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Dynamical Chaos in the Lorentz Lattice Gas

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This paper provides an introduction to the applications of dynamical systems theory to nonequilibrium statistical mechanics, in particular to a study of non-equilibrium phenomena in Lorentz lattice gases with stochastic collision rules. Using simple arguments, based upon discussions in the mathematical literature, we show that such lattice gases belong to the category of dynamical systems with positive Lyapunov exponents. This is accomplished by showing how such systems can be expressed in terms of continuous phase space variables. Expressions for the Lyapunov exponent of a one-dimensional Lorentz lattice gas with periodic boundaries are derived. Other quantities of interest for the theory of irreversible processes are discussed.

KEY WORDS: Lorentz lattice gas; Lyapunov exponents; dynamical chaos; KS entropy; diffusion, kinetic theory of gases, random walks.

1. INTRODUCTION

Over the past several years a number of workers have begun to explore the connections between the statistical mechanics of irreversible processes in fluids and the ergodic behavior of dynamical systems. Studies by Posch and Hoover[(1)] and Evans *et al.*[(2)] of fluid systems subjected to external forces producing shear flows or electric currents with internal Gaussian thermostats maintaining a constant kinetic or total energy led to very interesting connections between the transport coefficients and the Lyapunov exponents for the thermostatted systems. A good example of the work is the study of shear flows by Evans *et al.*[(2)]. They were able to relate the coefficient of shear viscosity $\eta(\gamma)$ of a thermostatted system subjected to an external force

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providing a shear flow, with $\gamma = (\partial u_y/\partial x)$, to the most positive Lyapunov exponent, $\lambda_{\max}(\gamma)$ and the most negative Lyapunov exponent, $\lambda_{\min}(\gamma)$ through the relation

$$\eta(\gamma) = -\frac{3nk_B T}{\gamma^2}(\lambda_{\max}(\gamma) + \lambda_{\min}(\gamma)) \tag{1.1}$$

Here, we imagine a shear flow with an x-dependent velocity in the y direction, $u_y(x)$, the system is maintained at temperature T by the thermostat, n is the number density of the fluid, and k_B is Boltzmann's constant. The positive (or negative) Lyapunov exponents characterize the exponential separation (or convergence) rates of two nearby trajectories in the $2dN$-dimensional phase space, Γ, for N particles each of which moves in a d-dimensional space. The classical mechanics of Hamiltonian systems requires that the most positive and the most negative Lyapunov exponents have exactly the same magnitude, so the right-hand side of Eq. (1.1) might appear to vanish, but the presence of the Gaussian thermostat prevents the system from being a Hamiltonian system. For finite η the sum $[\lambda_{\max}(\gamma) + \lambda_{\min}(\gamma)]$ is at least of order γ^2 as the shear rate becomes small. A rigorous mathematical study of the electrical conductivity of an electron moving in a periodic array of fixed scatterers, *also* with a thermostat to maintain the constant energy of the electron in the presence of an applied external force, leads to results very similar to Eq. (1.1), where η becomes the electrical conductivity and γ the applied electric field strength.[3]

A study of the relation between transport coefficients and chaotic behavior for purely Hamiltonian systems has been initiated by Gaspard and Nicolis[4] and Gaspard and co-workers.[5,6] These authors relate transport coefficients for fluid systems to the escape rate of a set of trajectories from a certain well defined region in the appropriate phase space. Typical of the results of this approach is the expression for the coefficient of diffusions D of a single moving particle in an unbounded region with a fixed array of scatterers. Then

$$D = \lim_{L\to\infty} \left(\frac{L}{\pi}\right)^2 \left[\sum_{\lambda_i > 0} \lambda_i(F_L) - h_{KS}(F_L)\right] \tag{1.2}$$

Here one considers all trajectories of the moving particles such that their x coordinate remains within the interval

$$-L/2 \leqslant x \leqslant L/2 \tag{1.3}$$

Most trajectories, except for a set of measure zero, will eventually leave the interval. However there is a fractal set of trajectories F_L that *never* leave the interval. Then $\lambda_i(F_L)$ is a Lyapunov exponent for trajectories on the fractal set, $h_{KS}(F_L)$ is the Kolmogorov–Sinai entropy per unit time for trajectories on the fractal set, and only the positive (separating) Lyapunov exponents are summed over in Eq. (1.2). While expressions (1.1) and (1.2) have some structural similarities, the connection between them remains obscure. Nevertheless, the fact is that a direct relation exists between quantities of interest for the description of irreversible processes in fluids and quantities such as the Lyapunov exponents and KS entropies that describe the fundamental dynamical behavior of the phase space trajectories of the same system.

