking time derivatives and integrating by parts we find that

$$\frac{dS_G}{dt} = -k_B \int d\vec{r} \int d\vec{v} \alpha \rho = -k_B \langle \alpha \rangle. \quad (36)$$

The average value is taken with respect to the phase space distribution function for the moving particles, ρ .

It is found that the system approaches a non-equilibrium stationary state in the course of time where all of the averages taken with respect to ρ reach constant values. One might expect the average value of the friction coefficient to be positive, so as to keep the kinetic energy constant. Thus, this Gibbs entropy decreases with time, making its way to negative infinity! This can be understood by the observation that if the trajectories of the moving particles are getting concentrated on an attractor, we will be gaining more information about the system as time goes on, hence the Gibbs entropy will decrease. This decrease in entropy must be matched, at least, by an increase in entropy of the reservoir that is responsible for the additional frictional force. Thus

$$\frac{dS_{\text{reservoir}}}{dt} \geq k_B \langle \alpha \rangle \geq 0. \quad (37)$$

We now take the entropy production in the reservoir to be given by the usual macroscopic laws, in particular,

$$\frac{dS_{\text{reservoir}}}{dt} = \frac{\vec{J} \cdot \vec{E}}{T} = \frac{\sigma \vec{E}^2}{T}, \quad (38)$$

where $\vec{J} = \sigma \vec{E}$ is the electrical current produced by the moving particles and σ is the coefficient of electrical conductivity. Then, by combining Eqs. (37) and (38), and assuming that we take the entropy production in the reservoir to be exactly $k_B \langle \alpha \rangle$, we obtain an expression for σ as

$$\sigma = \frac{k_B T \langle \alpha \rangle}{\vec{E}^2}. \quad (39)$$

The final step in this process is to relate the average friction coefficient, $\langle \alpha \rangle$, to the Lyapunov exponents for the trajectories of the moving particles. We note, first of all, that the volume, $\mathcal{V}$ of a small region in phase space will change exponentially in time with an exponent equal to the sum of all the Lyapunov exponents, as

$$\mathcal{V}(t) = \mathcal{V}(0) \exp \left[t \sum_i \lambda_i \right], \quad (40)$$

since the Lyapunov exponents describe the rates of stretching or of contracting of small distances in phase space. If we now use a representation of ρ in terms of phase space volumes, $\rho = \mathcal{N}/\mathcal{V}$, where $\mathcal{N}$ is the number of members of the ensemble in phase space volume $\mathcal{V}$. The quantity $\mathcal{N}$ remains constant in time while the phase space volume varies as described above. In fact, the modified Liouville equation, Eq. (34), shows that

$$\left\langle \frac{d \ln \mathcal{V}}{dt} \right\rangle = -\langle \alpha \rangle = \left\langle \sum_i \lambda_i \right\rangle. \quad (41)$$

We remind the reader that in the non-equilibrium stationary state, all averages remain constant with time, so that we can now use Eq. (39) to obtain the desired connection between a transport coefficient, in this case the conductivity σ , and the average Lyapunov exponents,

$$\sigma = -\frac{k_B T}{\vec{E}^2} \left\langle \sum_i \lambda_i \right\rangle. \quad (42)$$

This result has been used to determine the conductivity and the diffusion coefficient of the moving particles in the Lorentz gas by means of efficient computer algorithms for determining the Lyapunov exponents. Similar methods

have been used to determine the shear viscosity of a gas of hard balls, or a gas of particles that interact with WCA potentials [40, 41].

One important result of the analysis of these thermostatted systems is the “conjugate pairing rule”. This is a generalization of the result for Anosov, Hamiltonian systems that non-zero Lyapunov exponents come in pairs, with the same magnitude but with opposite signs so that members of each conjugate pair sum to zero. This is called the symplectic conjugate pairing rule. For Anosov systems on an attractor produced by a Gaussian thermostat, there is also a “conjugate pairing rule”, where the Lyapunov exponents appear to form conjugate pairs which sum to a constant, non zero, value [42]. The conjugate pairing rule is very helpful for analyzing relations such as that given by Eq. (42), since the right hand side is completely determined by the sum of any given conjugate pair. The easiest pair to use is the pair formed by the positive and negative exponents with the largest magnitude.

