ELSEVIER

Physica A 240 (1997) 12–42

PHYSICA A

Dynamical systems theory and transport coefficients: A survey with applications to Lorentz gases

J.R. Dorfman[a,*], Henk van Beijeren[b]

[a] *Institute for Physical Science and Technology, and Department of Physics, University of Maryland, College Park, MD 20742, USA*

[b] *Institute for Theoretical Physics, University of Utrecht, Postbus 80006, Utrecht, Netherlands*

Abstract

Recent developments in the applications of ideas from dynamical systems theory to transport phenomena in non-equilibrium fluids are reviewed. We discuss methods for expressing transport coefficients for fluid systems in terms of dynamical quantities that characterize the chaotic behavior of the phase-space trajectories of such systems. We describe two such methods: the escape rate method of Gaspard and co-workers, and the Gaussian thermostat method of Hoover, Posch and co-workers, and of Evans and Morriss and co-workers. Related issues such as the properties of repellers and attractors and of entropy production in such systems will be discussed. As examples of these formal developments, we describe recent work on Lorentz gases where the escape rate and Gaussian thermostat approaches to transport can be implemented in detail and the results compared with both numerical simulations and with the results of kinetic theory of gases.

1. Introduction

It is not immediately obvious that there should be a close relation between the chaotic properties of statistical mechanical systems, describing, for example, fluids, and their transport properties, such as shear viscosity, heat conductivity and diffusion coefficients. After all, the kinetic equations that are used to compute transport coefficients, such as the Boltzmann equation, the Enskog equation, and their generalizations, are derived by kinetic theory arguments based either on some rather straightforward stochastic reasoning (e.g. Boltzmann's *Stoßzahlansatz*) or on cluster expansion solutions of the Liouville equation (more precisely, the BBGKY hierarchy equations)

* Corresponding author. E-mail: jrd@ipst.umd.edu.

PII S0378-4371(97)00128-3

obtained under reasonable assumptions on the initial state of the system[1] [1,2]. In this way excellent predictions are obtained for transport coefficients of a wide class of fluid systems, though no mention is made anywhere of the chaotic properties of the system. Nevertheless, it is widely realized that the foundations of kinetic theory must be based, for classical systems, at least, on the ergodic and mixing properties of the phase-space trajectories for the system, considered as an isolated, Hamiltonian, mechanical system [3]. The aim of the research directions surveyed in this paper is to make the connection between the transport properties of the system and the underlying chaotic properties much more apparent, and to relate, whenever possible, quantities characterizing transport processes, such as transport coefficients, to quantities characterizing the system's chaotic properties, such as Lyapunov exponents, Kolmogorov–Sinai entropies, and so on. That it has been possible to make this connection has been one of the most interesting developments in transport theory over the past decade. Moreover, we will show that several quantities that are defined in dynamical systems theory, such as Lyapunov exponents, KS-entropies and the dimensions of fractal repellers and attractors, are amenable to calculation by familiar techniques in statistical mechanics. The results may be compared with computer simulations, presently, and perhaps with experiment, in the future.

In order to give a first, simple example of how one can understand the connection between chaos and transport, we will discuss a well-known model for a chaotic system, the baker's map, in Section 2. In Section 3 we will present the escape rate method of Gaspard and co-workers which introduces the construction of a fractal repeller in phase-space, and relates transport coefficients to the dynamical properties of trajectories confined to this repeller, and to the geometric structure of the repeller. In the escape rate formalism, transport coefficients are expressed in terms of the mean first passage time of trajectories through appropriately constructed boundaries in phase-space. The connection to chaotic properties of the system is made by expressing the escape rate in terms of Lyapunov exponents and the KS-entropy of trajectories on the fractal repeller [4]. In Section 4 we present an alternative approach due to Hoover, Posch, Evans, Morriss and co-workers [5], which considers the dynamical behavior of a system in contact with an external force field as well as with a Gaussian thermostat which maintains a constant kinetic or total energy in the system. Here the combination of the external field and the thermostat forces the phase-space trajectories onto an attractor, generally a fractal of lower dimension than the phase-space itself, and the transport coefficients are determined by the average rate of contraction of the phase-space volume along the trajectories of the system. This rate of contraction is also determined by the Lyapunov exponents for the trajectories in phase-space, so the connection between chaotic and

[1] Here we regard the hypothesis of "molecular chaos" used in the derivation of the Boltzmann equation as a stochastic assumption. Our ultimate goal is to justify this assumption on the basis of a more fundamental approach to molecular dynamics, using methods based on recent advances in dynamical systems ("chaos") theory.

transport properties can be easily obtained, at least in a formal way. Of course, the second law of thermodynamics is at the center of our discussions, so in Section 5 we consider the definition and role of entropy production in these systems and discuss briefly some of the current thinking on this issue [6–8]. In Section 6 we illustrate the formal developments discussed in the earlier sections by applying them to the case of the diffusion of a moving particle in a random array of fixed hard disk or hard sphere scatterers. This is the Lorentz gas, and for it, we can calculate all of the transport and chaos quantities that appear in the various expressions under discussion, at least if the density of scatterers is low enough [9–11]. We also compare the theoretical results with the computer simulations of Dellago and Posch, and find excellent agreement [10,12]. We conclude in Section 7 with a number of remarks about current and future research directions.

2. The baker's map

The clearest and simplest example of a dynamical system that exhibits all of the features one would like to see in a fundamental description of transport in a fluid system is provided by the baker's map of a unit square in a plane onto itself. We think of the unit square as a "metaphorical" form of a phase-space for a large system of particles. We discretize the time so that phase-space trajectories move only at unit time steps rather than continuously in time. The baker's map is an invertible, measure-preserving transformation of the square given by

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \mathbf{B} \cdot \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 2x \\ y/2 \end{pmatrix} \qquad \text{for } 0 \leqslant x \leqslant \tfrac{1}{2}\,,$$

$$= \begin{pmatrix} 2x-1 \\ (y+1)/2 \end{pmatrix} \quad \text{for } \tfrac{1}{2} < x \leqslant 1\,. \tag{1}$$

One sees immediately that there is a stretching of intervals in the x direction by a factor of 2, and a contraction of y intervals by a factor of $\frac{1}{2}$. This is accompanied by a shifting of the right-half of the resulting rectangle in order to recover a unit square, as illustrated in Fig. 1. The inverse transformation is easily obtained, and is

$$\begin{pmatrix} x'' \\ y'' \end{pmatrix} = \mathbf{B}^{-1} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x/2 \\ 2y \end{pmatrix} \qquad \text{for } 0 \leqslant y \leqslant \tfrac{1}{2}\,,$$

$$= \begin{pmatrix} (x+1)/2 \\ 2y-1 \end{pmatrix} \quad \text{for } \tfrac{1}{2} < y \leqslant 1\,. \tag{2}$$

The baker's transformation is ergodic and mixing, so that on repeated application non-equilibrium averages of microscopic functions on this "phase-space" approach their equilibrium values, obtained from a uniform distribution on the unit square [2,13]. Given the inverse transformation, we can write down a discrete version of Liouville's

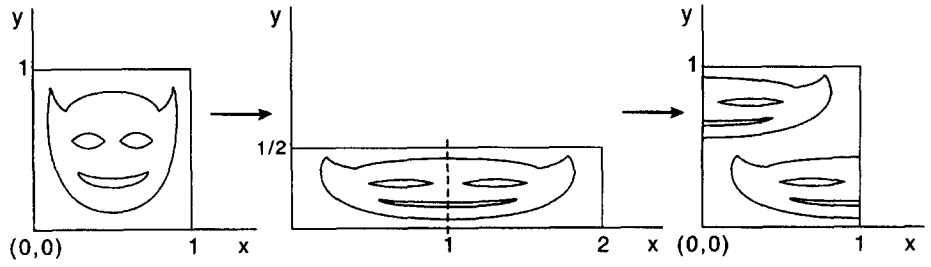

Fig. 1. The baker's map on the unit square. The square is stretched by a factor of 2 in the x- direction, and by a factor of $\frac{1}{2}$ in the y-direction, and then rearranged to form a unit square.

equation for a non-equilibrium distribution on the unit square, which is

$$\begin{aligned}\rho_n(x,y) &= \rho_{n-1}(\mathbf{B}^{-1}(x,y)) \\ &= \rho_{n-1}(x/2, 2y) \qquad \text{for } 0 \leqslant y \leqslant \tfrac{1}{2}, \\ &= \rho_{n-1}((x+1)/2, 2y-1) \quad \text{for } \tfrac{1}{2} < y \leqslant 1. \end{aligned} \tag{3}$$

Here $\rho_n(x,y)$ is the phase-space distribution function at the nth time step.

Now for many particle systems one derives useful transport equations from the Liouville equation by integrating the equation over all but a few degrees of freedom so as to obtain equations for reduced distribution functions (i.e. the BBGKY hierarchy equations) [1]. It is useful and instructive to see how a similar procedure works for this simple "Liouville" equation in the baker's transformation. In keeping with this picture, we now derive an irreversible transport equation by integrating $\rho_n(x,y)$ over the y variable to obtain a function $W_n(x)$. For reasons to be made clear in a moment, this would correspond, in a more complete discussion of transport theory, to a projection of the full phase-space distribution function onto the distribution function that describes slow, hydrodynamic processes taking place in the system. An elementary integration over the y variable in Eq. (3) leads to

$$\begin{aligned} W_n(x) &= \int_0^1 \rho_n(x,y)\,dy \\ &= \int_0^1 \rho_{n-1}(\mathbf{B}^{-1}(x,y))\,dy \\ &= \frac{1}{2}\left[W_{n-1}\left(\frac{x}{2}\right) + W_{n-1}\left(\frac{x+1}{2}\right)\right]. \end{aligned} \tag{4}$$

The resulting equation is familiar to dynamical systems theorists who know it as the Perron–Frobenius equation for the dyadic map $x' = 2x \bmod 1$ [14]. A great deal is known about its properties [15,16], but here we will concentrate on its properties as a model for an irreversible transport equation. This equation has many features

similar to those of the Boltzmann equation in kinetic theory, as well as some important differences. First we note the similarities.

There is an H-theorem for this equation indicating a monotonic approach to equilibrium from some arbitrary non-equilibrium initial state. Here the H-function is defined by

$$H_n = \int_0^1 W_n(x) \ln W_n(x)\, dx\,. \tag{5}$$

The H-theorem, $H_n \leqslant H_{n-1}$, follows from the observation that $z \ln z$ is a convex function of z such that any chord connecting two points on the curve lies above the curve. One can also verify that solutions to Eq. (4) approach a uniform distribution $W_{eq}(x) = 1$, exponentially rapidly with a decay rate of $\ln 2$. In this respect, Eq. (4) displays the properties of a typical transport equation, but it is not quite analogous to a Boltzmann equation. It rather resembles a master equation for a diffusion process. In a generalization of the baker map to systems of macroscopic scale, the multibaker map, described by Gaspard and Tasaki [18,19], the corresponding distribution function satisfies an equation similar to Eq. (4) on a microscopic scale and reduces to a macroscopic diffusion equation on a large spatial scale. By extending this further to multibaker maps on phase-space one can derive generalized Fokker–Planck equations for the distribution functions for mass, momentum, and energy of the type introduced by Green [17]. We conclude from this that the function $W_n(x)$ is not quite a direct analog of the single-particle distribution function that satisfies the Boltzmann equation.

