Mean-Field Theory for Lyapunov Exponents and Kolmogorov-Sinai Entropy in Lorentz Lattice Gases

M. H. Ernst, J. R. Dorfman,* R. Nix, and D. Jacobs†

Institute for Theoretical Physics, Utrecht University, P.O. Box 80006, 3508 TA Utrecht, The Netherlands

(Received 21 December 1994)

Chaotic properties of a Lorentz lattice gas are studied analytically and by computer simulations. The escape rates, Lyapunov exponents, and Kolmogorov-Sinai entropies are estimated for a 1D example using mean-field theory, and the results are compared with simulations for a range of densities and scattering parameters of the lattice gas. Computer results show a distribution of values for the dynamical quantities with average values in good agreement with mean-field theory, and consistent with the escape-rate formalism for the coefficient of diffusion.

PACS numbers: 05.45.+b, 05.20.Dd, 05.60.+w

The purpose of this Letter is to describe a simple model of interest for nonequilibrium statistical mechanics, the Lorentz lattice gas (LLG), that allows a detailed calculation of its chaotic dynamical properties as well as its transport properties. Here we show that such quantities as Lyapunov exponents, Kolmogorov-Sinai (KS) entropies, and dynamical partition functions can be calculated for LLG's over a full range of densities, using analytical methods as well as computer simulations for closed, periodic, and open systems. The latter case is of particular interest, since Gaspard and Nicolis [1] have established a relation between the transport coefficients of hydrodynamics and the Lyapunov exponents and KS entropies of a fractal set of trapped trajectories in open systems. Although LLG's are random systems and not of the type usually accessible by the methods used widely in dynamical systems theory, we are able to compute their dynamical properties using techniques of statistical mechanics. Most of our calculations will focus on the dynamical partition function which can be used to obtain all of the other dynamical quantities of interest [2,3].

A Lorentz lattice gas consists of a moving particle (MP) traveling on the sites of a d-dimensional lattice with unit lattice distance and having allowed velocities equal to nearest-neighbor lattice vectors. The dynamical state of the particle at any time t is given by its position $\mathbf{r}$ and its velocity $\mathbf{c}$. A fixed number of scatterers N is placed at random on lattice sites, and the density ρ denotes the fraction of occupied sites. We will average over all *quenched* configurations of scatterers. The dynamics of the MP at every time step consists of instantaneous collisions with a scatterer, followed by propagation, in which the MP travels from a site to a nearest neighbor. If the MP arrives at a scattering site with velocity $\mathbf{c}$, it will be transmitted, reflected, or deflected with probabilities p, q, s, respectively, normalized as $p + q + 2(d - 1)s = 1$. If the MP arrives at a nonscattering site, its velocity remains unchanged. The special case of full coverage ($\rho = 1$) is an example of a persistent random walk, studied by Haus and Kehr [4].

The diffusion of the MP in a LLG has been studied in considerable detail, and the density dependence of the diffusion coefficient is well approximated by a simple expression, which is exact in the one-dimensional case for all densities [5]. Here we address the chaotic properties of this system. Although the method described here can be used for cubic lattices in any dimension, we will consider one-dimensional systems for simplicity.

We consider a line of lattice points with sites, labeled $r = 1, 2, \dots, L$. The sites at $r = 0$ and $r = L + 1$ are occupied by absorbers, so that no particle (re)enters the region $r = 1, \dots, L$ from these sites, and any particle leaving this region is absorbed. This construction is of importance for determining the set of trajectories of the MP that are trapped forever in the bounded region. The dynamical properties of this set of trajectories determine the coefficient of diffusion in the escape-rate formalism.

We begin by considering a quenched configuration of scatterers at density ρ, and define the matrix of transition probabilities $w(x|y)$ to be the probability for the MP to go from a precollision state $y = \{r', c'\}$ at time t to the precollision state $x = \{r, c\}$ at time $t + 1$. For our one-dimensional example, the velocity of the MP c can only take on the values ± 1. For a quenched configuration of scatterers with escape the matrix $w(x|y)$ has dimension $2(L - 1)$ and is given by

$$w(x|y) = w(r, c|r', c') = [a_1(r')\delta(c, c') + b_1(r')\delta(c, -c')] \times \delta(r, r' + c). \quad (1)$$