In this paper we describe the methods by which dynamical systems theory can be applied to Lorentz lattice gases with stochastic collision rules governing the interactions between a moving particle on the lattice and fixed scatterers distributed on lattice sites.[7] This system is simple enough that the applications of dynamical systems theory to it can be made very clear, and all transport and dynamical properties of interest can be calculated in full detail. These properties include the diffusion coefficient, Lyapunov exponents, KS entropies, and a number of related quantities. This paper is intended to introduce some of the essential ideas of this approach to nonequilibrium processes for a simple example. It draws upon elementary mathematical arguments and models to show that the Lorentz lattice gas can be thought of as a dynamical system with many of the properties normally present in chaotic Hamiltonian systems. A full description of this line of research on Lorentz lattice gases will be presented elsewhere.[8] There we will show that the Lorentz lattice gas belongs to the category of systems discussed by Gaspard *et al.*, such that its transport properties can be characterized by the dynamics of a fractal set of trapped trajectories. We will compute these chaotic properties of open systems using both analytical and computational methods, in order to illustrate Eq. (1.2) for Lorentz lattice gases and to develop further consequences of the approach to transport phenomena.

The outline of this paper is as follows. In Section 2 we describe Lorentz lattice gas systems and give the stochastic collision rules. In Section 3 we provide a basic introduction to the chaotic dynamics of a simple stochastic system, the coin toss system, in order to develop the ideas needed for the Lorentz lattice gas. This section is largely based upon the mathematical literature. In Section 4 we discuss the one-dimensional Lorentz lattice gas and compute the Lyapunov exponent, the KS entropy, and other quantities, all for closed periodic systems. We summarize this paper in Section 5, and describe the extensions to open systems which will be presented in further publications.

2. THE LORENTZ LATTICE GAS

We consider a regular lattice of points in d dimensions. The dynamical state of a particle moving on the lattice is described by its position $\mathbf{r}$ and by its velocity $\mathbf{c}$. The positions are restricted to lattice sites and the velocity is restricted to lie along a lattice vector. The spacing between nearest neighbor lattice sites will be taken to be unity, and the magnitude of $\mathbf{c}$ will be set equal to one, $|\mathbf{c}| = 1$, so that at each unit interval of time the moving particle travels from one site to a nearest neighbor along one of the lattice directions. We suppose that fixed scatterers are placed at lattice sites at random with density ρ such that $\rho = 1$ corresponds to full coverage of the lattice by scatterers and $\rho = 0$ corresponds to a lattice without scatterers. We will refer to a given configuration of scatterers as a "quenched" configuration and we may wish to average over all configurations of scatterers at a fixed density or with a fixed number of scatterers. The dynamics of the moving particle on the lattice is determined by the rules governing the collision of the moving particle with a scatterer. The collision rules are as follows:

1. If the moving particle arrives at a site where there is *no* scatterer, then its velocity does not change and at the next instant of time it proceeds to the nearest neighbor in the direction of its velocity.

2. If the particle arrives at a site where a scatterer is situated, then a collision instantaneously takes place which transforms a "precollision" into a "postcollision" velocity.

   (a) The precollision velocity is the velocity of the moving particle when it arrives at the site with the scatterer. It lies along the vector connecting the site with the scatterer and the previous site.

   (b) The postcollision velocity is chosen according to a stochastic rule: with probability p the particle will have a postcollision velocity parallel to the precollision velocity, with probability q the postcollision velocity will be opposite to the precollision velocity, and with probability s it will lie along one of the other lattice directions. The probabilities p, q, s satisfy

$$p + q + (b - 2)s = 1 \tag{2.1}$$

where b is the coordination number of a lattice site.

3. At the next instant of time the particle moves to the nearest neighbor site in the direction of its postcollision velocity.

The Lorentz lattice gas (LLG) represents a discretization of the usual Lorentz gas of kinetic theory. Its transport properties and velocity autocorrelation functions have been studied in considerable detail by Ernst and co-workers.[7] Here we focus on the LLG as a dynamical system.

3. STOCHASTIC PROCESSES AS DYNAMICAL SYSTEMS: A SIMPLE EXAMPLE

One ordinarily thinks of dynamical systems as having a differential structure so that the concept of nearby and exponentially separating trajectories needed to define, among other things, Lyapunov exponents can be applied to them. Such a differential structure does not appear to be appropriate for LLGs at first sight, since the dynamics takes place on a set of discrete positions and velocities and the collision rules are stochastic rather than deterministic. There is a large and very useful literature which shows how one can map many discrete stochastic processes onto differentiable dynamical systems and vice versa, so that it is not unusual to be able to define Lyapunov exponents and KS entropies for such systems.[9-11] What is lost in the mapping of a stochastic system onto a deterministic one is the dimensionality of the phase space, so that instead of getting a set of individual Lyapunov exponents for these stochastic systems, one obtains a quantity which can be interpreted as the sum of all the positive Lyapunov exponents.[9-12] However, for the connection between dynamical quantities and transport coefficients, as typified by Eq. (1.2), this sum is all that is needed.