4.3. Entropy production in non-equilibrium, Hamiltonian systems

One of the subjects of most active research in recent years has been the theory of entropy production in non-equilibrium systems. Dynamical systems theory has provided some new insights into this old problem. Briefly formulated, the problem is to explain the positive, irreversible production of entropy using the fundamental ideas in statistical mechanics, particularly the Liouville equation. The obstacle in this direction that must be overcome somehow is the fact that the Gibbs entropy

$$S_G(t) = -k_B \int d\Gamma \rho(\Gamma, t) [\ln \rho(\Gamma, t) - 1], \quad (43)$$

remains constant in time if $\rho(\Gamma, t)$ satisfies the Liouville equation for Hamiltonian systems

$$\frac{d\rho(\Gamma, t)}{dt} = 0. \quad (44)$$

Here Γ represents all of the coordinate and momentum variables of the system. The usual way around this difficulty is to introduce a coarse grained entropy, obtained by either defining an entropy in terms of reduced distribution functions, as is done in Boltzmann’s famous H-theorem, or by coarse graining the phase space itself, and defining an entropy in terms of the average phase space distribution in each of the coarse graining regions. In either case, it is possible to show that the rate of production of the redefined entropy is positive, and for the Boltzmann case at least, is in agreement with the predictions of irreversible thermodynamics when the gas is close to a local equilibrium state.

Ideas from dynamical systems theory have not changed the fundamental need for coarse graining. Instead they have provided strong reasons for doing it, reasons that were lacking in the previous approaches, where the motivation for coarse graining seemed only to be that it was necessary to coarse grain in some way to get a positive entropy production. The central new idea in this area is that the phase space description of a non-equilibrium process requires, in the thermodynamic limit at least, the use of distribution functions that are characterized by singular SRB measures. A simple example is provided by a system in which diffusion can take place in a region between two particle reservoirs, each reservoir being maintained at a different density of particles. Then if the dynamics that leads to transport of the particles between the reservoirs is Anosov-like, one can argue, and in simple enough cases show explicitly [1], that the regions in phase space that correspond to regions of different density in the system get so tangled up and enmeshed that the distribution function is a wildly varying, fractal function. As such, it is no longer differentiable and the steps that lead to the proof of the constancy of the Gibbs entropy can no longer be justified. The only way to treat this kind of fractal behavior of the distribution function is to smooth the function in one or another way, typically by defining cumulative distribution functions over small regions of phase space, leading to the construction of SRB measures. In simple cases, one can show that fractal forms appear in the phase space distribution function for systems in non-equilibrium stationary states produced by particle reservoirs, or in the relaxation of a system with particle diffusion to equilibrium, and that the rate of entropy production agrees with the predictions of irreversible thermodynamics [24, 25, 43]. However, much needs to be done to extend this work to other hydrodynamic processes and to understand why the results of macroscopic theory is obtained in this way.

4.4. Entropy production in systems with Gaussian thermostats and the Cohen–Gallavotti fluctuation theorem

As a final example of the applications of dynamical systems theory to non-equilibrium statistical mechanics we briefly discuss the Gallavotti–Cohen fluctuation theorem. In our discussion of systems with energy conserving thermostats, we have introduced another idea for entropy production, namely entropy production in a reservoir associated with phase space contraction of a thermostatted system. Here the central idea is that the thermostatted dynamics makes the phase space available to the system contract onto an attractor. However, the friction coefficient, which we denoted by α , is a dynamical function taking on positive or negative values depending on the trajectory of the system in phase space. To produce an overall

phase space contraction, the average value of the friction coefficient should be positive, but from time to time it may be negative. For example, in the Lorentz gas that we have been discussing, when the particle moves in the direction of the field, α is positive, and when it moves opposite to the direction of the field, α is negative, provided the charge q is positive. One might imagine some time interval τ , say, and ask for the probability that the time-averaged entropy production, ϵ_τ , as measured by the phase space contraction, has a value a over this time interval. This probability can be expressed in terms of the SRB measure on the attractor of the steady state system. The Gallavotti–Cohen fluctuation theorem is a result for the ratio of the probability that the time-average entropy production over an interval τ will be the value a , to the probability that this value will be $-a$. They show that for a reversible, Anosov-like system with a frictional thermostat,

$$\frac{\text{Prob}(\epsilon_\tau = a)}{\text{Prob}(\epsilon_\tau = -a)} = e^{a\tau}. \quad (45)$$

Note that for long times this ratio approaches zero or infinity depending upon the sign of a .