However, with almost no effort whatsoever we have been able to go from a time-reversible Liouville equation to an irreversible transport equation simply by integrating over one of the degrees of freedom of the system. In order to understand this at a somewhat deeper level, we first note that we did not integrate over the x variable, and that if we had, we would have obtained a much less transparent equation for the distribution function in y. The reason for this is connected to the fact that the baker's map is expanding in the x direction and contracting in the y direction. Any small region of the unit square will, as time increases, become stretched in the x direction, with a projection along the x-axis that looks more and more uniform. However, its projection along the y-axis becomes more and more fragmented as time increases, becoming a fractal set in the limit as $n \to \infty$. Consequently, any initial distribution in x and y, $\rho_0(x, y)$ will lead to a $\rho_n(x, y)$ which becomes smooth as a function of x for large n, but very rapidly changing with y. Integrating over the y variable, we obtain a function of x, $W_n(x)$, which is approaching a uniform equilibrium distribution $W_{eq}(x) = 1$.

The x direction, which is the direction of stretching or expansion, is called the *unstable* direction, and the y, or contracting direction, is called the *stable* direction [14]. The reason for these names is that the distance, $|\mathbf{B}^n(x, y) - \mathbf{B}^n(x + \delta x, y)|$, between the nth image, under the baker's map, of an arbitrary point (x, y) in the plane and the nth image of nearby points with the same y coordinate, but slightly differing x coordinates will separate exponentially with n as 2^n, for almost all x. However, the

distance $|\mathbf{B}^n(x,y) - \mathbf{B}^n(x,y+\delta y)|$ approaches zero with n as 2^{-n}, for almost all y. The exponential separation is characterized by a *Lyapunov* exponent of $\ln 2$, and the exponential approach is characterized by a negative Lyapunov exponent $\ln(\frac{1}{2})$. Note that the sum of the two Lyapunov exponents is zero, which is a consequence of the conservation of volume in our phase space, the unit square. It is also worth noting that the images of almost any two nearby points will separate exponentially with n for large n, as a consequence of the fact that two nearby points chosen at random will have different x-coordinates, with probability 1. Finally, we remark that it is possible to extend the dynamics of the baker's transformation to a model for diffusion of particles in the x-direction, which is a deterministic form of the usual random walk on a one-dimensional lattice with equal probabilities of jumping to the right or to the left [19,20].

Our analysis has assumed that the initial distribution $W_0(x)$ is reasonably smooth. There are initial values of this distribution which do not lead to an equilibrium distribution. Examples are distributions containing delta functions on the periodic points of the map $x' = 2x \bmod 1$. E.g. one can easily check that $W_0(x) = \frac{1}{2}[\delta(x-\frac{1}{3}) + \delta(x-\frac{2}{3})]$ is a solution of Eq. (4) which does not approach equilibrium but instead stays constant with n. Other examples involve distributions that are non-zero on a fractal subset of the unit interval and zero everywhere else. E.g. one can choose the subset of all points with a binary expansion without consecutive zeroes. Later on we will encounter invariant distributions on fractal repellers that are precisely of this nature. For instance, in the appendix we consider a map closely related to Eq. (4) which has the form

$$W_n(x) = \frac{1}{2}\left[W_{n-1}\left(\frac{x}{4}\right) + W_{n-1}\left(\frac{x+3}{4}\right)\right]. \tag{6}$$

It has an invariant solution which is a uniform distribution on the "middle-$\frac{1}{2}$" Cantor set, which is obtained by deleting from the unit interval first the interval $[\frac{1}{4}, \frac{3}{4}]$, next the intervals $[\frac{1}{16}, \frac{3}{16}]$ and $[\frac{13}{16}, \frac{15}{16}]$, etc. [21].

In summary, the ingredients in the derivation of the transport equation from the Liouville equation for the baker's map are: (1) Under this map the phase space can be decomposed into stable and unstable directions about almost every point, with associated non-zero Lyapunov exponents. (2) One considers reduced distribution functions where the dependence upon the coordinates in the stable directions is removed by integration. (3) The initial distributions are sufficiently smooth functions of their coordinates, certainly not containing delta functions on dynamically periodic points or distributions that are concentrated on fractal subsets of the unit square. (4) If one considers the time-reversed motion, then the stable and unstable directions are interchanged, and the appropriate reduced distribution functions must be defined on the coordinates associated with the "new" unstable directions. The fact that distributions become smooth with time in the unstable directions has led to the development of a theory for SRB (Sinai–Ruelle–Bowen) distributions in phase space. We refer the reader to [22,23] for details.

We see in this simple model that an understanding of the transitions from the Liouville equation to irreversible transport equations with well-defined transport

coefficients can be based upon the analysis of trajectories in phase-space, the existence of stable and unstable directions about almost any point in phase-space, and upon the Lyapunov exponents that characterize the rates of expansion and contraction of intervals in phase-space along these various directions. However, there is still much that needs to be clarified before we can say that the transition from the Liouville equation to transport equations in general can be understood from this more fundamental point of view. Here we mention that the Boltzmann equation for the single-particle distribution function for a dilute gas is obtained by integrating the N-particle distribution function over the phases of all but one particle, and by making some assumptions about the properties of the N-particle function at some initial time. This does not directly correspond to a projection onto an unstable manifold, so that the decay to equilibrium obtained from the Boltzmann equation cannot be interpreted precisely the same way as the decay of $W_n(x)$ in the baker's map. Exactly how these things are connected is one of the interesting open questions which we discuss further in Section 6.

In the baker's map we see ingredients which are common to all of the recent studies of the dynamical foundations of transport theory for fluids. One typically assumes that the forces between the particles are such that the system can be described as a hyperbolic dynamical system [22]. That is, one supposes that stable and unstable directions can be defined at almost every point in the (generally high-dimensional) phase-space of the system and that the directions are all transverse to one another so as to avoid complications due to tangent directions. Further, one supposes that all of the Lyapunov exponents associated with these directions are bounded away from zero, with the exception of zero exponents connected with the usual symmetries of the system – time translations, spatial translations and rotations and Galilean boosts – as far as compatible with the boundary conditions imposed on the system. Gallavotti and Cohen [24], following a similar suggestion of Ruelle [25] for the study of turbulence, have emphasized that this hypothesis – which they denote as the Chaotic Hypothesis – forms an excellent starting point for the analysis of fluid systems from a dynamical point of view.

In the next section we will discuss the escape rate formalism, which shows how one can connect transport coefficients and dynamical quantities for fluid systems obeying classical mechanics.

3. The escape rate formalism

The escape rate formalism makes the connection between transport coefficients and dynamical quantities by showing that an exponential decay of the density of particles on some bounded region in space, or more generally, of a phase-space density on some bounded region in phase-space, can be expressed in terms of a macroscopic "diffusion coefficient" as well as a simple combination of microscopic dynamical quantities [4,26]. For example, consider some region of space, $\mathscr{R}$, in d dimensions that is occupied by fixed scatterers placed at random in the region. Suppose further that $\mathscr{R}$ is characterized

by some length L which is much larger than the average spacing, l, between the scatterers as well as the mean free path ℓ between subsequent collisions of a small moving particle with the scatterers. Then such a particle will undergo a diffusive motion in $\mathscr{R}$ on a length scale that is large compared to l and to ℓ, but small compared to L, provided the interaction potential between the particle and the scatterers is such that the dynamics of the moving particle is hyperbolic – think of hard-sphere-type interactions. Suppose further that the region $\mathscr{R}$ is surrounded by absorbing boundaries so that if the particle crosses a boundary it is removed from the system. Then it follows from the diffusion equation that if the particle is placed in the region at $t=0$ with some velocity, the probability $P(t)$ that the particle will still be in the region at time t later is, for large t, given by

$$P(t) \sim e^{-\gamma t}, \tag{7}$$

where the escape rate γ is

$$\gamma = D\frac{a}{L^2}, \tag{8}$$

with D the diffusion coefficient, and a a constant determined by the geometric structure of $\mathscr{R}$. Typically it is of order π^2. This is the macroscopic approach to the escape rate. There is another approach based upon dynamical considerations which leads to the expression

$$\gamma = \sum_{\lambda_i > 0} \lambda_i(\mathscr{R}) - h_{KS}(\mathscr{R}). \tag{9}$$

To understand this expression, one considers the set of initial positions and velocities of the moving particle in $\mathscr{R}$ such that: (a) the particle never leaves $\mathscr{R}$ for arbitrarily long times t; and, (b) if one follows the time-reversed motion of the particle from the initial point, the particle never leaves the system as $t \to -\infty$. This set of initial points is called a *repeller*. That is, this set defines trajectories that never leave $\mathscr{R}$. It is generally a fractal set of measure zero in the phase-space of the moving particle, and its name derives from the fact that particles starting from points near the repeller will eventually leave the system. The quantities $\lambda_i(\mathscr{R})$ are the Lyapunov exponents for the trajectories on the fractal repeller. The quantity h_{KS} is the Kolmogorov–Sinai entropy of the repeller [14]. This is a somewhat complicated object, but it can be understood intuitively in the following way: Suppose one can distinguish points in phase space with a finite resolution δ (if needed coordinates may be rescaled so as to obtain the same resolution in all directions). Then phase-space can be divided into $\mathscr{N} = \mathscr{V}(\mathscr{R})/\delta^d$ subvolumes, with $\mathscr{V}(\mathscr{R})$ the accessible phase-space volume of $\mathscr{R}$ and d its dimensionality, such that one can just distinguish in which of these subvolumes, say $\mathscr{V}_0$, an initial point is located. If subsequently one follows this initial point and observes where it is found at a sequence of later times, one can determine with ever increasing accuracy in which part of $\mathscr{V}_0$ the point actually was located initially. How this goes becomes most transparent if one chooses the subvolumes in such a way that their boundaries run

along the expanding and contracting directions (e.g. for the baker's transformation one chooses them as squares with sides parallel to the x- and y-axis). Such a division is known as a *Markov partition* [27]. After a long time t the cross section of an initial subvolume in the subspace spanned by the expanding directions has increased by a factor $\exp(\sum_{\lambda_i>0}\lambda_i t)$, so, with the same resolution δ the number of distinguishable initial boxes to which the phase point can be assigned has increased by the same factor. However, of all these boxes only a fraction $\exp(-\gamma t)$ has remained inside $\mathscr{R}$, the other ones having escaped through the boundaries. So the number of distinguishable boxes *on the repeller* increases as the product of the above two exponential factors. The logarithm of this therefore is the rate at which information is gained on the initial location of a typical phase point and it can be used to define the Kolmogorov–Sinai entropy, h_{KS}. That is, one writes

$$e^{th_{KS}} = e^{t\sum_{\lambda_i>0}\lambda_i} \cdot e^{-t\gamma}. \tag{10}$$

By taking logarithms and dividing by the time we obtain the escape rate formula (9). The construction given here leads to the observation that the trajectories which never escape from the region form a fractal structure, which we have called a repeller. Here we see that the escape rate formula is a natural result of this intuitive definition of h_{KS} as the rate of information retrieval. In the appendix we illustrate the construction and properties of a simple one-dimensional repeller based upon a generalization of the dyadic map of the previous section. There we will compute the escape rate, Lyapunov exponent, and KS-entropy appropriate for the repeller, and show that a generalized Perron–Frobenius equation, given by Eq. (6), governs an invariant distribution on this fractal repeller.