There are a number of equivalent methods by means of which stochastic process can be described as dynamical systems with Lyapunov exponents, KS entropies, and related quantities. There are also a number of papers that introduce dynamical systems methods for studies of cellular automata.[13] Here we shall use a method based upon linear one-dimensional maps, which is conceptually very simple and leads immediately to simple expressions for Lyapunov exponents. While the examples studied here are quite elementary and almost self-evident, the strategy used here can easily be extended to the more complicated case of open systems or higher dimensions, as discussed in Section 1.

We begin the discussion with a well-known, simple stochastic system that can be mapped onto a differentiable dynamical system, a coin toss experiment with a probability of p for finding heads and q for tails, with $p+q=1$. The phase space of such a system consists of the set of all possible infinite sequences of 0's and 1's of the form

$$\boldsymbol{\alpha} = \alpha_0 \alpha_1 \alpha_2 \dots \tag{3.1}$$

where $\alpha_i = 0, 1$, with 0 representing tails and 1 representing heads, and hence

α_i has an expectation value $\langle \alpha_i \rangle = p$. For a given set of $\{\alpha_i\}$ Eq. (3.1) represents one particular run of the experiment starting from $t = 0$ and continuing to $t = +\infty$ with the outcome at time $t = i$ taking the value α_i. If $\boldsymbol{\alpha}(0)$ denotes a particular sequence

$$\boldsymbol{\alpha}(0) = \alpha_0 \alpha_1 \alpha_2 \cdots$$

the effect of tossing the coin once is to generate a new sequence

$$\boldsymbol{\alpha}(1) = \alpha_1 \alpha_2 \alpha_3 \cdots$$

where each α_i is replaced by $\alpha_i' = \alpha_{i+1}$ and the α_0 dropped. Thus the dynamics of the coin toss is represented by a shift of the entire sequence one unit to the left and dropping the leftmost term. Consequently, after t tosses of the coin, one obtains $\boldsymbol{\alpha}(t)$ with

$$\boldsymbol{\alpha}(t) = \alpha_t \alpha_{t+1} \alpha_{t+2} \cdots \tag{3.2}$$

Of course in each of these infinite sequences, heads will occur a fraction p of the time and tails a fraction q of the time. These sequences are commonly referred to as (one-sided)) Bernoulli sequences, and the transition from $\boldsymbol{\alpha}(0)$ to $\boldsymbol{\alpha}(1)$, is known as a Bernoulli shift.[9-11]

There is an uncountable infinity of sequences of the type (3.1) and they can be put into one-to-one correspondence with points on the interval $0 \leqslant x \leqslant 1$. The dynamical process of tossing a coin can be put into a one-to-one correspondence with a map of this unit interval onto itself. To illustrate this point, we first consider the case where $p = q = 1/2$. Then the value of x corresponding to $\boldsymbol{\alpha}(0) = \alpha_0 \alpha_1 \alpha_2 \cdots$ is given by the binary representation of a fraction

$$x(0) = \sum_{i=0}^{\infty} \frac{\alpha_i}{2^{i+1}} \tag{3.3}$$

where the α_i are always 0 or 1. These α_i, taken in order, represent the Bernoulli sequence $\boldsymbol{\alpha}(0)$, Eq. (3.1). Similarly the value of $x(t)$ corresponding to $\boldsymbol{\alpha}(t)$ is

$$x(t) = \sum_{i=0}^{\infty} \frac{\alpha_{t+i}}{2^{i+1}} \tag{3.4}$$

where again the α_i are always 0 or 1, and $x(t)$ corresponds to the sequence $\boldsymbol{\alpha}(t) = \alpha_t \alpha_{t+1} \alpha_{t+2} \cdots$, as in Eq. (3.2). The map M which replaces $x(t)$ by $x(t+1)$, representing a coin toss, is the binary map

$$x(t+1) = M(x(t)) = 2x(t) \qquad (\text{mod } 1) \tag{3.5}$$

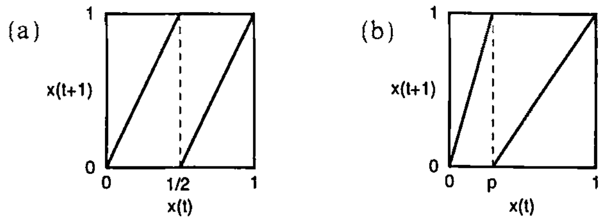

Fig. 1. Continuous maps associated with coin toss sequences. (a) The map appropriate for the case $p=q=1/2$, Eq. (3.5). (b) is the map appropriate for the case $p \neq q$, Eq. (3.6).