This result was first discovered by means of computer simulations by Evans, Cohen, and Morris [44], and this observation was explained on the basis of Anosov-like dynamics by Gallavotti and Cohen [20]. By now this result has been generalized considerably to include analogous results for stochastic and other kinds of systems. We refer to the literature for further details [26,27].

5. Pseudochaotic systems

We begin a brief discussion of pseudochaotic systems with an observation: *Microscopic, chaotic dynamics is neither necessary nor sufficient for normal transport.* There are simple examples of non-chaotic systems which have normal diffusion. Such an example would be the wind-tree model which is a Lorentz gas with oriented squares as scatterers [7]. The most often discussed case has squares placed at random in the plane, the diagonals of the square scatterers oriented along the x and y -directions, and the moving particles traveling only in the $\pm x$ and $\pm y$ -directions. The diffusion of the moving particles is normal if the squares are not allowed to overlap, and, at low enough density, for squares that are allowed to overlap. Since the sides of the squares are flat, the Lyapunov exponents are zero for this model. It is not chaotic. A chaotic Lorentz gas that has abnormal diffusion properties is a periodic Lorentz gas with circular scatterers and with “corridors” along which the moving particles can travel arbitrarily far without encountering a scatterer.

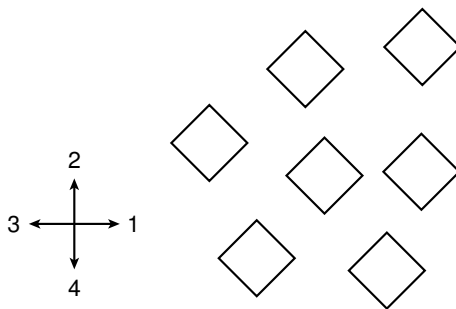


Fig. 9. The Ehrenfest wind-tree model. The trees are diamonds with axes oriented along the x and y directions. The wind is a collection of point particles that can only move in the $\pm x$ or $\pm y$ directions with unit speed.

The wind tree model is an example of a system that is pseudochaotic [8]. That is, it has zero Lyapunov exponents but trajectories still separate in time, but only algebraically instead of exponentially. The algebraic separation of trajectories is due to the sharp corners of the scatterers, which can cause the separation of two, nearby trajectories.

Pseudochaotic systems often have a weak mixing property [10]. For weak mixing systems, Eq. (3) is not satisfied, but a weaker property is, namely

$$\lim_{T \rightarrow \infty} \frac{1}{T} \sum_0^{(T-1)} [\mu(A_\tau \cap B) - \mu(A)\mu(B)] = 0. \quad (46)$$

Here we have taken the measure of the phase space to be finite and normalized to unity. The origin of the weak mixing property is, of course, the algebraic separation of trajectories caused by the corners of the scatterers.

There have been many studies of pseudochaotic systems, and many issues remain to be resolved. The mathematical descriptions of these systems can be quite profound, and require the application of deep results from number theory and differential geometry, among others, when solutions are available at all. A good introduction to the mathematical issues can be found in the small book of Tabachnikov [45].

Here we wish to mention a few issues that seem to be more easily resolvable than some others. It is of some interest to study partial van Hove functions for pseudochaotic systems, with normal as well as abnormal diffusive properties, either super-diffusive, where the mean square displacement grows faster than the first power of time, or sub-diffusive, where the growth of the mean square displacement is slower than the first power of the time. Figure 11 shows a partial van Hove function for a particle moving through a channel of 20-sided scatterers, as illustrated in Fig. 10. The partial van Hove