The crucial step of Gaspard and Nicolis [4] was to combine the two expressions for the escape rate, Eqs. (8) and (9), so as to obtain a relation between the diffusion coefficient and the dynamical quantities given by

$$D = \lim_{L\to\infty} \frac{L^2}{a}\left[\sum_{\lambda_i>0}\lambda_i(\mathscr{R}) - h_{KS}(\mathscr{R})\right]. \tag{11}$$

This is the main result of the escape rate formalism applied to the diffusion coefficient of a moving particle in an array of scatterers. A number of points are in order. There is a theorem due to Pesin that shows that for *closed* hyperbolic systems the KS entropy is equal to the sum of the positive Lyapunov exponents [22]. We have been discussing *open* systems and Eq. (11) shows that the sum of the positive Lyapunov exponents on the repeller is equal to the KS entropy on the repeller plus terms of order L^{-2}, if a normal diffusion coefficient exists. If the difference decays to zero faster than L^{-2} the diffusion coefficient must vanish, while if the difference decays more slowly, the diffusion is anomalous, with infinite diffusion coefficient implying a breakdown of normal diffusion, as one might expect for the case of self-diffusion in two-dimensional hydrodynamical systems [1,28] or for periodic billiards with infinite horizon [29]. The geometric factor a must not appear in the final expression for the diffusion coefficient.

Therefore, the difference between the sum of the positive Lyapunov exponents and h_{KS} on the repeller must be proportional to a for large systems. The limit $L \to \infty$ should also take care of any other finite-size effects, say of order L^{-3}, which are not needed for the diffusion coefficient.

This method has been extended to all of the other transport coefficients for simple fluids [30]. The main idea behind this extension is the following. We relate the diffusion coefficient to the mean square displacement of the moving particle with time, i.e., by the Einstein relation

$$\langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \rangle = 2dDt \quad \text{as } t \to \infty . \tag{12}$$

Here $\mathbf{r}(t)$ is the position of the moving particle in d-dimensional space at time t, and the angular brackets denote an average over an equilibrium ensemble of scatterers and moving particles. The linear growth of the mean square displacement with t indicates the diffusive nature of the motion of the moving particle, of course. All other transport coefficients for simple fluids also can be expressed in terms of the mean square fluctuation with time of an associated quantity called a Helfand moment. For example, the coefficient of shear viscosity, η, can be expressed in terms of the equilibrium fluctuations of its associated Helfand moment M_η, as

$$\langle (M_\eta(t) - M_\eta(0))^2 \rangle = 2\eta t \quad \text{as } t \to \infty , \tag{13}$$

where the angular brackets denote an average over the equilibrium canonical ensemble for an N particle system in a volume V, taken in the thermodynamic limit $N \to \infty, V \to \infty$, $N/V = n$, and the Helfand moment is

$$M_\eta = (Vk_BT)^{-1/2} \sum_{i=1}^{N} x_i p_{iy} . \tag{14}$$

Here T is the temperature, k_B is Boltzmann's constant, x_i is the x-coordinate of particle i and p_{iy} is the component of its momentum in the y-direction. Therefore, the Helfand moment undergoes a random walk in phase-space like the random walk that the position vector of a diffusing particle undergoes in ordinary configuration space. Thus, the basic idea of the escape rate method can be applied to a phase-space region, $\mathscr{X}$ on which the Helfand moment is bounded, say $|M_\eta| \leqslant X$, where X is some finite number, and from which most trajectories will escape through the boundaries on which M_η assumes the values $\pm X$. Thus, we can express the shear viscosity η as

$$\eta = \lim_{X \to \infty} \frac{X^2}{a_\eta} \left[\sum_{\lambda_i > 0} \lambda_i(\mathscr{X}) - h_{KS}(\mathscr{X}) \right] . \tag{15}$$

Similar results obtain for the other transport coefficients, such as thermal conductivity, and for reaction rate coefficients, as well. The escape rate method has been applied to a number of model systems. Gaspard has investigated the application to the multibaker map mentioned earlier [18]. Gaspard and Baras have studied the application to diffusion

of a moving particle in a periodic, triangular array of hard disk scatterers (the periodic Lorentz gas) at sufficiently high density that it is impossible for a particle to move through the lattice without collisions with the scatterers, i.e., the case of a "finite horizon" [31]. Van Beijeren et al. [9,32] have studied the escape rate formalism for the diffusion of a moving particle in a system of hard sphere or hard disk scatterers placed at random in space or in the plane, respectively (the random Lorentz gas). For the case where the density of scatterers is low, it has been possible to compute the Lyapunov exponents on the repeller using methods familiar from the kinetic theory of gases. We will discuss these latter calculations in Section 6. Ernst and co-workers have made an extensive analytical and numerical study of the application of the escape rate formalism to diffusion in a Lorentz lattice gas (LLG) [33]. This is a model in which a moving particle is placed on a lattice with a velocity in one of the lattice directions. Fixed scatterers are distributed at random on the lattice with a certain density. The moving particle travels from site to site at unit intervals. If at a given site there is no scatterer, the particle retains its velocity and moves to the next site in the same direction. However, if the particle encounters a scatterer at a given site, the direction of its velocity is changed to a new lattice direction according to some collision rule. If the collision rule is stochastic, that is, the change of velocity direction at a collision is determined by some pre-assigned probability, then the diffusion is normal. Kinetic theory and mean field theory methods can be used to compute the diffusion coefficient as a function of the density of scatterers [34]. The same or similar methods can be used to calculate the quantities appearing in the escape rate formula, as well. In this way it has been possible to compute the sum of the positive Lyapunov exponents on the repeller and to compare the results with numerical simulations. In the limit that the scatterers occupy all of the sites on the lattice the LLG model reduces to the so-called persistent random walk model. For this case, Ernst and Dorfman have made a rather detailed study of the Lyapunov exponents and other properties of the repeller [35]. This model is somewhat simpler than the general LLG model because density fluctuations in the distribution of scatterers do not occur.

There are many open problems in the escape rate method waiting for solution. We know very little about the structure of the repellers that appear to underly transport processes. For two-dimensional systems one knows something about the fractal dimension of the repeller from Young's formula [14], since the fractal dimension of the repeller is then equal to $h_{KS}(\mathscr{R})/\lambda^{+}(\mathscr{R})$, where $\lambda^{+}(\mathscr{R})$ is the positive Lyapunov exponent on the repeller. However, very little is known about the fractal dimensions of repellers in higher dimensions or about their very complicated structures in phase-space. One problem with the method is that we have as yet no way of computing the KS entropy on the repeller other than by computing the escape rate from the known values of the transport coefficient and doing an independent calculation of the sum of the positive Lyapunov exponents on the repeller. It would be more satisfactory if the escape rate formula could be used as a predictive method for computing transport coefficients and not only as a method for computing h_{KS} on the repeller. Perhaps Young's formula or the Kaplan–Yorke formula [14] can be of help here: if one finds ways to determine the

fractal dimensions of the repeller, the KS entropy can probably be obtained from them. Finally, we need more specific calculations of the Lyapunov exponents for repellers. It would be interesting to see what happens if one extends the currently available random Lorentz gas results to higher densities and to systems where all of the particles move. Also, the well-known long time tails and density logarithms in transport coefficients for moderately dense gases have yet to make their appearance in this dynamical approach to transport.

In the next section we will turn our attention to another method for relating transport coefficients to Lyapunov exponents, this time on an attractor.

4. Systems with Gaussian thermostats

The use of computer-simulated molecular dynamics to study transport coefficients has led to a number of innovations in transport theory. One of the most interesting innovations, due to Hoover, Evans, Posch, Morriss and other co-workers [5], has been the use of Gaussian thermostats in the simulations. They were introduced to provide a means whereby the heat generated in an irreversible flow could be eliminated and the temperature maintained at a constant value. Examples include the Joule heating of particles moving in external electric fields [36] or the viscous heating produced in a shear flow [5,37]. The idea is to add to the equations of motion of the particles a fictitious force which keeps either the total kinetic energy of the system or the overall total energy (kinetic + potential) constant despite the irreversible production of heat. The resulting equations of motion are no longer of a simple Hamiltonian form and the conservation of volume in phase-space, typical of Hamiltonian systems, is no longer valid for thermostated systems. This is reflected in the properties of the Lyapunov exponents for the thermostated system. In particular, the sum of *all* of the Lyapunov exponents is no longer zero, as it is for a Hamiltonian system. Instead one finds that starting from some initial state, a typical phase-space distribution concentrates on a fractal attractor of lower dimension than the full phase-space. In this case the sum of the Lyapunov exponents is negative, indicating a contraction of phase-space volume. Furthermore, the sum of the Lyapunov exponents can be related to the transport coefficients of the system.

To illustrate we consider the motion of a charged particle in an array, periodic or random, of fixed scatterers, with an external electric field that acts on the particle to induce an electric current [36,38]. The collisions of the particle with the scatterers will be taken to be instantaneous and elastic. Between collisions the particle satisfies the equations of motion

$$\dot{\mathbf{r}} = \mathbf{v}\,,$$

$$\dot{\mathbf{v}} = \frac{q}{m}\mathbf{E} - \alpha\mathbf{v}\,. \tag{16}$$

Here q and m are the charge and mass of the moving particle, $\mathbf{E}$ is the external electric field, and $-\alpha\mathbf{v}$ is the force that is added to the equation of motion to keep the kinetic energy of the moving particle constant. That is, we set $\dot{\mathbf{v}}\cdot\mathbf{v}=0$, so as to obtain an expression for α,

$$\alpha=\frac{q\mathbf{E}\cdot\mathbf{v}}{mv^2}\,. \tag{17}$$

Notice that the equations of motion are time reversible (under the transformation $t\to -t, \mathbf{v}\to -\mathbf{v}$), and that the flow in phase-space is not incompressible, since

$$\frac{\partial\dot{\mathbf{r}}}{\partial\mathbf{r}}+\frac{\partial\dot{\mathbf{v}}}{\partial\mathbf{v}}=-(d-1)\alpha\,, \tag{18}$$

where d is the number of spatial dimensions of the system. It is found that the distribution function for an ensemble of similarly prepared systems reaches a non-equilibrium steady state under the combined action of the electric field, the thermostating force, and the collisions of the moving particle with the fixed scatterers.