Here δ denotes a Kronecker delta function; if there is no scatterer at the point r', then $a_1(r') = 1$ and $b_1(r') = 0$; if there is a scatterer, then $a_1(r') = p$ and $b_1(r') = q$. In constructing the dynamical partition function we will need $[w(x|y)]^\beta \equiv w_\beta(x|y)$, where β is an "inverse-temperature-like" parameter, which might be negative as well. The random matrix $w_\beta(x|y)$ is also given by Eq. (1) with $a_1(r)$ replaced by $a(r) \equiv a_1^\beta(r)$ and $b_1(r)$ replaced by $b(r) \equiv b_1^\beta(r)$. Further, w_β is a periodic matrix [6] with period 2. This follows from the dynamics where the particle will necessarily move alternately from even

 0031-9007/95/74(22)/4416(4)$06.00

to odd numbered sites or vice versa. This has important consequences for the proper ergodic decomposition of the ergodic states of this system.

To construct the dynamical partition function we imagine that the MP is initially placed on the lattice with an initial phase $x_0 = (r_0, c_0)$ and we ask for the probability $P(\Omega, t; x_0)$ that in t time steps the particle follows a trajectory $\Omega = \{x_0, x_1, \dots, x_t\}$ starting at x_0 and always remaining within the boundaries of the system. Knowing the hierarchy of t-point functions we can construct the dynamical partition function as [2,3]

$$Z_\beta(L, t; x_0) = \sum_\Omega [P(\Omega, t, x_0)]^\beta = \sum_{x_1,\dots,x_t} w_\beta(x_t|x_{t-1}) \cdots w_\beta(x_1|x_0). \quad (2)$$

With the help of the thermodynamic formalism all dynamical quantities of interest can be obtained from the *topological pressure* $\psi_\beta(L; x_0)$, defined by

$$\psi_\beta(L; x_0) = \lim_{t\to\infty} (1/t) \ \ln Z_\beta(L, t; x_0) = \ln\Lambda(\beta, L), \quad (3)$$

where $\Lambda(\beta, L)$ is the largest eigenvalue of the random matrix w_β. This can be understood by observing that (2) for long times is essentially the trace of a matrix, i.e., $(2L)^{-1}\mathrm{Tr}(w_\beta)^t$. To obtain the average pressure we have to calculate the quenched average $\langle \ln Z_\beta \rangle$ over all distributions of scatterers, formally analogous to spin glasses with random interactions [7]. We note that w_β is the analog of the transfer matrix in statistical mechanical calculations of the partition function of Ising-type lattice models with random interactions. The large-t limit is the analog of the thermodynamic limit.

The dynamical quantities of interest here are the escape rate $\gamma(L)$ of the particle from the lattice, the Lyapunov exponent $\lambda(L)$, and the KS entropy $h_{\mathrm{KS}}(L)$ for the fractal set of trajectories that are forever trapped on the lattice. According to the thermodynamic formalism these quantities are given by

$$\gamma(L) = -\psi_1, \qquad \lambda(L) = -\psi_1', \qquad h_{\mathrm{KS}}(L) = \lambda(L) - \gamma(L), \quad (4)$$

where the prime denotes a derivative with respect to β. For a LLG *without* escape ($\gamma = 0$) the Lyapunov exponent is *independent* of the configuration of scatterers, and is given by $\lambda_0 = -\rho p \ln p - \rho q \ln q$ [8], and $\lambda_0 = h_{\mathrm{KS}}$ (Pésin's theorem). In a LLG *with* escape the exponents $\gamma(L)$ and $\lambda(L)$ depend on the configurations.

In general, it is difficult to evaluate Z_β or $\Lambda(\beta)$, except for the special case $\rho = 1$. Elsewhere we will show that methods based on the kinetic theory of gases can be used to compute the various quantities of interest. Here we show how simple mean-field and scaling approximations can be used to obtain useful approximations for Z_β which compare well with computer simulations over a wide range of densities and reflection probabilities. Suppose the system has a given number of N scatterers distributed in some way over the L lattice sites. For large N and L the average distance between scatterers is $R = L/N = 1/\rho$. We replace our random lattice with a regular lattice with scatterers placed a distance R apart. Thus we can pretend that we are evaluating the dynamical partition function for a persistent random walk of a MP on an effective lattice of L/R sites and for an effective time of t/R steps. To simplify matters further we can suppose that the initial state x_0 is located on a scatterer. Then we obtain the result

$$Z_\beta(L, t; x_0) \simeq Z_\beta(L/R, t/R). \quad (5)$$

Here Z_β is the dynamical partition function for a persistent random walk on a lattice of $L/R = \mathcal{N}$ sites during a time $t/R = \mathcal{T}$ with absorbing boundaries.