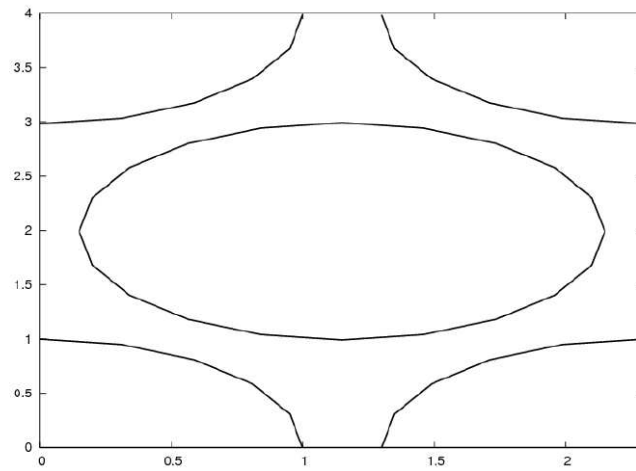


Fig. 10. A pseudo-chaotic system consisting of point particles moving among twenty sided scatterers placed in a cell which is repeated periodically along the horizontal direction. In addition to the central scatterer, there are half-scatterers placed along the top and bottom sides of the channel.

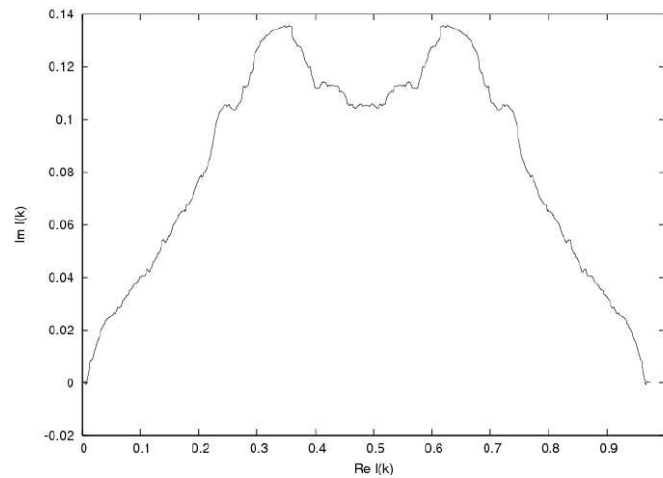


Fig. 11. The real vs imaginary parts of the partial van Hove function for the channel of twenty-sided scatterers as illustrated in Fig. 10.

function looks similar to those of chaotic systems, and seems, at first sight, to have a fractal structure. How this structure evolves with time and with the number of sides of the scatterers is currently under study.

6. The quantum chaos and the quantum multi-baker map

6.1. Quantum chaos

In this section we will briefly consider some results in the area of quantum chaos. Quantum chaos is a subject with a vast literature, starting with a paper of Einstein's who pointed out problems with the Bohr–Sommerfeld quantization conditions for non-integrable systems [46]. Much of the current understanding of the subject is described in the books of Stöckmann [47] and Haake [48]. The definition of quantum chaos is not clear, at first sight, since there are no quantum analog for Lyapunov exponents, separation of trajectories, and the quantum analogs of the Kolmogorov–Sinai entropy is still very much a topic of research. The simplest definition of quantum chaos is that it is the quantum mechanics of systems whose classical counterparts are chaotic. Berry refers to this as *quantum chaology* [49]. Such systems should exhibit features of classical chaos in the semiclassical limit.

There are a number of fundamental results obtained by workers in quantum chaos. These include Gutzwiller's trace formula [50], Schnirelman's Theorem [51], and Random Matrix Theory [47, 48, 52]. Gutzwiller's trace formula allows one to calculate the density of quantum states for a (classically chaotic) system in terms of a sum over all of the periodic orbits of the classical system. The quantity being summed depends on the action of the classical periodic orbit. Random Matrix Theory supposes that the eigenstates of a quantum system are distributed, typically, as if the Hamiltonian of the system were taken at random from an ensemble of Hamiltonians whose matrix elements are random variables with a particular distribution. For classically non-chaotic systems, the distribution of matrix elements obeys Poisson statistics, while for classically chaotic systems, the appropriate ensemble is Gaussian, with a detailed structure that depends upon the symmetries of the Hamiltonian. It has been conjectured by Bohigas, Gianonni, and Schmidt that this result is generic [53], and recently some progress has been made on proving this conjecture [54]. Schnirelman's Theorem is the one rigorous result in this field and it states that the wave function of a system whose classical counterpart is chaotic, becomes, in the semi-classical limit, $\hbar \rightarrow 0$, uniformly distributed over the constant energy surface. For further discussion of these topics, we refer to the books of Haake and of Stöckmann. Finally we mention that there are typically two well-separated time scales that are of importance for quantum chaos. The shorter of the two is called the *Ehrenfest time*, τ_E . The Ehrenfest time, τ_E , is roughly the time it would take for a minimal wave packet to grow to the size of some characteristic microscopic length of the system, which in turn is determined by a classical Lyapunov exponent [55]. In a Lorentz gas, this length would typically be the size of a scatterer. The typically longer time scale is called the *Heisenberg*