In the same spirit as in the escape rate method, the connection between transport coefficients and dynamical quantities for this system is made by combining macroscopic descriptions of some property of the system with microscopic ones for the same property. In this case we express the average value of the "friction coefficient" α as

$$\langle\alpha\rangle=\frac{\langle\mathbf{j}\rangle\cdot\mathbf{E}}{k_BT}=\frac{\sigma E^2}{k_BT}\,, \tag{19}$$

where we identified $q\mathbf{v}$ as the microscopic current and used the macroscopic relation $\langle\mathbf{j}\rangle=\sigma\mathbf{E}$, with σ the conductivity. In addition, the kinetic energy of the moving particle was identified with k_BT. Next we show that $\langle\alpha\rangle$ is also related to the rate of phase-space contraction of the system. We consider the phase-space density for the moving particle, $\rho(\mathbf{r},\mathbf{v},t)$. Using Eq. (18), we find that ρ satisfies

$$\frac{d\rho}{dt}=(d-1)\alpha\rho\,. \tag{20}$$

If we now express ρ as a constant number of replicas of the system, $\mathcal{N}$, divided by a phase-space volume $\mathcal{V}(t)$, we find the time rate of change of this volume is given by

$$\frac{d\ln\mathcal{V}(t)}{dt}=-(d-1)\alpha\,. \tag{21}$$

If we take the steady-state ensemble average of this equation we find that

$$\left\langle\frac{d\ln\mathcal{V}(t)}{dt}\right\rangle=-(d-1)\langle\alpha\rangle\,. \tag{22}$$

We know that for long enough times, the phase-space volume changes in time as $\ln[\mathcal{V}(t)/\mathcal{V}(0)]\sim t\sum_i\lambda_i(E)$, where the $\lambda_i(E)$ are the Lyapunov exponents for the

system in the field and thermostat, so that we find

$$(d-1)\langle\alpha\rangle = -\left\langle \sum_i \lambda_i(E) \right\rangle . \tag{23}$$

This then is the microscopic identification of the friction coefficient with the sum of the Lyapunov exponents for the system. As we expect the average friction coefficient to be positive in order to remove heat from the system, we note that the phase-space volume must be decreasing. As a macroscopic steady state is reached, we conclude that the system is approaching an attractor in phase-space.

Identification of Eqs. (23) and (19) yields the desired relation between the Lyapunov exponents and the conductivity (which can be related immediately to the diffusion coefficient D through the Einstein relation $\sigma = Dq^2/k_BT$). It is very interesting to reinterpret this relation in terms of entropy production in the system. It is not altogether clear a priori how to define this entropy production, but we will take the usual Boltzmann–Gibbs expression for the entropy of the system at time t as [38]

$$S(t) = -k_B \int d\mathbf{r} \int d\mathbf{v}\, \rho[\ln \rho - 1] . \tag{24}$$

If we differentiate this expression with respect to time, use Eq. (20), and carry out two partial integrations over the phase-space variables, we easily obtain

$$\frac{dS}{dt} = -k_B(d-1) \int d\mathbf{r} \int d\mathbf{v}\, \rho\alpha = -k_B(d-1)\langle\alpha\rangle . \tag{25}$$

Notice that if $\langle\alpha\rangle$ is positive, as expected, the entropy production is negative! This can be understood by realizing that if the phase-space volume is decreasing, we are learning more about the microscopic state of the system as time increases, hence a decrease in entropy. This must be compensated for by a parallel increase in entropy of the reservoir that is responsible for the thermostat [38]. The minimum rate of entropy increase in the reservoir must then be

$$\frac{dS_{reservoir}}{dt} = k_B(d-1)\langle\alpha\rangle . \tag{26}$$

So far there is no net entropy production, there is just a transport of entropy from the system to the reservoir. However, macroscopically the system just appears to be in a steady state; the ever-continuing contraction of phase-space density onto the attractor eventually is completely lost to any macroscopic observer and to the latter the entropy of the system soon reaches a constant value. That is, the difference between the macroscopic entropy and the Gibbs' entropy will keep increasing forever and it is this increase that should be identified as the irreversible entropy production of the system [7]. From Eqs. (25) and (19) it follows that the irreversible entropy production has exactly the value one expects from irreversible thermodynamics.

Similar results obtain for other transport coefficients as well. One of the most studied cases is that of a thermostated viscous flow produced by an externally imposed shearing

of the fluid [5,37]. Numerically, at least, one can go to rather large electric fields, in the case of the conductivity, or to large shearing fields, in the case of viscous flow. In any case, the transport coefficients obtained this way should reduce to their zero-field values as the field approaches zero. This implies, as we see from Eq. (19), that the sum of the Lyapunov exponents on the attractor should approach zero quadratically in the field as the field goes to zero, if the coefficients are well-defined. The structural similarities to the escape rate formalism should be emphasized. In the escape rate formulae, the difference between the KS entropy and the positive Lyapunov exponents on the repeller has to scale inversely as the square of the system size. In the Gaussian thermostat formalism the sum of all of the Lyapunov exponents on the attractor has to scale as the square of the external field. The reason for this formal similarity is not clear, yet [39]. The repeller of escape rate theory has a much different fractal structure than the attractor of the thermostat theory. The repeller is a fractal in all directions in phase-space, while the attractor is smooth in the expanding directions and has a well-defined SRB measure [24]. The relation between the two structures for the same transport coefficients awaits further elucidation.

The analysis so far has been completely formal, only relationships were established, but no explicit calculations of the quantities have been presented here. Results from computer simulation studies have been abundant, but, until recently, there have not been many analytical results for the same quantities. Gallavotti and Cohen have developed the theory for the SRB measures on the attractors in non-equilibrium steady states, and shown, among many other things, that the SRB measures can be used to compute the probabilities of fluctuations in entropy production in the steady states [24]. These predictions agree very well with the results of computer simulations of Evans, Morriss and Cohen [40]. These latter authors also discovered a very important "conjugate pairing rule" for the Lyapunov exponents of thermostated systems [37]. This rule states that the Lyapunov exponents of such systems can be ordered in pairs in such a way that the same value is obtained for the sum of each pair of exponents. For an isolated system with a symplectic Hamiltonian dynamics, it is known that conjugate pairs of exponents exist, and that their sum is zero [41]. Evans, Cohen and Morriss, and more recently, Dettmann and Morriss have provided strong arguments, and for some systems, proofs, for the correctness of the pairing rule – though not with a zero sum – for the exponents in a thermostated system [37,42]. The importance of the conjugate pairing rule resides in the fact that one only needs to calculate the sum of *one* conjugate pair of exponents in order to compute the associated transport coefficient, instead of having to compute all of them. This is a considerable simplification in systems with many particles, or for Lorentz gases in more than two space dimensions, since for the latter case, there are typically $2(d-1)$ non-zero exponents, where d is the number of space dimensions. Recently, van Beijeren et al. have been able to compute the Lyapunov exponents for random Lorentz gases at low densities, both for an isolated system and for a system in a thermostated electric field [9–11]. The appropriate E^2 scaling was confirmed, as well as the conjugate pairing rule for the case of $d=3$. This work will be discussed in Section 6, below. Before doing so, we turn our attention in the next section

to the fascinating questions related to the entropy production results discussed above.

5. Entropy production

In the previous section we could invoke the irreversible production of entropy in order to connect transport coefficients to Lyapunov exponents. Entropy production is involved in the escape rate method as well, although its role in the discussion is not so obvious. A number of authors have been working on clarifying the connections between these methods and the usual methods for calculating the entropy production in irreversible mechanical systems [6–8]. We have already encountered the situation in the thermostat method that an entropy current from the system to the reservoirs was counterbalanced by a positive entropy production in the system due to coarse graining. Breymann et al. [7] have recently shown that something very similar occurs in Hamiltonian systems with escape, as treated in the escape rate methods. They present a reasonable definition for the rate of entropy increase in these systems and show that it too is negative due to exchange with the environment, and equal to $-k_B\gamma$, where γ is the (positive) escape rate. Their argument, essentially, is to define an entropy for a system with escape in terms of a normalized phase-space density on the sets of initial points in phase-space that do not lead to escape over some time interval, say $0 \leqslant t \leqslant T$:

$$S(T) = -k_B \sum_i \int d\Gamma \chi_t(\Gamma_i)\tilde{\rho}(\Gamma_i)[\ln \tilde{\rho}(\Gamma_i) - 1] . \tag{27}$$

Here $\chi_t(\Gamma)$ equals unity for all initial points which do not lead to escape in the specified time interval and zero for all other points. $\tilde{\rho}(\Gamma)$ is a normalized phase-space density so that

$$\sum_i \int d\Gamma \chi_t(\Gamma_i)\tilde{\rho}(\Gamma_i) = 1 . \tag{28}$$

and the sum is over all the disjoint sets of points that do not escape in time T. This entropy can be evaluated using arguments given in Section 3, by noticing that for large T the number of sets becomes very large and each of them becomes of very small measure. We can then safely approximate the normalized density by a uniform value given by $\tilde{\rho}(\Gamma_i) = [\int d\Gamma \chi_t(\Gamma)\rho(\Gamma)]^{-1}$. Further, since we are describing a system with escape, one immediately sees that for large T, $[\int d\Gamma \chi_t(\Gamma)\rho(\Gamma)] \sim \exp(-\gamma T)$. Then the entropy at time T becomes

$$S(T) = -Tk_B\gamma + k_B . \tag{29}$$

The rate of entropy change is then the time derivative of $S(T)$, that is

$$\frac{dS(T)}{dT} = -k_B\gamma . \tag{30}$$

Breymann et al. [7] also make the important observation, described in the previous section on thermostated systems, that the coarse graining of phase-space required by the finite ability of measuring instruments would lead automatically to a positive entropy production if one takes the entropy production to be the rate of change of the difference between the coarse grained entropy and the microscopic entropy. At some point again changes in the structure of the sets of points that remain trapped in the system, i.e., the sets of the repeller, would be too small to be noticed within the experimental resolution. The coarse grained entropy would be constant thereafter, but the microscopic entropy would continue to change, and the rate of entropy production so defined would be positive. In a closely related study, Ruelle has recently considered the problem of entropy production in non-equilibrium systems and carefully discussed the mathematical properties of expressions for the rate of entropy production in thermostated systems, as well as for Hamiltonian systems with escape, among others [8]. He has been able to prove that for systems with Gaussian thermostats, the rate of increase of the entropy of the thermostating reservoir is strictly positive for hyperbolic dynamical systems, and that the rate of entropy loss of the repeller in a Hamiltonian system with escape, is at least non-negative. Ruelle does not consider coarse grained entropies, however.