Analogous results obtain in the case that $p \neq q \neq 1/2$. Here the map $M(x(t))$ is

$$x(t+1) = M(x(t)) = \begin{cases} \dfrac{1}{p}\, x(t) & \text{for} \quad 0 \leqslant x(t) < p \\ \dfrac{1}{q}\,(x(t) - p) & \text{for} \quad p \leqslant x(t) < 1 \end{cases} \tag{3.6}$$

and the corresponding value for $x(0)$ is

$$x(0) = \alpha_0(1 - \Pi_{\alpha_0}) + \alpha_1(1 - \Pi_{\alpha_1})\, \Pi_{\alpha_0} + \alpha_2(1 - \Pi_{\alpha_2})\, \Pi_{\alpha_0} \Pi_{\alpha_1} + \cdots$$

where $\Pi_0 = p$ and $\Pi_1 = q$.

These maps are illustrated in Figs. 1a and 1b. Since the coin tossing experiment can be expressed in terms of a map on a continuous variable $x(t)$, one can easily define a positive, nonzero Lyapunov exponent that characterizes coin tossing as a chaotic process.

Imagine, then, two sequences $\boldsymbol{\alpha}_i(0)$ and $\boldsymbol{\alpha}_2(0)$ which are represented by very nearby points $x(0)$ and $x_1(0) = x(0) + \delta x(0)$ on the unit interval. The Lyapunov exponent characterizes the exponential separation of the phase points $x(t)$ and $x_1(t)$ with time t. To see this exponential separation, suppose $\delta x(0)$ is very small, and compute $\delta x(t) = x_1(t) - x(t)$ as

$$\begin{aligned} |\delta x(t)| &= |M^t(x(0) + \delta x(0)) - M^t(x(0))| \\ &= \left| \frac{dM^t(x(0))}{dx(0)} \right| \cdot |\delta x(0)| \\ &= \prod_{\tau=0}^{t-1} |M'(x(\tau))| \cdot |\delta x(0)| \\ &= \left(\frac{1}{p}\right)^{t_1} \left(\frac{1}{q}\right)^{t_2} |\delta x(0)| \end{aligned} \tag{3.7}$$

where M^t is the tth iterate of the map M and $dx(t+1)/dx(t) = M'(x(t))$ is the derivative of the map at $x(t)$. We have used the mapping (3.6), and t_1 is the number of times that heads appears in t trials, and $t_2 = t - t_1$ is the number of times that tails appears. The right-hand side of Eq. (3.7) can be written in an exponential form

$$|\delta x(t)| = e^{t\lambda(t)}\, |\delta x(0)|$$

with

$$\lambda(t) = (t_1/t)\log(1/p) + (t_2/t)\log(1/q) \tag{3.8}$$

Since, as $t \to \infty$, the fraction of the time that heads appears, t_1/t approaches the value p, and the fraction of time that tails appears t_2/t approaches q, we find that

$$\lambda = \lim_{t\to\infty} \lambda(t) = p\log(1/p) + q\log(1/q) \tag{3.9}$$

It is important to note that we have defined the Lyapunov exponent λ in Eq. (3.9) as the *time* average of the rate of the exponential separation of two nearby points in the appropriate phase space. In replacing the quantities t_1/t and t_2/t by p and by q, respectively, in the transition from Eq. (3.8) to Eq. (3.9), we have made use of the ergodic properties of the coin toss system to replace a time average by an ensemble average. Therefore starting from Eq. (3.7) and using an ergodic theorem, we can also express the Lyapunov exponent as an ensemble average

$$\begin{aligned}\lambda &= \lim_{t\to\infty} \frac{1}{t}\langle \log|\delta x(t)/\delta x(0)|\rangle \\ &= \lim_{t\to\infty} \frac{1}{t}\sum_{\tau=0}^{t-1} \log|M'(x(\tau))| = \langle \log|M'(x)|\rangle \end{aligned} \tag{3.10}$$

where the angular brackets denote an average over all possible realizations of coin toss experiments with probability p for heads and q for tails.

The first line of Eq. (3.10) expresses the Lyapunov exponent in terms of the ensemble average of the logarithm of the stretching factor $|\delta x(t)/\delta x(0)|$ for a given trajectory. Due to the ensemble average, the time dependence is very simple and this expression is a constant for $t > 0$. One might ask if the distribution of values of the separation factor is sharp or broad, and a convenient measure of this distribution is found by computing the quantity $t^{-1}\log\langle \delta x(t)/\delta x(0)\rangle$, where the ensemble average and the logarithm have been interchanged. In dynamical systems theory, the latter quantity is called the "topological entropy" h_T. Several equivalent definitions of h_T for stochastic systems are possible.[9-11, 14] Here we follow the line developed so far, and define h_T by

$$h_T = \frac{1}{t} \log\langle |\delta x(t)/\delta x(0)| \rangle \qquad \text{for} \quad t > 0 \tag{3.11}$$