This can be evaluated by noting that the dynamical partition function for this case is

$$Z_\beta(\mathcal{N}, \mathcal{T}) \simeq (1/2\mathcal{N})\mathrm{Tr}(\tilde{w}_\beta)^{\mathcal{T}}, \quad (6)$$

where $\tilde{w}_\beta$ is the transition matrix for the persistent random walk, given by Eq. (1) with all a's replaced by $a = p^\beta$ and all b's by $b = q^\beta$. Since $\tilde{w}_\beta$ is a $2(\mathcal{N} - 1)$-dimensional matrix with period 2, its square can be put in block-diagonal form, each block corresponding to an invariant, ergodic subspace where particles on even (odd) sites remain on even (odd) sites for every *two* time steps. We then look for the eigenstates of each of the two separate blocks of $\tilde{w}_\beta^2$ and find that the largest eigenvalues of both blocks are identical, and denote them by $\Lambda^2(\beta, \mathcal{N})$. Thus we evaluate $Z_\beta \simeq \Lambda^{\mathcal{T}}(\beta, \mathcal{N})$. For *closed* systems the matrix $\tilde{w}_\beta$ is cyclic, and one easily finds $\Lambda(\beta, \mathcal{N}) = a + b$, from which the above result for λ_0 can be recovered. For *open* systems and large $\mathcal{N}$ there is a correction of $\mathcal{O}(1/\mathcal{N}^2)$, and the topological pressure is found to be

$$\psi_\beta(\mathcal{N}) = \ln(a + b) - \frac{a}{2b}\left(\frac{\pi}{\mathcal{N} + a/b}\right)^2. \quad (7)$$

Our main result is obtained from this equation by scaling $\mathcal{N} = L/R$ and $\mathcal{T} = t/R$ with the expected free interval between scatterers $R = 1/\rho$. We find that for a LLG with N scatterers, distributed at random over L sites, the mean-field value for the topological pressure is found from (3) and (6) as

$$\psi_\beta(N, L) = \rho\left\{\ln(a + b) - \frac{a}{2b}\left(\frac{\pi}{\rho L + a/b}\right)^2\right\}. \quad (8)$$

Using Eqs. (4) one readily finds

$$\gamma(L) = \left(\frac{\rho p}{2q}\right)\left(\frac{\pi}{\rho L + p/q}\right)^2,$$
$$\lambda(L) = \lambda_0 + \left(\frac{\rho p}{2q}\right)\ln(p/q)\left(\frac{\pi}{\rho L + 2p/q}\right)^2. \quad (9)$$

The terms of $\mathcal{O}(1/L^2)$ are the corrections due to the absorbing boundary conditions. They have the size dependence expected from the escape-rate formalism [1,9], which suggests to write $\gamma(L) \equiv Dk_0^2$, where $k_0 = \pi/(L +$

$p/\rho q$) is the wave number of the slowest decaying diffusive mode, and $D = p/2q\rho$ is the mean-field value of the diffusion coefficient of the LLG. This expression is exact for one-dimensional systems [5]. Combination of $\gamma(L) \equiv Dk_0^2$ with the last line of (4) clearly exhibits the intimate connection between chaos properties and transport properties, as referred to in the introduction. It has the same form as the corresponding relation derived by Gaspard and Nicolis for the continuous Lorentz gas in a periodic array of scatterers.

We now discuss the comparison of these results with our computer simulations. In order to test to what extent the mean-field results capture the essence of the chaos properties for the LLG, we numerically determine the largest eigenvalue of the large random matrix $\tilde{w}_\beta^2$ of linear dimension $2(L-1)$. In every quenched distribution of scatterers the secular determinant of this rather sparse random matrix is calculated from a two step recursion relation. Its largest root $\Lambda(\beta, \mathcal{N})$, the topological pressure $\psi_\beta(\mathcal{N})$, and its derivative in Eq. (9) are computed numerically. Then we average over an ensemble of different configurations of N scatterers, placed at random on a lattice of L sites.