In order to have a totally satisfactory theory of entropy production, one would like to consider systems together with their thermostats and surroundings, as complete mechanical systems to be analyzed together. For example, one might consider setting up a stationary-state situation for diffusion by having a system connected to two reservoirs with different densities of particles in such a way that a constant density gradient is established across the system. Then the methods of irreversible thermodynamics would provide the macroscopic expression for the rate of entropy production, and one could use dynamical expressions like the ones used above to construct microscopic expressions for the same quantity. One would like to find unambiguously positive expressions for the rate of entropy production under all circumstances by considering the dynamics of the system plus reservoir carefully. In the escape rate formalism this is what we found above indeed under the assumption that *for long times the coarse grained normalized phase-space density* $\tilde{\rho}(\Gamma_i)$ *becomes stationary*. In a complete theory one ought to prove this is the case indeed, in addition one would like to be able to treat more general situations including stationary non-equilibrium states. An important advance in this direction has been made by Gaspard, who has analyzed a simple diffusive system and discovered an important dynamical mechanism for entropy production related to the microscopically fractal structure of the interface between sets of phase points corresponding to particles injected into the system at different boundaries [6]. Since this work is included in these proceedings, we refer the reader to his paper for more details. Here we only mention that Gaspard has taken fractal structures into account when defining the entropy of a system representing a steady-state diffusion experiment. This seems to be a promising direction for a careful proof of the positivity of the rate of entropy production using purely dynamical arguments. It is important to note the differences between the approaches of Breymann et al. [7], and that of Gaspard [6]. The former authors consider either thermostated or open systems and suppose that the macroscopic

entropy production is the difference between a coarse-grained Boltzmann–Gibbs entropy production (which eventually vanishes) and a fine-grained entropy production (which approaches negative infinity as the system contracts to an attractor or consists more and more of those trajectories on a fractal repeller). Gaspard sets up a non-equilibrium steady-state situation and shows that a fractal structure appears due to the different conditions present at the boundaries of the system that maintain the steady state. He then shows that this structure can be identified as the source of the positive entropy production of the system, with a properly defined coarse grained entropy.

6. The random Lorentz gas

In Section 4 we already introduced the Lorentz gas as a system of fixed scatterers with a charged particle moving among them at a constant speed v. At low scatterer densities and for a random distribution of scatterer positions the Lyapunov exponents and KS entropy of this system can be calculated explicitly [9–11].

6.1. Expressing the Lyapunov exponent in terms of the radius of curvature

Our starting point is a relation obtained by Sinai [43] in which the positive Lyapunov exponents are expressed in terms of the curvature matrix of a diverging bundle of infinitesimally close trajectories in phase-space. For a two-dimensional system this relation is very simple. In this case, there is only one positive Lyapunov exponent,[2] it suffices to consider the separation of trajectories in position space; since its time derivative is the separation in velocity space, both have to grow with the same exponential [26]. Following the bundle backwards in time, one finds all trajectories go through a common point of intersection. The distance from the present position to this intersection point is the radius of curvature ρ of the bundle. Calling the distance between two representative trajectories in the bundle Δ one sees immediately from Fig. 2 that this quantity satisfies the differential equation

$$\frac{d\Delta}{\Delta} = \frac{v\,dt}{\rho}\,, \tag{31}$$

which can be solved in the form

$$\Delta(t) = \exp\left(\int_0^t d\tau\, v/\rho(\tau)\right)\Delta(0)\,. \tag{32}$$

Hence, one finds the positive Lyapunov exponent must be of the form

$$\lambda^+ = v\left\langle\frac{1}{\rho}\right\rangle\,, \tag{33}$$

[2] This is a system with four phase-space dimensions. The energy of the particle is constant, and two points on the same trajectory do not separate at all since the speed remains constant. Thus, there is only one possible direction for exponential separation and one for exponential approach of trajectories in phase-space.

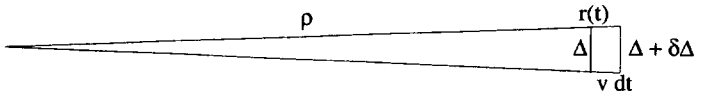

Fig. 2. The geometry of two nearby trajectories. Δ is the distance between the trajectories, ρ the radius of curvature of the bundle to which they belong and $d\Delta$ the change of Δ during a small time dt.

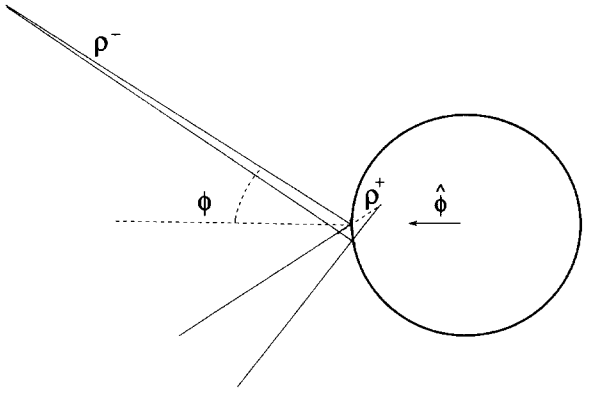

Fig. 3. The change in ρ in a collision. ρ^- and ρ^+ are the radius of curvature just before and just after the collision and ϕ is the angle of incidence.

where the brackets denote a time average along the trajectory and λ^+ may in principle be different for different trajectories. To calculate λ^+ one needs the time evolution of ρ. For zero electric field this time evolution in between collisions simply is described by $d\rho/dt = v$. In a collision ρ changes instantaneously from a pre-collisional value ρ^- to a post-collisional value ρ^+, as illustrated in Fig. 3. The relation between these is given by [26,43]

$$\frac{1}{\rho^+} = \frac{1}{\rho^-} + \frac{2}{a\cos\phi}\,, \tag{34}$$

where ϕ is the angle of incidence at the collision. So one sees that at each collision ρ is reduced to a value which is less than or equal to $a/2$. Then ρ grows during the subsequent free streaming to a value of order ℓ, the mean free path between collisions. Hence, λ^+ has to be bounded somewhere between v/ℓ and $2v/a$.

Iterating Eq. (34) over all the collisions along a given trajectory one obtains Sinai's continued fraction expression for $\rho(t)$,

$$\rho = v\tau_0 + \cfrac{1}{\cfrac{2}{a\cos\phi_1} + \cfrac{1}{v\tau_1 + \cfrac{1}{\cfrac{2}{\cos\phi_2} + \cfrac{1}{v\tau_2 + \cdots}}}}\,.$$

Here the τ_i's are the times between collisions and the ϕ_i's are the incidence angles, as illustrated in Fig. 4. As one moves back the initial point along the trajectory, ρ rapidly converges to a value that is independent of this initial point and only depends

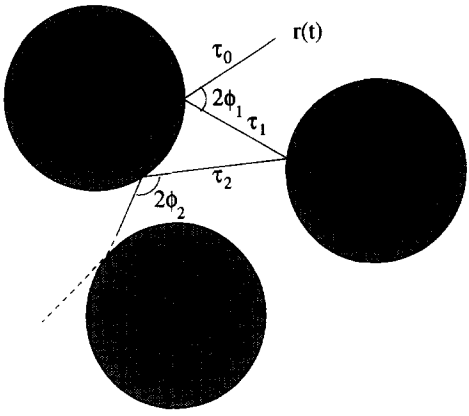

Fig. 4. A trajectory among three scatterers. τ_0 is the time elapsed since the last scattering, τ_1 the time between the last and the second last scattering, etc. The angles are defined as in Fig. 3.

in a smooth way on the final position and velocity of the moving particle and the positions of the fixed scatterers. Therefore, if the motion of the light particle is ergodic, the time average $\langle 1/\rho \rangle$ in Eq. (33) may be replaced by an ensemble average over all accessible initial positions and all initial velocity directions for the moving particle.

6.2. *The generalized Lorentz–Boltzmann equation*

One step further is to extend this ensemble average so as to also include an average over all allowed configurations of scatterers. For this extended ensemble one may then introduce a distribution function $P(\mathbf{r}, \mathbf{v}, \rho, t)$ describing the probability density for finding the trajectory bundle at time t at position $\mathbf{r}$ with velocity $\mathbf{v}$ and radius of curvature ρ. At low scatterer densities, and at zero field, the time evolution of this distribution is described by an extended Lorentz–Boltzmann equation [9] of the form

$$\{\partial/\partial t + \mathbf{v}\cdot\nabla\}P(\mathbf{r},\mathbf{v},\rho,t) = -v\partial/\partial\rho\, P(\mathbf{r},\mathbf{v},\rho,t)$$

$$- vP(\mathbf{r},\mathbf{v},\rho,t) + v/2 \int_{-\pi/2}^{\pi/2} d\phi \int_0^{\infty} d\rho' \cos\phi$$

$$\times \delta\left(\rho - \frac{a\cos\phi/2}{1 + a\cos\phi/2\,\rho'}\right) P(\mathbf{r},\mathbf{v}',\rho',t)\,. \tag{35}$$

Here $v = 2anv$ is the average collision frequency, where n is the number density of the scatterers, and we assume that $na^2 \ll 1$.

Comparing Eq. (35) to the ordinary Lorentz–Boltzmann equation [44] one sees an extra term (the first term on the right-hand side) describing the effects of free streaming on ρ; collisions with scatterers produce a standard loss term $-vP$, whereas the gain term takes into account the change in ρ at a collision described by Eq. (34) and also

depends on the restituting velocity $\mathbf{v}'$. In equilibrium both terms on the l.h.s. vanish and for $\rho > a/2$ the last term on the r.h.s. vanishes as well. The remaining terms give rise to a simple exponential decay of the form $\exp(-\rho/\ell)$, where we used the identity $v = v/\ell$. To lowest order in the scatterer density the solution of Eq. (35) for $\rho < a/2$ is simple as well and, setting $P(\rho, \mathbf{v}) = \phi_0(v) f(\rho)$, where $\phi_0(v) = (1/2\pi v)\delta(|\mathbf{v}| - v)$, one obtains the result, up to corrections of relative order a/ℓ [9],

$$f(\rho) = \begin{cases} (1/\ell) e^{-\rho/\ell}, & \rho > a/2\,, \\ (1/\ell)[1 - (1 - (2\rho/a)^2)^{1/2}], & \rho < a/2\,. \end{cases} \tag{36}$$

From this, λ^+ at low densities is obtained as

$$\lambda^+ = v \int_0^\infty d\rho \, \frac{1}{\rho} f(\rho) = 2nav(1 - \ln 2 - C - \ln \tilde{n})\,, \tag{37}$$

with $\tilde{n} = na^2$ and C Euler's constant. This result agrees with a conjecture of Krylov [45] for the leading low-density behavior of λ^+. The coefficient of the $n \ln \tilde{n}$ term agrees with a similar result, [46,47], obtained for the periodic case as the radius of the disks becomes small. The coefficient of the order n term however, is new. Further, the KS entropy follows from Pesin's Theorem [22] for closed systems as $h_{KS} = \lambda^+$.