time and it is the time needed to see the effects of the spacing of energy levels. The Ehrenfest time is of the order of $\ln \hbar$ while the Heisenberg time is of the order of $\hbar^{-1}$ for small values of Planck's constant.

6.2. The quantum baker map

To illustrate some simple features of quantum chaos, we will describe the quantum version of the multi-baker map and compare some features of transport in a quantum multi-baker map with their classical counterparts, in the semi-classical limit. For further details, we refer to papers of Wojcik [9]. There is no unique way to quantize a map. In fact there are a few different ways of doing it, and one is allowed to work with the quantization one prefers. The only controlling feature is that in the classical limit, one should recover the classical map. It is typical for quantum versions of maps on the unit square, to have a range of values for Planck's constant. A simple reason is that the number of quantum states associated with an area, A in a $2d$ -dimensional phase space should be equal to A/h^d , where h is Planck's constant. For a map on a unit square, one can take $A = 1$, the number of quantum states, N is an integer, leading to the value for Planck's constant $h = N^{-1}$. Thus the classical limit can be associated with N large, while small $N = 1, 2, 3 \dots$ is the deep quantum regime.

Here we turn our attention to the quantum baker map and use a quantization method due to Balazs and Voros [56], and to Saraceno [57]. We begin with the quantized baker map and then proceed to the multi-baker map. We take the number of quantum states in the unit square to be an even integer, and associate half of them with the "right" quantum states $|q_n\rangle$, with $n = 0, \dots, N/2 - 1$, and the other half with the "left" quantum states, $|q_n\rangle$, with $n = N/2, \dots, N - 1$ in the position representation. There is a corresponding momentum representation of any quantum state, related to its position representation by a Fourier transform, according to

$$\langle q_n | p_m \rangle = \frac{1}{N^{1/2}} e^{i2\pi q_n p_m / N}, \text{ for } n, m = 0, \dots, N - 1. \quad (47)$$

Any state $|\Psi\rangle$ has representations as

$$|\Psi\rangle = \sum |q_n\rangle \langle q_n | \Psi \rangle = \sum |p_m\rangle \langle p_m | \Psi \rangle. \quad (48)$$

The specific values of q_n and p_m in Eq. (47) can be specified up to a phase angle, with $q_n = n + \phi_n$, with $0 \leq \phi_n \leq 1$ and $p_m = m + \phi_m$, with $0 \leq \phi_m \leq 1$. This sets up the quantum kinematics used in the baker map.

The Balazs-Voros formulation for the quantum-baker dynamics defines a time translation operator acting on the quantum state at discrete time

intervals. This time translation operator, or propagator, $\mathcal{B}$ is given, in the position representation, by

$$\Psi(t+1) = \mathcal{B}\Psi(t) = \mathbf{F}_N^{-1} \cdot \begin{pmatrix} \mathbf{F}_{N/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{F}_{N/2} \end{pmatrix} \Psi(t), \quad (49)$$

where $\mathbf{F}_N$ is an $N \times N$ matrix with elements

$$\mathbf{F}_N = \frac{1}{N^{1/2}} e^{-i2\pi q_n p_m / N}, \text{ for } n, m = 0, \dots, N-1. \quad (50)$$