For the coin toss system, h_T can be easily computed as

$$h_T = \frac{1}{t} \log \left[\sum_{t_1=0}^{t} \left(\frac{1}{p}\right)^{t_1} \left(\frac{1}{q}\right)^{t-t_1} \frac{t!}{t_1!(t-t_1)!} p^{t_1} q^{t-t_1} \right] = \log 2 \tag{3.12}$$

Here we have used the facts that the probability that t_1 heads and $t-t_1$ tails will occur is $p^{t_1}q^{t-t_1}$, and the binomial factorial accounts for the number of different ways t_1 heads and $t-t_1$ tails can occur in t steps. The topological entropy is independent of p and for $p \neq q$ is very different from λ, showing that there is a broad distribution of $|\delta x(t)/\delta x(0)|$ over the ensemble of possible trajectories.

Although we will not present the details here, a calculation of the Kolmogorov–Sinai entropy per unit time can be given for the coin toss sequences as well.[9-11, 14] To do this one must examine the rate at which small subregions of the unit interval get distributed over the entire unit interval with time. Then the KS entropy measures a global mixing property of the dynamics, while the Lyapunov exponents measure the rate of separation of trajectories from a nearby reference trajectory. For the coin tossing sequences described above, one finds

$$h_{KS} = p \log(1/p) + q \log(1/p) = \lambda \tag{3.13}$$

The equality $h_{KS} = \lambda$ is an example, for coin toss sequences, of a more general theorem known as Pesin's theorem.[9-14]

4. THE LLG AS A DYNAMICAL SYSTEM

The point of the discussion in Section 3 is, of course, to show that some classes of stochastic processes can be mapped onto differentiable dynamical systems, and thus the methods of dynamical systems theory can be applied to them. The LLGs described in Section 2 fall into this class, so that the dynamics of a LLG can be characterized by a KS entropy and by λ, where λ is the analog of the sum of positive Lyapunov exponents. It is possible to formulate the dynamics of a LLG as a Markov process, similar to the formulation of the coin toss system as a Bernoulli process, and to employ some usual methods of dynamical systems theory appropriate for Markov systems.[9-11] Here we will instead use simple linear mapping methods to provide an immediate introduction to the subject and to show that Lyapunov exponents, etc., are natural objects for study in LLGs.[4] In our further work, we use Markov methods or maps as convenient. The results presented here for closed, periodic systems are quite elementary, but form a useful starting point for further work.

We illustrate this method for the case of a one-dimensional LLG at density ρ on a lattice of L sites ($L \gg 1/\rho$) and with periodic boundary conditions imposed. The phase space necessary for a description of the dynamical properties of this system must be more elaborate than that for a coin toss since at every instant of time the particle has both a velocity, which can take two values (± 1), and a location on the lattice. Furthermore, the lattice itself has a fixed configuration of scatterers, so the dynamical state of the moving particle depends on the quenched configuration of scatterers as well as on its position on the lattice and on the direction of its motion.

The phase space necessary to keep track of these various quantities can be described as follows.[8] We consider the particle moving on a one-dimensional lattice with a quenched configuration of scatterers. Each of the lattice sites is labeled by an integer n, where n ranges from 1 to L, and the periodic boundary conditions imply site $L+j$ is to be identified with site j, where j is an integer. The motion of the particle on this lattice can be modeled as a dynamic process by associating with each lattice site n a half-open unit interval, $[n, n+1)$ and supposing that at each instant of time there is a map which moves points on the interval to points on the adjacent intervals associated with the sites $(n+1)$ and $(n-1)$ according to a deterministic rule. It is convenient to think of a moving particle at site n as being somewhere in the interval $[n, n+1)$ and that its motion from one lattice site to the next is determined by its specific location on the interval and by the direction of the precollision velocity when the particle arrives at the point.

The dynamical phase space variable describing the location and direction of the moving particle will be denoted by $x_t = (r_t, c_t)$, where c_t is the precollision velocity of the particle when it arrives at the point r_t at the tth time step and r_t is a continuous variable, $r_t = [r_t] + \tilde{r}_t$. Here $[r_t]$ denotes the integer part of r_t, which we associate with lattice site n, and $\tilde{r}_t$ is a continuous variable, $0 \leqslant \tilde{r}_t < 1$ which locates the position of the moving particle in the interval $[[r_t], [r_t] + 1)$ at the tth time step. The dynamics of the moving particle at each time step is given by a map $x_{t+1} = \mathbf{M}(x_t)$

[4] It is worth mentioning that a closely related idea of using a baker's transformation to describe a collision process leading to ergodic behavior appears in Ref. 15. We thank Prof. Lebowitz for calling this reference to our attention.