6.3. *Systems with open boundaries*

Next, let us consider the case of open-boundary conditions. Now one may apply the standard Chapman–Enskog method for solving the extended Lorentz–Boltzmann equation, under the boundary conditions that P vanishes outside the region occupied by scatterers. This procedure is an expansion method in which the expansion parameter is ℓ/L, where L measures the system size and is a characteristic length for gradients in the moving particle density. The details are described in Ref. [9], here we just quote the main results: Through first order in the gradient of the moving particle density $n_m(\mathbf{r}, t)$ the distribution function for the surviving particles at time t takes the form

$$P(\mathbf{r}, \mathbf{v}, \rho, t) = \phi_0(v)[n_m(\mathbf{r}, t) f_0(\rho) + f_1(\rho)\, \mathbf{v} \cdot \nabla n_m(\mathbf{r}, t) + \cdots]\,. \tag{38}$$

The form of f_1 is given in Ref. [9]. For large systems and for long times (i.e. system size $\gg \ell$ and $vt \gg 1$) $n_m(\mathbf{r}, t)$ satisfies the diffusion equation

$$\partial n_m(\mathbf{r}, t)/\partial t = D \nabla^2 n_m(\mathbf{r}, t) \tag{39}$$

with absorbing boundary conditions and diffusion coefficient,

$$D = \tfrac{3}{8} \ell v\,, \tag{40}$$

as follows from the solution of the ordinary Lorentz–Boltzmann equation [44]. However, now an important subtlety arises: Eq. (38) does not suffice to calculate λ^+ on the repeller. The reason is that it describes the distribution function of particles (or

trajectories) that survive within the system through time t, but the repeller is defined as the set of trajectories (or particles) that survive within the system forever. Therefore, the relevant distribution function is obtained by multiplying the result of Eq. (38) by a function $S(\mathbf{r},\mathbf{v},t|T)$ describing the probability that a particle with velocity $\mathbf{v}$ and position $\mathbf{r}$ at time t will survive within the system through time T, and by considering the limit $T\to\infty$. This function S is obtained easily from the solution of the ordinary Lorentz–Boltzmann equation [9]. The calculation of the positive Lyapunov exponent now gives the result

$$\lambda^+ = \lambda_0^+ + \frac{3\ell^2}{8}\left[\lambda_0^+ - \frac{v}{2\ell}\right] J\,, \tag{41}$$

where λ_0^+ is the equilibrium Lyapunov exponent and J is

$$J = \left[\int (\nabla n_m(\mathbf{r},t))^2 d\mathbf{r}\right]\left[\int n_m(\mathbf{r},t)^2 d\mathbf{r}\right]^{-1}\,. \tag{42}$$

For large systems this expression can be simplified by using the diffusion equation (39). For large times only the most slowly decaying eigenmode of this equation survives, so $\partial n_m(\mathbf{r},t)/\partial t$ may be replaced by $-\gamma n_m(\mathbf{r},t)$, as the decay rate of the density must equal the escape rate. Substituting this into Eq. (41) after applying a partial integration, and using Eq. (39) one obtains the result

$$\lambda^+ = \lambda_0^+ + \gamma\left(\frac{\lambda_0^+}{v} - \frac{1}{2}\right). \tag{43}$$

From Eq. (9) it then follows that the KS entropy is given by $h_{KS} = \lambda_0^+ + \gamma(\lambda_0^+/v - \frac{3}{2})$.

6.4. Driven systems

In the presence of an electric field and corresponding Gaussian thermostat the extended Lorentz–Boltzmann equation has to be supplemented by terms due to the external fields resulting from the changes in the direction of the velocity. The collision dynamics are not affected because the collisions are instantaneous. For the details we refer to Ref. [10]. For weak fields one can solve this equation again by applying the Chapman–Enskog method, treating this time the field strength as a small parameter instead of ℓ/L. To second order in $\varepsilon = qE/vm$ the positive Lyapunov exponent becomes

$$\lambda^+ = \lambda_0^+ - \frac{11}{48v}\varepsilon^2 + O(\varepsilon^4)\,. \tag{44}$$

Unlike in the previous cases the negative Lyapunov exponent is not just the opposite of the positive one. Calculating negative Lyapunov exponents by following trajectories in the forward time direction is somewhat cumbersome. One has to choose the initial curvature of the contracting bundle in such a way that it will keep contracting forever, which means that each time a new collision is encountered the initial condition on ρ

has to be adjusted a bit. This problem can be avoided by considering the time reversed motion starting from points on the attractor. In the kinetic equation this amounts to replacing the Stoßzahlansatz before collisions by a corresponding Ansatz for the post-collisional coordinates (which in fact *are* the pre-collisional coordinates, but in time reversed dynamics they appear as post-collisional ones). In other words, the generalized Lorentz–Boltzmann equation is replaced by an anti-Lorentz–Boltzmann equation. For details we refer to [10] again. Solution of this anti-Lorentz–Boltzmann equation to second order in ε yields

$$\lambda^- = -\lambda_0^+ - \frac{7}{48v}\varepsilon^2 + O(\varepsilon^4)\,. \tag{45}$$

Notice that the sum of λ^+ and λ^- indeed satisfies Eq. (23). It came rather as a surprise that λ^+ deviates more from λ_0^+ than $-\lambda^-$. In sheared thermostated systems λ^+ differs hardly, if at all, from its equilibrium value and so all deviations from equilibrium are found in the negative Lyapunov exponents alone [37,48]. There are some indications that this difference may be related to the small number of degrees of freedom in the Lorentz gas. For example, in the three-dimensional Lorentz gas, which has two more degrees of freedom, the deviation from equilibrium in the negative Lyapunov exponent exceeds that in the positive Lyapunov exponent.

The above predictions for the Lyapunov exponents in a field-driven system have been tested in molecular dynamics simulations by Posch and Dellago [10]. As shown in Fig. 5 the agreement of the field dependence of these exponents at densities of $\tilde{n} = 0.001$ or 0.002 with the theoretical predictions looks very good. The sum of the slopes of the two curves, however, differs beyond its error bars from the predicted value, if for D one uses the Lorentz–Boltzmann value (40). But if this value is corrected by adding higher-order terms in the density expansion of D, including logarithmic ones, as obtained by Van Leeuwen and Weyland [49] and Bruin [50], it agrees with the simulation results within error bars. So we may conclude that transport coefficients can be calculated from field-dependent Lyapunov exponents with almost the same accuracy as from direct simulation methods!

6.5. *The three-dimensional Lorentz gas*

Recently, the calculations for the low-density Lorentz gas have been extended to the case of three-dimensional spherical scatterers by Latz et al. [11]. Though these calculations are similar to those for the two-dimensional system a number of new complications do arise. First of all the spatial separation between two nearby trajectories becomes a two-dimensional vector and the radius of curvature has to be replaced by a 2×2 radius of curvature tensor. As a result the exponential on the r.h.s. of Eq. (32) becomes a time-ordered exponential of non-commuting 2×2 random matrices. Fortunately the distribution of these matrices is sufficiently well-behaved, even in the presence of a driving field, that it remains possible to calculate the largest Lyapunov exponent. The sum of the two positive Lyapunov exponents is a scalar, which can

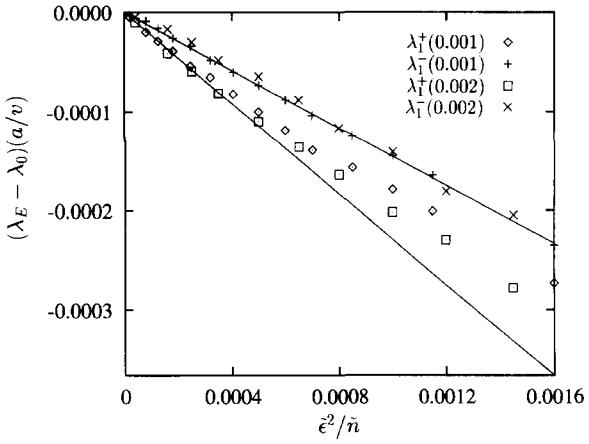

Fig. 5. Field dependence of the Lyapunov exponents for a two-dimensional-driven Lorentz gas at the dimensionless densities $\tilde{n} = na^2 = 0.001$ and 0.002. The deviations of the positive and negative Lyapunov exponent λ_1^+, respectively, λ_1^- vs. the square of the electric field, expressed in dimensionless units $\tilde{\epsilon}^2/\tilde{n}$, with $\tilde{\epsilon} = qEa/mv^2$. Courtesy of H.A. Posch and Ch. Dellago.

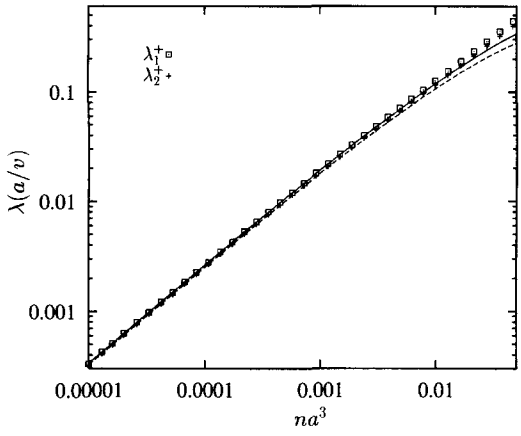

Fig. 6. The two positive Lyapunov exponents of a three-dimensional Lorentz gas in equilibrium, expressed in units of the collision frequency, as function of the dimensionless density $\tilde{n} = \pi na^3$. The solid line and the dashed line show the theoretical predictions for these exponents. Courtesy of H.A. Posch and Ch. Dellago.

be calculated much more easily. Obviously, the second positive Lyapunov exponent follows immediately from these results. The negative Lyapunov exponents, as in the two-dimensional case, can be calculated again from the time reversed evolution of the distribution function on the attractor. The results for the Lyapunov exponents in a