The differences between the Balazs–Voros quantization of the baker map and that of Saraceno, are different choices of the phase angles ϕ_n, ϕ_m . The Balazs–Voros phases are simply $\phi_{n,m} = 0$, while Saraceno’s phases, $\phi_{n,m} = 1/2$ are designed to preserve more of the symmetries in the classical map. The stretching and squeezing that defines the classical baker map is described in the quantum version by the block-diagonal matrix on the right in Eq. (49). It takes a state in the position representation and transforms it to a new state but in the momentum representation. Then the inverse matrix to its left transforms the new state in the momentum representation to its form in the position representation. The operator $\mathcal{B}$ is a unitary $N \times N$ matrix, so all of its N eigenvalues lie on the unit circle. That is

$$\mathcal{B}|\theta_i\rangle = e^{i\theta_i}|\theta_i\rangle \text{ for } i = 0, \dots, N-1, \quad (51)$$

in an obvious notation. Schnirelman’s theorem implies that as $N \rightarrow \infty$ the quantum states become uniformly distributed over the unit interval in position space and in momentum space.

6.3. The quantum multi-baker map

The properties of the quantized baker map are very interesting, in their own right, but for our purposes here, we pass immediately to the multi-baker map, which is quantized in a similar way but with a translation of quantum states from one cell to the next at each step. We label the sites of the unit squares by the index k , and group the quantum states in cell k at any time t into “left” and “right” states in an obvious way, where the states $n = 0, \dots, N/2 - 1$ are included in the left state, $|\Psi^{(L)}(k, t)\rangle$, and the rest are included in the right state $|\Psi^{(R)}(k, t)\rangle$. The time translation operation for the multi-baker is then defined by

$$\begin{pmatrix} |\Psi^{(L)}(k, t+1)\rangle \\ |\Psi^{(R)}(k, t+1)\rangle \end{pmatrix} = \mathbf{F}(\mathbf{k})_N^{-1} \begin{pmatrix} \mathbf{F}(k-1)_{N/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{F}(k+1)_{N/2} \end{pmatrix} \begin{pmatrix} |\Psi^{(L)}(k-1, t)\rangle \\ |\Psi^{(R)}(k+1, t)\rangle \end{pmatrix}. \quad (52)$$

Here we have indicated that the left states from site $k - 1$ and the right states from site $k + 1$ all get transported to site k . The matrices can depend on the sites k through the choice of the phase angles. In this version the quantum states are “stretched and squeezed” at their “home” cells, which leaves the new state in the momentum representation. These states are then transformed to the position representation at the new cell.

The freedom to choose phases in the operators, which seems just an unnecessary complication for the quantum baker map, has some real value for the quantum multi-baker map. One can study periodic, crystal-like, systems by choosing the identical phases in every cell, or one can study localization by choosing phases randomly for one cell to the next. In fact, any kind of arrangement of the phases is possible so that with the wide range of choices, the model is quite rich and useful. It is interesting to note that for $N = 2$, and phase angles set equal to zero, the quantum multi-baker map is the *Hadamard walk*, a simple quantum random walk much studied in the theory of quantum computation, as an example of a search algorithm for a quantum computer [5]. The hope is to take advantage of the difference between the quantum mechanical, ballistic motion for a particle in a periodic lattice, as opposed to the classical diffusive motion in the same lattice.

Here we are going to discuss briefly the mean square displacement of a particle in the quantum mechanical, periodic, multi-baker system, with Balazs–Voros phases, $\phi_{n,m} = 0$. As just mentioned, we expect to see a difference between the classical and quantum cases. We will denote the propagator for the quantum multi-baker map with L sites, and with periodic boundary conditions by $\mathcal{M}$. The time dependence of an observable Ω is, as usual

$$\Omega(t) = \mathcal{M}^{\dagger t} \Omega \mathcal{M}^t. \quad (53)$$

The mean square displacement, δ_t^2 is defined by

$$\begin{aligned} \delta_t^2 &\equiv \left\langle (\delta \mathbf{r}(t) - \mathbf{r})^2 \right\rangle \\ &= \text{Tr} \left[\left(\mathcal{M}^{\dagger t} \mathbf{r} \mathcal{M}^t - \mathbf{r} \right)^2 \rho_{\text{eq}} \right], \end{aligned} \quad (54)$$

where a trace is taken over the equilibrium density matrix, given by

$$\rho_{\text{eq}} = \frac{\mathbf{1}}{NL}. \quad (55)$$

This density matrix is normalized over the N states in each of the L cells.