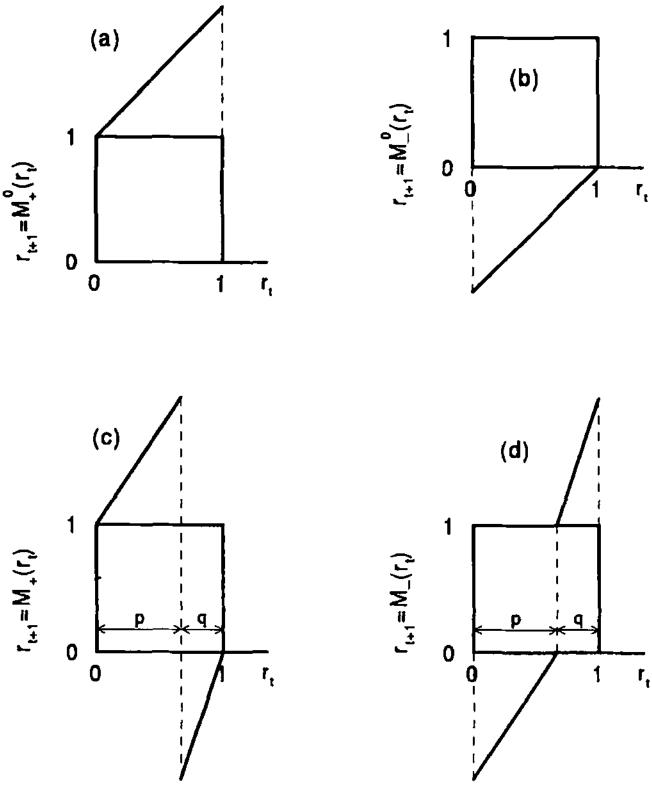

Fig. 2. Continuous maps associated with a one-dimensional Lorentz lattice gas. We show the interval (0, 1) for convenience. (a, b) The maps (4.1) that are appropriate when there is no scatterer at lattice site 0. (a) The map for a particle incident from the left ($c=+1$); (b) the map for a particle incident from the right ($c=-1$). (c, d) The maps (4.2) that are appropriate when a scatterer is present at site 0. (c) The case when a particle is incident from the left ($c=+1$); (d) the case when the particle is incident from the right ($c=-1$).

which gives the position and precollision velocity of the particle at time step $(t+1)$ in terms of its position and precollision velocity at time step t. The structure of the map depends upon whether or not there is a scatterer at site $[r_t]$ and upon the precollision velocity c_t. In Figs. 2a–2d we illustrate the map **M** for the four possible cases. Figures 2a and 2b, represent the maps appropriate for the case when there is no scatterer at $[r_t]$. These maps have the analytic form

$$\begin{aligned} r_{t+1} &= M^0_{c_t}(r_t) = r_t + c_t \\ c_{t+1} &= c_t \end{aligned} \tag{4.1}$$

Here, the superscript zero denotes the absence of a scatterer at $[r_t]$, and the postcollision velocity is the same as the precollision velocity, $c_t = (\pm 1)$. The absence of a scatterer means that at the next time step the particle proceeds to the next adjacent site in the direction of its velocity. Note also that these maps have *unit* slope. In Figs 2c and 2d we illustrate the maps appropriate for the cases where a scatterer is present at $[r_t]$. Then the maps $x_{t+1} = \mathbf{M}(x_t)$ has two possible analytic forms

$$r_{t+1} = M_{c_t}(r_t) = \begin{cases} [r_t] + c_t + \dfrac{1}{p}\tilde{r}_t, & 0 \leqslant \tilde{r}_t < p \\ [r_t] - c_t + \dfrac{1}{q}(\tilde{r}_t - p), & p \leqslant \tilde{r}_t < 1 \end{cases}$$
$$c_{t+1} = \begin{cases} c_t, & 0 \leqslant \tilde{r}_t < p \\ -c_t, & p \leqslant \tilde{r}_t < 1 \end{cases} \tag{4.2}$$

In a way similar to that for the coin tossing situation, the unit interval is divided into two regions of length p and of length q, with $p + q = 1$, such that the region of length p leads to forward scattering and that of length q leads to backscattering. Note that the slopes of the maps, needed for the computation of λ are $1/p$ for the forward scattering region and are $1/q$ for the backscattering regions.