For the escape rate the agreement between mean-field theory (MFT) and simulations is excellent, as would be expected, and we first consider the distribution of escape rates over the members of the ensemble. It appears to be a *very narrow* Gaussian-type distribution with a width less than 5% of the mean. We introduce the reduced escape rate $g \equiv (\gamma/\rho)(N + p/q)^2$, which is predicted to be independent of the density ρ, the number of scatterers $N = \rho L$, and system size L, and measure it typically over 3×10^6 configurations of scatterers. It varies by less than 0.5% over the whole density range ($0.1 \le \rho \le 0.9$), and over different system sizes ($N = \rho L = 50, 100, 200, 400$), and differs by less than 0.5% from the MFT prediction $\pi^2(p/2q)$. This also implies that $\langle \ln\Lambda(1)\rangle$ should be nearly equal to $\ln\langle\Lambda(1)\rangle$. In fact, they are found to be equal within statistical errors. At $N = 10$ there are sizable finite size effects as is to be expected on the basis of (9).

The measured Lyapunov exponents show huge variation over different placements of scatterers, resulting in a very broad distribution with a width much larger than the mean. This is illustrated in Fig. 1, which displays the probability distribution $P(\ell)$ of the reduced Lyapunov exponent $\ell \equiv (\Delta\lambda/\rho)(N + 2p/q)^2$, with $\Delta\lambda = \lambda(L) - \lambda_0$.

Table I compares the MFT results for the reduced Lyapunov exponent at different $(N;p)$ values with $\langle\ell\rangle$, resulting from computer simulations averaged over 3×10^6 scatterer configurations, except at $N = 200$ and $p = 0.2$, where 5×10^7 runs were used, and at $N = 200$ and $p = 0.5$, where 2×10^7 runs were used. The required CPU time on a DEC 3000 α machine is typically $10^{-3}N$ days per 10^6 runs.

The variance $w^2 = \langle\ell^2\rangle - \langle\ell\rangle^2$ depends strongly on N and only weakly on p. At $p = 0.8$ the ratio $w/\langle\ell\rangle$ is about 6, 20, 100 for $N = 50, 200, 400$, respectively. Nevertheless, when averaging over typically 3×10^6 runs the mean $\langle\ell\rangle$ remains independent of density and system size, and is in good agreement (within 2% to 4%) with the MFT prediction $\langle\ell\rangle = \pi^2(p/2q)\ln(p/q)$. One can also see a small systematic density variation in the results for $\langle\ell\rangle$. At small p values ($p \sim 0.2$) the distribution becomes very broad, as $\langle\ell\rangle$ and $\langle\ell\rangle/w$ decrease by a factor of 20. Finite size effects and density dependence of $\langle\ell\rangle$ become more pronounced with systematic deviations from MFT up to 7%. At $p = 0.5$ the MFT prediction is $\langle\ell\rangle = 0$. In an LLG with $N = 50$ scatterers, the mean $\langle\ell\rangle$ is nonvanishing ($w = 300\langle\ell\rangle$), and shows again a weak, but systematic density dependence. The deviations from the asymptotic MFT may be ascribed to finite size effects. For larger systems ($N = 200$) the simulation results are consistent with a vanishing MFT prediction, but the error bars are very large. Similar broad distributions are expected to occur in continuous Lorentz gases with escape [10].

It is important to emphasize two consequences of these very broad distributions: (i) The error bars, as listed

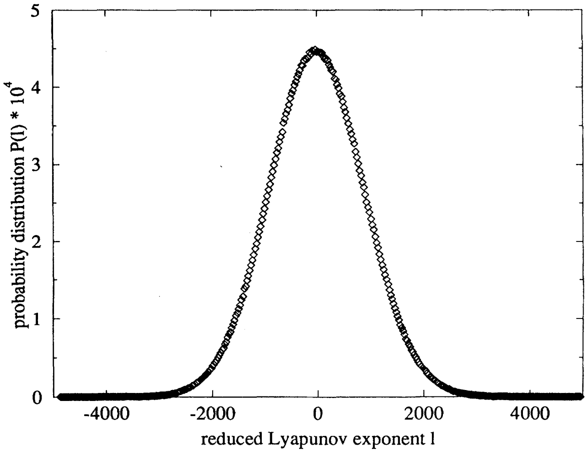

FIG. 1. Probability distribution $P(\ell)$ of reduced Lyapunov exponent ℓ in a LLG with $N = 200, L = 1000$, and $p = 0.2$, taken over 10^7 configurations. $P(\ell)$ is a very broad Gaussian distribution with $\langle\ell\rangle = -1.9 \pm 0.3$, width $w = 500|\langle\ell\rangle| = 900$, and kurtosis 0.02.