After some manipulations based upon the isotropy of the lattice — all the cells are identical and the phases are all the same — and upon the time

translation invariance of the equilibrium average, the mean square displacement can be expressed entirely in terms of the propagator for a single cell, $\mathcal{B}$ and written in the Green–Kubo form

$$\delta_t^2 = C_0 t + 2 \sum_{\tau=1}^{t-1} (t - \tau) C_\tau, \quad (56)$$

where C_τ is a time correlation function for the velocity of the particle given by

$$C_\tau = \frac{1}{N} \text{Tr} \left[(\mathcal{B}^\dagger)^t \mathbf{J} \mathcal{B}^t \mathbf{J} \right]. \quad (57)$$

The velocity operator $\mathbf{J}$ can be taken to have the simple form

$$\mathbf{J} = \begin{pmatrix} \mathbf{1}_{N/2} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1}_{N/2} \end{pmatrix}, \quad (58)$$

which expresses the fact that half the states move one unit to the right and half move one unit to the left. The trace in Eq. (57) is over the N states of the baker propagator $\mathcal{B}$. Except for small values of N where one can explicitly calculate the various matrix products needed above, it is useful to express the velocity correlation functions and the mean square displacement in terms of the eigenstates, $|j\rangle$, and eigenvalues, $\exp i\theta_j$ of $\mathcal{B}$. This leads in a straightforward way to an expression for the mean square displacement given by

$$\delta_t^2 = \frac{1}{N} \sum_{j,k} |J_{jk}|^2 \frac{\sin^2 \left[\frac{(\theta_j - \theta_k)t}{2} \right]}{\sin^2 \left[\frac{(\theta_j - \theta_k)}{2} \right]}. \quad (59)$$

This is about as far as one can go using simple analytical methods. To get explicit results one can use computational methods to determine the eigenvalues and eigenstates of $\mathcal{B}$, to provide a numerical result, or one can use random matrix theory to evaluate this expression, assuming that the eigenstates are sampled from those for a random distribution of unitary matrices, given by one of the random matrix ensembles for the quantum states of a classically chaotic system. These various distributions depend on the symmetry properties of the unitary matrices, but they are well known and called *circular ensembles* [52].

In figure 12 we show the results of both methods for comparison. Both calculations lead to a crossover from diffusive motion, with a linear growth in the mean square displacement with time, to ballistic motion, where the time dependence becomes quadratic. Roughly speaking, it takes the particle some time to notice the periodicity of the lattice and build a Bloch wave. Before that time, the motion is diffusive and afterwards, the motion is ballistic.

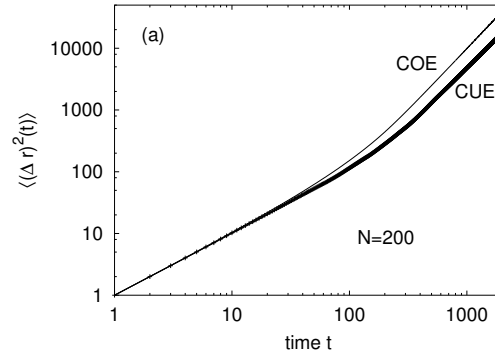


Fig. 12. The mean square displacement for a quantum multi-baker map as a function of time for a large value of the inverse Planck constant, $N = 200$. The two curves show results obtained by using the circular orthogonal ensemble (COE) and the circular unitary ensemble (CUE). The solid line shows results from the numerical simulation of the model.

This time is of the order of the Heisenberg time, namely, of the order of the inverse of Planck's constant, for small values of N^{-1} . Also evident in this figure is the fact that Random Matrix Theory, while not exact, gives a good approximation to the correct result for large N . There are also slight differences between the results obtained by using different ensembles.