Now that we have described the continuous phase-space variable x_t for the moving particle and the four possible analytic forms for the map $x_{t+1} = \mathbf{M}(x_t)$, at each step, we can outline the calculation of the exponential separation rate λ of trajectories which characterizes the chaotic dynamics of the LLG. If we denote the Jacobian of the map by $|\mathbf{M}'(x_\tau)| = |\partial x_{\tau+1}/\partial x_\tau|$, then we compute $|\delta x(t)/\delta x(0)|$ following the method outlined in Section 3,

$$\left|\frac{\delta x(t)}{\delta x(0)}\right| = \prod_{\tau=0}^{t-1} |\mathbf{M}'(x_\tau)| \tag{4.3}$$

The quantity λ is defined to be the limit as $t \to \infty$ of $\lambda(t|x(0))$ when

$$\lambda(t \mid x(0)) = \frac{1}{t}\log\left|\frac{\delta x(t)}{\delta x(0)}\right| = \frac{1}{t}\sum_{\tau=0}^{t-1} \log |\mathbf{M}'(x_\tau)| \tag{4.4}$$

In general $\lambda(t \mid x(0))$ depends upon time and upon the initial phase point $x(0)$. To evaluate $\lambda = \lim_{t\to\infty} \lambda(t \mid x(0))$, we can proceed in an intuitive way. The heuristic evaluation of λ is obtained by evaluating the right hand side of Eq. (4.3) by observing that the Jacobian of the map (4.1) and (4.2) is given by $|\mathbf{M}'(x_\tau)| = |dr_{t+1}/dr_t|$, where the derivative is either $1/p$, $1/q$, or 1, so that

$$\left|\frac{\delta x(t)}{\delta x(0)}\right| = \left(\frac{1}{p}\right)^{t_1} \left(\frac{1}{q}\right)^{t_2} (1)^{t_3} \tag{4.5}$$

Here the map $\mathbf{M}$ is such that:

(a) If the moving particle encounters a scatterer at a given time step and is scattered in the forward direction, the slope of the map is $1/p$. We suppose that in t time steps, t_1 collisions are of this type.

(b) If the particle encounters a scatterer at a given time step and is backscattered, the slope of the map is $1/q$. We suppose that in t time steps, t_2 collisions are of this type.

(c) If the particle arrives at a site which is not occupied by a scatterer, then the map has unit slope. We suppose that this happens t_3 times in t time steps, where $t_1 + t_2 + t_3 = t$.

Then $\lambda(t|x(0))$ is clearly

$$\lambda(t \mid x(0)) = (t_1/t)\log(1/p) + (t_2/t)\log(1/q) \tag{4.6}$$

The quantity of interest to us is $\langle \lambda(t \mid x(0)\rangle = (1/t)\langle \log \mid \delta x(t)/\delta x(0)| \rangle$, where the angular brackets denote an average over (a) an ensemble of replicas of the LLG with different configurations of scatterers with average density ρ and (b) all starting configurations $x(0)$ of the moving particle. One can now argue that with this ensemble

$$\langle t_1/t \rangle = \rho p \qquad \text{and} \qquad \langle t_2/t \rangle = \rho q \tag{4.7}$$

since for long times and for large systems the fraction of the times that a particle encounters a scatterer and maintains/reverses its original direction is equal to the product of the probability ρ that a particle will encounter a scatterer with the probability p/q that it will maintain/reverse its velocity direction. Thus we obtain

$$\lambda = \lim_{t \to \infty} \langle \lambda(t \mid x(0)) \rangle = \rho[p \log(1/p) + q \log(1/q)] \tag{4.8}$$

This result can be confirmed by a more careful argument using the Frobenius–Perron equation, but since the result is rather clear, we will not pursue this point further. We also note that simple arguments based on the Frobenius–Perron equation show that the result, Eq. (4.8), applies for a quenched configuration of scatterers as well.

We wish to point out one feature of the expression (4.6) for λ that is important for making the connection between dynamical systems theory and the kinetic theory of gases. The quantities t_1 and t_2 appearing as the right-hand side of Eq. (4.6) can be interpreted respectively as the number of "transmitting" collisions and the number of "reflecting" collisions of the moving particle with the scatterers in time interval t. These "collision numbers" are typical quantities of interest in kinetic theory, and their average values, taken over an ensemble of configurations of scatterers, can easily be computed by means of a kinetic equation. Of course, the results, Eq. (4.7) are recovered by this means, but one can also determine the rate at which the asymptotically long-time results are achieved. The connection between dynamical systems theory and kinetic theory, so simply illustrated here, is of considerable interest in more general cases.[16]

In fact, by using methods of kinetic theory, we have computed $\langle \lambda(t \mid x(0)) \rangle_{\text{scatt}}$, where the average is over an ensemble of scatterer configurations, for a fixed $x(0)$. These calculations show that as $t \to \infty$,

$$\langle \lambda(t \mid x(0)) \rangle_{\text{scatt}} = \rho[p \log(1/p) + q \log(1/q)] + O(t^{-1}) + O(t^{-3/2}) \qquad (4.9)$$