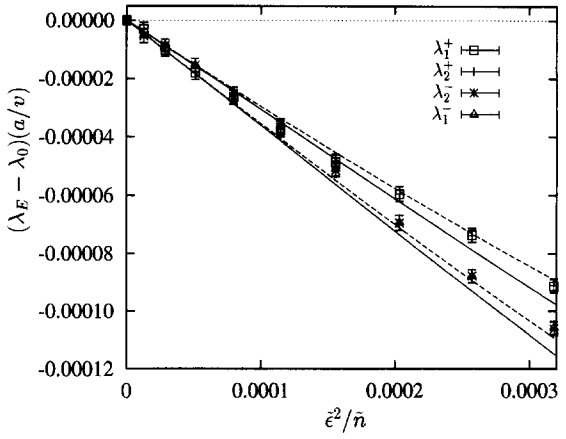

Fig. 7. Field dependence of the positive and negative Lyapunov exponents for the three dimensional Lorentz gas at $\tilde{n} = 0.001\pi$. The solid lines show the theoretical predictions for the deviations of the positive respectively the negative lyapunov exponents from their equilibrium values. The dashed lines present results from a numerical solution of the extended Lorentz–Boltzmann equation [35]. Courtesy of H.A. Posch and Ch. Dellago.

driving field are found as

$$\lambda_1^{\pm} = \mp\frac{v}{a}\tilde{n}\left(\log\frac{\tilde{n}}{2} + \mathscr{C} - \log 2 + \frac{1}{2}\right) - \left(\frac{1}{3} \mp \frac{1}{36}\right)\frac{a}{v}\frac{\varepsilon^2}{\tilde{n}},$$
$$\lambda_2^{\pm} = \mp\frac{v}{a}\tilde{n}\left(\log\frac{\tilde{n}}{2} + \mathscr{C} + \log 2 - \frac{1}{2}\right) - \left(\frac{1}{3} \mp \frac{1}{36}\right)\frac{a}{v}\frac{\varepsilon^2}{\tilde{n}}. \tag{46}$$

Here $\tilde{n} = \pi n a^3$. One sees that, at least through order E^2, both positive Lyapunov exponents are shifted from their equilibrium values by equal amounts and the same is true for the negative Lyapunov exponents. Therefore the conjugate pairing rule obviously is satisfied. Notice that in MD simulations of thermostated *sheared* systems all positive Lyapunov exponents also were found to be shifted by about the same small value, while the negative exponents were shifted by nearly the same larger value [37,48].

Also for the three-dimensional Lorentz gas, Dellago and Posch did MD simulations to calculate the Lyapunov exponents both in equilibrium and for a field-driven Lorentz gas [12]. Their results are compared to the theoretical ones in Figs. 6 and 7. Again, the agreement is excellent.

7. Conclusion

Here we have summarized the connections that are becoming evident between non-equilibrium transport theory and dynamical systems theory. There are other, closely related, approaches to this topic which we have not included in this discussion, mainly in the interest of brevity. However, there is a large literature on periodic orbit

expansions as a method for relating transport coefficients to dynamical quantities [51–53], and a developing literature using a method based on Ruelle–Pollicott resonances for classical dynamical systems [16,54]. All cases of the applications of these analyses to fluid systems are based upon the assumptions that the particles interact with strong, short ranged potentials, have non-zero Lyapunov exponents and KS-entropies, and can be thought of as in hyperbolic dynamical systems. However, it is only for systems of hard-sphere-like potentials that any rigorous results exist. Nevertheless, the results obtained so far show that there is indeed a useful connection between transport coefficients and dynamical quantities, useful in the sense that methods inspired by dynamical systems theory can be used to compute transport coefficients for interesting systems, or that the connection provides a deeper understanding of methods already in use to compute transport coefficients. Further, one of the striking results mentioned here is the fact that well-developed techniques from kinetic theory and statistical mechanics, in general, can be employed to compute dynamical quantities such as Lyapunov exponents. One of the deepest results emerging from these studies is the intimate connection between the positive entropy production in irreversible processes and fractal structures that underly these processes.

One of the stimulating features of this area of research is that there are so many open and interesting problems which are awaiting solution. Here we summarize those that have come up in the course of our discussions:

(1) It is not clear how the irreversible time dependence of few-particle distribution functions is determined by the projection of the dynamics of the system onto the unstable manifolds. In our discussion of the transport equation for the baker's map, we projected the "Liouville" equation onto the unstable manifold to obtain an irreversible equation. This projection introduced a time direction and the subsequent approach to equilibrium. However, in a typical derivation of the Boltzmann equation, for example, one never considers stable and unstable manifolds. Somehow the steps taken to derive the Boltzmann equation from Liouville's equation must implicitly involve a projection onto a space that includes contributions from unstable manifolds, which are ultimately responsible for the approach to smooth, equilibrium distributions. In this connection the rate of the approach to equilibrium in closed systems ought to be expressible in terms of Lyapunov exponents and KS-entropies in a manner similar to the relation between these quantities and transport coefficients for open systems as embodied by the escape-rate formula. Is there such a general formula for the approach to equilibrium in closed systems?

(2) As mentioned earlier in our discussion of the escape-rate formula, the fractal repeller for a large open system with many particles is a very complicated object about which we know almost nothing. Only for very simple systems like that discussed in the appendix do we know anything in much detail. It would be useful to understand how to compute the dimension of the repeller, the Lyapunov exponents and the KS-entropy for trajectories confined to the repeller.

(3) An important advance has been made by showing that standard techniques of non-equilibrium statistical mechanics can be used to compute Lyapunov exponents, and

KS-entropies of open systems, systems in Gaussian thermostats, or equilibrium systems. However, the only analytical results known so far for Lyapunov exponents, etc., are for disordered systems with independent particles moving in an arrangement of fixed scatterers. With one exception where a mean-field theory can be easily constructed [33], the calculations are carried out where the scatterers are placed at random in space at low densities. It would be desirable to extend these results in two directions: (a) to systems where all of the particles are moving; and (b) to higher densities of scatterers. It would also be interesting to know how the long time tails and other non-analytic phenomena of transport theory appear in this dynamical systems approach. These remarks apply to closed, to open and to thermostated systems. In any of these cases, it seems non-trivial to extend the known results to the more complicated cases listed here.

(4) There still remains the question of the precise connection between the various approaches to transport discussed here. Although the formal results of the escape-rate method and the thermostated system method look very similar, the underlying fractal structures appear to be different. We would like to understand why the formulae look so similar, though, and what the relation is between the quantities defined on the repeller of an open system and those on the attractor of a thermostated system. The precise connection is not so obvious.

(5) The deepest issue discussed here, perhaps, is the connection between the phenomenon of entropy production in an irreversible process and the fractal structures that underly the dynamics of the process. The recent works of Ruelle [8], of Breymann et al. [7], and of Gaspard [6] on simple models have given us some strong and encouraging directions for future research designed to clarify and to formalize this connection for a general class of systems. However, these approaches differ in detail, and open questions remain concerning: (a) the proper definition of a non-equilibrium entropy; (b) why one should take the difference between the coarse and fine scale changes in entropy as the appropriate definition of entropy production in an attractor or a repeller; and (c) whether Gaspard's steady-state model can be extended to provide a general approach to entropy production in non-equilibrium states.

(6) We have not discussed here the thermodynamic formalism of Bowen Ruelle and Sinai which allows close, albeit often formal, connections between dynamical systems theory and equilibrium statistical mechanics [55,56]. It embodies a broad generalization of the ideas discussed here to a new set of dynamical quantities related to a dynamical free energy (usually called the Ruelle pressure or the topological pressure), and its derivatives. The interesting questions related to the use and relevance of this formalism for transport theory would take us outside the scope of our discussions; we refer the reader to the literature for further details [55,56]. However it is important to mention that this formalism allows for the possibility of dynamical "phase transitions" as functions of the temperature-like variable that appears in the definition of the Ruelle pressure, or of other variables such as density. These phase transitions may have important consequences for transport theory but only a few models have been examined so far [57].

Acknowledgements

We benefitted from extensive discussions with C. Appert, E.G.D. Cohen, Ch. Dellago, M.H. Ernst, P. Gaspard, R. Klages, A. Latz, H.A. Posch and R. van Zon.

J.R.D. acknowledges support by the National Science Foundation under Grants No. PHY-93-21312 and PHY-96-00428. H.v.B was supported by FOM, SMC and by the NWO Priority Program Non-Linear Systems, which are financially supported by the "Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO)".

Appendix. The escape rate method for a simple map

Here we illustrate the construction and properties of a fractal repeller in order to illustrate the escape rate method for a simple one-dimensional map. We consider the map on the unit interval $0 \leqslant x \leqslant 1$:

$$x' = \begin{cases} px & \text{for } x \leqslant \frac{1}{2}, \\ p(x-1)+1 & \text{for } \frac{1}{2} \leqslant x \leqslant 1, \end{cases} \tag{A.1}$$

with $p > 2$. Here we take a map consisting of two pieces with equal slope. The more general case with different slopes has interesting ergodic properties and is discussed by Gaspard [31] and in Ref. [2]. Points which eventually fall into the interval $(1/p, 1-1/p)$ upon repeated applications of the map, are mapped outside of $[0,1]$ and discarded, as illustrated in Fig. 8. Thus, we see that the set of points in the interval $(1/p, 1-1/p)$ are lost in the first application of the map, points in the intervals $(1/p^2, (p-1)/p^2)$ and $((p^2-p+1)/p^2, 1-1/p^2)$ in the second iterate and so on. The total length of the sets of points that remain in the interval after n iterations is easily seen to be $(2/p)^n$ since there are 2^n separate intervals, each of length p^{-n}. Thus, there is an exponential escape of points and the escape rate γ is $\gamma = \ln p - \ln 2$. The repeller is the Cantor set of points that remain in the unit interval for all times. This is an uncountable number of points that can be coded by semi-infinite sequences of 0's and 1's, corresponding to the order in which they are mapped either to the left of $\frac{1}{2}$ for a "0", or to the right of $\frac{1}{2}$ for a "1", as illustrated in Fig. 8. The Lyapunov exponent, $\lambda(\mathscr{R})$, for the points on the repeller is easily seen to be $\ln p$, since any two infinitesimally close points on the repeller will separate by a factor of p at each iteration of the map. Thus, their separation after n iterates will be p^n. The KS-entropy for the repeller is $\ln 2$. This follows from Eq. (10) using

$$e^{nh_{KS}} = e^{n\lambda(\mathscr{R})} \cdot e^{-n\gamma} = e^{n(\ln p - \ln(p/2))} = e^{n \ln 2}. \tag{A.2}$$

Thus, $h_{KS} = \ln 2$, provides the rate at which information is gained when distinguishing nearby points on the repeller.