7. Discussion

These notes have attempted to describe some of the insights gained by looking at the theory of irreversible processes from the point of view of dynamical systems theory. The mathematical description of isolated systems of particles with chaotic dynamics provides useful notions for understanding the approach of a non-equilibrium system to a state of local equilibrium. These notions include the exponential separation of phase space trajectories and the existence of stable and unstable manifolds in phase space. Since statistical mechanics is primarily concerned with projections of phase space distributions of many variables onto space of only a few variables, the smoothing provided by the motion of phase points in unstable directions can be seen as a source of an approach of reduced distributions to local equilibrium forms. This picture has been verified in detail only for systems with very few degrees of freedom in total, such as the baker map or the Arnold cat map. While it is reasonable to expect that a similar picture applies to chaotic systems with many more degrees of freedom, this has by no means been verified by analytical methods. It is important to note that ergodic

and mixing properties of a dynamical system are insufficient for a full explanation of the approach to equilibrium as seen on laboratory time scales. However, we argued that if the microscopic system has positive Lyapunov exponents connected to unstable manifolds in the phase space, an approach to equilibrium of reduced distribution functions can occur on much shorter times scales than those needed to establish the mixing of phase space regions throughout the entire phase space. Once local equilibrium has been established in a fluid, then the possibility exists for hydrodynamic type motion of the system on time and space scales that are determined by the macroscopic boundary conditions and typically much larger than the time and spatial scales on which local equilibrium is established.

While the above qualitative description of the approach to local equilibrium is plausible for systems with chaotic dynamics, chaotic dynamics is neither necessary nor sufficient for the appearance of normal transport processes. Examples of non-chaotic systems with normal diffusive properties are provided by pseudochaotic systems, such as the random wind-tree model. While such models cannot represent a real system of particles, the mathematical questions they raise are often important for a full understanding of more realistic systems. In order to understand the behavior of pseudochaotic systems, one needs to extend dynamical systems theory to cover situations where the separation of trajectories is algebraic rather than exponential. While there has been considerable progress in this direction, there appear to be some mathematical issues to be resolved, for some cases, at least, and, as in the case of chaotic dynamics, the full picture is far from completion.

Most realistic systems of particles are not fully chaotic. Instead they are *mixed* systems, in which the phase space has both chaotic and non-chaotic regions. This is true even of systems of interacting spheres with softer potentials than hard spheres [16]. What effect the non-chaotic regions have on the non-equilibrium behavior of such systems is still a largely open problem. Moreover, as external perturbations are very likely to play a role in the approach of a system, chaotic or not, to equilibrium, if only to help the system explore more of the phase space on a short time scale, one needs to continue the study of the behavior of all these types of systems under the influence of random perturbations.

In these lectures we only touched upon the behavior of quantum systems, in so far as transport processes and the approach to thermodynamic equilibrium is concerned. This subject is very complex since quantum mechanics requires a different way of looking at transport phenomena and provides a richer variety of behaviors than classical mechanics. This subject is clearly of great importance for understanding the behavior of *mesoscopic* quantum devices such as quantum dots and related materials. The understanding of the approach to equilibrium in macroscopic systems, requires a treatment of

quantum systems with a very large number of degrees of freedom. Such systems are not likely to be in one or in a superposition of a few quantum states. Instead, such systems are likely to be in a state that is a superposition of a huge number of quantum states, and destructive interference of the phase relations among the states is an important ingredient of the behavior of such systems. In fact there is a large literature that deals with the phenomenon of the loss of coherence, or *decoherence*, of superpositions of large numbers of quantum states for a macroscopic system, and helps us understand a bit more clearly why classical mechanics is a good approximation for describing systems that we know to be intrinsically quantum mechanical. An important role in this area is played by the notion of looking at projections of wavefunctions onto various subspaces of the system [58]. Thus we appear to come full circle, the need for projecting functions onto subspaces of lower dimension is common to both classical and quantum statistical mechanics. This topic, too, is in need of further study and improvement.

It is a pleasure to thank my hosts for this summer school, The Institute of Theoretical Physics, University of Warsaw, particularly Jarosław Piasecki, Marek Napiórkowski, and Bogdan Cichocki, for their kind hospitality and for the opportunity to be a part of this program. Much of what is discussed here has been the result of work and many conversations, with Pierre Gaspard, Henk van Beijeren, Thomas Gilbert, Daniel Wójcik, and many others. I wish to acknowledge their help and their insights into the physics discussed here. I also thank Matthew Reames for help with some of the figures. Finally I acknowledge the National Science Foundation for support under NSF Grant PHY-01-38697.

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