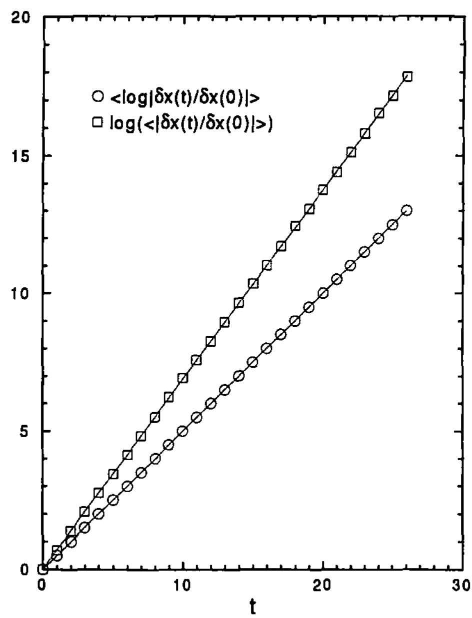

Fig. 3. Results from computer simulations illustrating the exponential separation of trajectories for the filled ($\rho = 1$) Lorentz lattice gas for $p = 0.8$, $q = 0.2$. The circles represent the average needed or the Lyapunov exponent. The slope of the line is 0.500, in excellent agreement with the value 0.504 predicted by Eq. (4.8). The squares represent the average needed for the topological entropy h_T. The slope of the line is 0.687, and the theoretical prediction is $\log 2 = 0.693$, We used 2×10^5 nearby pairs of trajectories in the simulations to compute these curves.

The coefficients of all terms in Eq. (4.9), those of $O(t^{-1})$, and mode-coupling terms of order $t^{-3/2}$, or $t^{-1-d/2}$ for a LLG in d-dimensions, can be computed explicitly.

It is important to note that:

(a) The methods of kinetic theory have a valuable role to play in the evaluation of dynamical quantities for systems such as a LLG where the statistical randomness of collisions is important.

(b) One might also wish to compute the average value $\log\langle |\delta x(t)/\delta x(0)| \rangle$ rather than the average value $\langle \log |\delta x(t)/\delta x(0)| \rangle$ as calculated above. As in Section 3, for the coin toss, one can use ergodic theory arguments to show that the former quantity, $\log\langle \cdot \rangle$, is related to the topological entropy[9-11, 13] of the system, while the latter quantity, $\langle \log(\cdot) \rangle$, is the proper Lyapunov exponent and thus related to the KS entropy. The difference between these two quantities as determined by computer simulation is illustrated in Fig. 3 for the case $\rho = 1$.

5. CONCLUSION

We conclude this paper with a brief discussion of open LLG systems and some general remarks.

The purpose of our research on open systems is to study the connection between nonequilibrium statistical mechanics and chaos theory, and more specifically between transport coefficients and Lyapunov exponents and the KS entropy.[8] To do this one has to study λ and h_{KS} for the set of trajectories that remain in a bounded region of the lattice for an infinite time.

For example, suppose that instead of imposing periodic boundary conditions on a system of L sites, we place absorbers at both ends of the line, i.e., at sites 0 and $L+1$, such that a particle starting as one of the sites $1, 2, \ldots, L$ will be absorbed if it reaches 0 or $L+1$. Then almost all of the trajectories for the moving particle will eventually lead to absorption at the boundaries. However, in the continuous phase space of trajectories there will always be a set of trajectories of measure zero that never lead to absorption. To compute the coefficient of diffusion for the LLG one has to determine λ and h_{KS} for the zero-measure set of trajectories. This requires a very detailed study of the system, keeping track of the location of the moving particle at each time step, and always restricting trajectories to those which do not lead to absorption. Both analytic and computer studies of the properties of these trajectories, the Lyapunov exponents, and KS entropy associated with them and of the escape rate formula are currently underway.[8]

We also note that dynamical systems can be described by a quantity, the topological pressure, that plays a role in chaotic systems similar to that of the Helmholtz free energy of statistical mechanical systems in the canonical ensemble.[7] For several reasons this topological pressure is an interesting quantity for study, and it, too, is accessible to both analytical and computer studies.[8]

In this paper we have tried to emphasize a few central points that motivate our interest in the chaotic dynamics of Lorentz lattice gases. These points are:

1. There exist interesting and general connections between transport properties of nonequilibrium systems and the dynamical properties of these systems when the phase space trajectories of the system are studied in detail.

2. Lattice gas automata, and Lorentz lattice gases in particular, represent simple systems in which both the transport and dynamic properties can be studied in considerable detail using analytic methods as well as computer simulations.

3. Methods traditionally used to study the statistical mechanics of nonequilibrium systems can be very useful also to study the chaotic properties of the same systems. This fact illustrates the deep connection between the chaotic properties of a dynamical system and the possible existence of an equilibrium state of the system. In our work we have used techniques from the kinetic theory of gases—kinetic equations, cluster expansions, mode coupling analyses, as well as techniques based on the Chapman–Kolmogorov equations familiar from probability theory.

4. The interface between dynamical system theory and nonequilibrium statistical mechanics is a new area of research and it promises to be very fruitful.

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