It is also useful to consider the Perron–Frobenius equation for the map (A.1). This equation is a discrete version of the Liouville equation which relates a distribution of

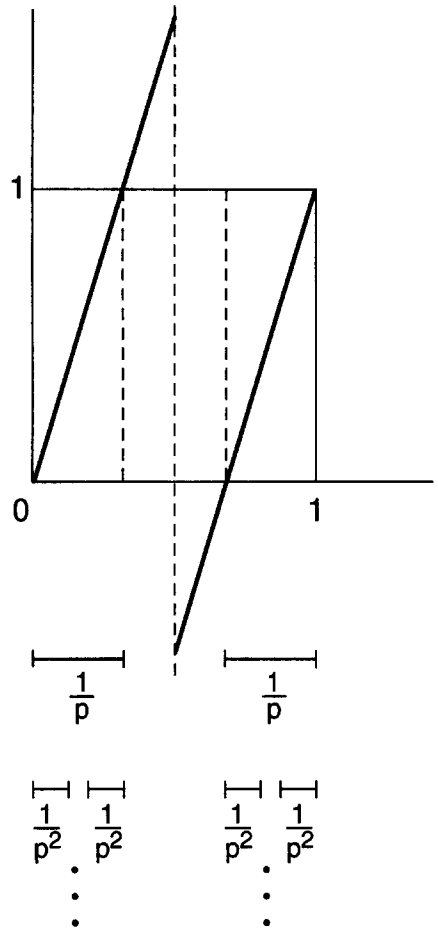

Fig. 8. A one-dimensional map with escape. Illustrated are the points on the unit interval which escape after $1, 2, \ldots$ iterations of the map given by Eq. (A.1).

points on the interval, $\rho_n(x)$, at the nth time step, to the distribution at the previous time step, when the points are acted upon by the map $x = M(y)$. That is,

$$\rho_n(x) = \int_0^1 dy\, \delta(x - M(y))\, \rho_{n-1}(y)\,. \tag{A.3}$$

This equation is reasonably self-evident. When applied to the map in Eq. (A.1), we obtain

$$\rho_n(x) = \frac{1}{p}\left[\rho_{n-1}\left(\frac{x}{p}\right) + \rho_{n-1}\left(\frac{x+p-1}{p}\right)\right]. \tag{A.4}$$

Note that this equation is exactly the "transport" equation, Eq. (4), when applied to the dyadic map for which $p = 2$. For this map there is no escape from the unit interval.

However, if $p > 2$, there is escape and the density of points on the unit interval approaches zero. Nevertheless, an interesting equation for the "density" of points on the repeller can be obtained from Eq. (A.4) by multiplying the r.h.s. by a factor that renormalizes the density at each step, boosting the density by a factor that exactly compensates for the escaping points [21]. It is easily seen that this factor is $\exp\gamma$, so that the equation for the renormalized density, $\hat{\rho}_n(x)$ is

$$\hat{\rho}_n(x) = \frac{1}{2}\left[\hat{\rho}_{n-1}\left(\frac{x}{p}\right) + \hat{\rho}_{n-1}\left(\frac{p-1}{p}\right)\right]. \tag{A.5}$$

This equation for the case $p = 4$ was discussed in Section 2 as an example of an equation which has a uniform distribution on a fractal set, there the "middle $-\frac{1}{2}$" Cantor set.

References

[1] J.R. Dorfman, H. van Beijeren, in: B. Berne (Ed.), Statistical Mechanics, B, Plenum, New York, 1977, p. 65.
[2] J.R. Dorfman, From Molecular Chaos to Dynamical Chaos, Lecture Notes, University of Utrecht and University of Maryland, 1995.
[3] B. Hunt, J. Yorke, Non. Linear Sci. Today 3 (1993) 2.
[4] P. Gaspard, G. Nicolis, Phys. Rev. Lett. 65 (1990) 1693.
[5] D.J. Evans, G.P. Morriss, Statistical Mechanics of Nonequilibrium Liquids, Academic Press, London, 1990; W.G. Hoover, Computational Statistical Mechanics, Elsevier, Amsterdam, 1991.
[6] P. Gaspard, Entropy production in open volume-preserving systems, J. Stat. Phys., submitted. A summary of this paper, under the title "Chaos and hydrodynamics", is contained in Physica A 240 (1997) 54, these Proceedings.
[7] W. Breymann, T. Tel, J. Vollmer, Phys. Rev. Lett. 77 (1996) 2945.
[8] D. Ruelle, Positivity of entropy production in nonequilibrium statistical mechanics, J. Stat. Phys., to appear.
[9] H. van Beijeren, J.R. Dorfman, Phys. Rev. Lett. 74 (1995) 4412; 76 (1996) 3238(E).
[10] H. van Beijeren, J.R. Dorfman, E.G.D. Cohen, Ch. Dellago, H. Posch, Phys. Rev. Lett. 77 (1996) 1974.
[11] A. Latz, H. van Beijeren, J.R. Dorfman, Phys. Rev. Lett. 78 (1997) 207.
[12] Ch. Dellago, H. Posch, Phys. Rev. Lett. 78 (1997) 211.
[13] M. Berry, in: S. Jorna (Ed.), Topics in Nonlinear Dynamics, American Institute of Physics, New York, 1978, p. 16.
[14] E. Ott, Chaos in Dynamical Systems, Cambridge Univ. Press, Cambridge, 1993.
[15] P. Gaspard, J. Phys. A: Math. Gen. 25 (1992) L483; Phys. Lett. A 168 (1992) 13; Chaos 3 (1993) 427.
[16] R. Fox, Chaos 5 (1995) 619; H.H. Hasegawa, W.C. Saphir, Phys. Rev. A 46 (1992) 7401; H.H. Hasegawa, D.J. Driebe, Phys. Rev. E 50 (1994) 1781.
[17] M.S. Green, J. Chem. Phys. 19 (1951) 1036; 20 (1952) 1281; 22 (1954) 398; Phys. Rev. 119 (1960) 829.
[18] P. Gaspard, J. Stat. Phys. 68 (1992) 673.
[19] S. Tasaki, P. Gaspard, J. Stat. Phys. 81 (1995) 935.
[20] J.R. Dorfman, M.H. Ernst, D. Jacobs, J. Stat. Phys. 81 (1995) 497.
[21] A. Csordás, G. Györgi, P. Szépfalusy, T. Tél, Chaos 3 (1993) 31.
[22] J.-P. Eckmann, D. Ruelle, Rev. Mod. Phys. 57 (1985) 617.
[23] A. Katok, B. Hasselblatt, Introduction to the Modern Theory of Dynamical Systems, Cambridge Univ. Press, Cambridge, 1995.
[24] G. Gallavotti, E.G.D. Cohen, Phys. Rev. Lett. 74 (1995) 2694; J. Stat. Phys. 80 (1995) 931.
[25] D. Ruelle, Ann. N. Y. Acad. Sci. 357 (1980) 1.

[26] P. Gaspard, J.R. Dorfman, Phys. Rev. E 52 (1995) 3525.
[27] R. Bowen, Am. J. Math. 92 (1970) 725; D. Ruelle, Am. J. Math. 98 (1976) 619; see also Ref. [24].
[28] Y. Pomeau, P. Resibois, Phys. Rep. C 19 (1975) 63.
[29] P. Bleher, J. Stat. Phys. 66 (1992) 315.
[30] J.R. Dorfman, P. Gaspard, Phys. Rev. E 51 (1995) 28.
[31] P. Gaspard, F. Baras, in: M. Maréschal, B. Holian (Eds.), Microscopic Simulations of Complex Hydrodynamic Phenomena, Plenum Press, New York, 1992, p. 301; Phys. Rev. E 51 (1995) 5332.
[32] H. van Beijeren, A. Latz, J.R. Dorfman, to be published.
[33] M.H. Ernst, J.R. Dorfman, R. Nix, D. Jacobs, Phys. Rev. Lett. 74 (1995) 4416.
[34] M.H. Ernst, G.A. van Velsen, J. Phys. A 22 (1989) 4337; J. Stat. Phys. 71 (1993) 1015; see also H. van Beijeren, M.H. Ernst, J. Stat. Phys. 70 (1993) 793.
[35] M.H. Ernst, J.R. Dorfman, to be published; C. Appert, M.H. Ernst, to be published.
[36] A. Baranyai, D.J. Evans, E.G.D. Cohen, J. Stat. Phys. 70 (1993) 1085.
[37] D.J. Evans, E.G.D. Cohen, G.P. Morriss, Phys. Rev. A 42 (1990) 5990.
[38] N.I. Chernov, G.L. Eyink, J.L. Lebowitz, Ya.G. Sinai, Phys. Rev. Lett. 70 (1993) 2209; Comm. Math. Phys. 154 (1993) 569.
[39] T. Tél, J. Vollmer, W. Breymann, Europhys. Lett. 35 (1996) 659.
[40] D.J. Evans, G.P. Morriss, E.G.D. Cohen, Phys. Rev. Lett. 71 (1993) 2401.
[41] V.I. Arnol'd, Mathematical Methods in Classical Mechanics, 2nd ed., Springer Verlag, Berlin, 1989.
[42] C. Dettmann, G.P. Morriss, Phys. Rev. E 53 (1996) R5545.
[43] Ya.G. Sinai, Russ. Math. Surv., 25 (1970) 137. See also S. Tabachnikov, Billiards, Panoramas et Synthèses 1 (1995).
[44] E.H. Hauge, What can one learn from Lorentz models?, in: G. Kirczenow, J. Marro (Eds.), Transport Phenomena, Springer, Berlin, 1974.
[45] N.S. Krylov, in: Ya.G. Sinai (Ed.), Works on the Foundations of Statistical Physics, Princeton Univ. Press, Princeton, 1979.
[46] B. Friedman, Y. Oono, I. Kubo, Phys. Rev. Lett. 52 (1984) 709.
[47] N.I. Chernov, Funct. Anal. Appl. 25 (1991) 204.
[48] S. Sarman, D.J. Evans, G.P. Morriss, Phys. Rev. A 45 (1992) 2233.
[49] J.M.J. van Leeuwen, A. Weyland, Physica 36 (1967) 457; 38 (1968) 35.
[50] C. Bruin, Physica 72 (1974) 261.
[51] R. Artuso, E. Aurell, P. Cvitanovic, Nonlinearity 3 (1990) 325.
[52] G.P. Morriss, L. Rondoni, J. Stat. Phys. 75 (1994) 553; G.P. Morriss, L. Rondoni, E.G.D. Cohen, J. Stat. Phys. 80 (1995) 35; J. Lloyd, M. Niemeyer, L. Rondoni, G.P. Morriss, Chaos 5 (1995) 536.
[53] P. Cvitanovic, P. Gaspard, T. Schreiber, Chaos 2 (1992) 85.
[54] P. Gaspard, Phys. Rev. E 53 (1996) 4379.
[55] D. Ruelle, Thermodynamic Formalism, Addison-Wesley, Reading, MA, 1978.
[56] C. Beck, F. Schlögl, Thermodynamics of Chaotic Systems, Cambridge Univ. Press, Cambridge, 1993.
[57] C. Appert, M.H. Ernst, H. van Beijeren, J.R. Dorfman, Phys. Rev. E 54 (1996) R1013; J. Stat. Phys., to appear.