TABLE I. Average reduced Lyapunov exponent $\langle\ell\rangle$ at different $(N;p)$ values. A superscript a denotes a statistical error of $\pm a$ in the last digit.

	Density ρ			MFT
$(N;p)$	0.2	0.5	0.8	1
(50;0.2)	-1.28^5	-1.30^5	-1.40^2	-1.71
(200;0.2)	-1.7^1	-1.4^1	-1.4^1	-1.71
(50;0.5)	0.7^1	0.6^1	0.5^1	0
(200;0.5)	0.3^3	0.3^2	0.5^1	0
(50; 0.8)	29.0^1	28.7^5	28.4^5	27.35
(200;0.8)	27.7^6	28.1^4	27.6^3	27.35

in Table I, have little bearing on the predictability of the outcome of a single measurement. For instance, the data used in Fig. 1 yield $\langle \ell \rangle = -1.9 \pm 0.3$, where the statistical uncertainty ± 0.3 in the average is calculated over 10^7 runs. On the other hand, the distribution $P(\ell)$ in Fig. 1 gives only the very weak prediction that the outcome of a single measurement ℓ will be in the interval $(-1.9 - 900, -1.9 + 900)$ with a 66% confidence limit. (ii) According to Eqs. (3) and (4) the proper way to obtain mean values of Lyapunov exponents is to calculate $\langle \Lambda'(1)/\Lambda(1) \rangle$, rather than $\langle \Lambda'(1) \rangle / \langle \Lambda(1) \rangle$, i.e., taking the logarithm and the quenched average should not be interchanged. Following the latter prescription leads to values that may be up to factors of 6 larger or smaller than $\langle \ell \rangle$, depending on density and transmission rate.

More details about the derivations of the theoretical results, about the numerical analysis of our sparse matrices with random elements, and about the effects of rare configurations will be published elsewhere. Calculations of topological entropies, and studies of possible dynamical phase transitions in higher-dimensional LLG's are in progress, as well as extensions of these ideas to random walks in random environments.

We conclude with the following remarks:

(i) The average values of the dynamical quantities, escape rates, Lyapunov exponents, and KS entropies [through Eq. (9)], averaged over a large number of 3×10^6 to 5×10^7, are close to the predictions of mean-field theory for all densities, sufficiently large system sizes, and all model parameters describing the scattering of MP's in LLG's. The probability distributions of these quantities over different placements of scatterers are very broad and of Gaussian form, and the mean values do not seem to be affected by rare events.

(ii) We have been able to show that a variety of methods from statistical mechanics can be usefully applied to determine properties that characterize the chaotic behavior of nonequilibrium systems. The present results for LLG's are closely related to the calculation presented in the preceding Letter by van Beijeren and Dorfman for the continuous Lorentz gas in two dimensions [10]. The simplifications present in LLG models allow a deeper exploration of systems at high density, but there are many close connections between the two systems, as well as with systems with other transport processes taking place.

(iii) A more systematic approach to the calculations of dynamical quantities for LLG's can be based on kinetic theory methods. Such a study will lead to an understanding of the contributions to Lyapunov exponents of the detailed dynamical events taking place in the system.

We thank H. van Beijeren, P. Gaspard, C. Beck, H. Bussemaker, and R. Brito for valuable discussions, for comments, and for help in realizing the computer simulations. One of us (D. J.) is financially supported by the "Stichting Fundamenteel Onderzoek der Materie (FOM)," which is sponsored by the "Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO)." J. R. D. thanks FOM for financial support during a visit in the summer of 1994 to the University of Utrecht, and acknowledges support from the National Science Foundation under Grant No. PHY-93-21312.

*Permanent address: IPST and Department of Physics, University of Maryland, College Park, MD 20742.

†Permanent address: Department of Physics, Michigan State University, East Lansing, MI 48824.

[1] P. Gaspard and G. Nicolis, Phys. Rev. Lett. **65**, 1693 (1990).

[2] C. Beck and F. Schlögl, *Thermodynamics of Chaotic Systems* (Cambridge University Press, Cambridge, 1993).

[3] P. Gaspard and J. R. Dorfman (unpublished).

[4] J. W. Haus and K. W. Kehr, J. Phys. Chem. Solids **40**, 1019 (1979).

[5] H. van Beijeren, Rev. Mod. Phys. **54**, 195 (1982); H. van Beijeren and M. H. Ernst, J. Stat. Phys. **70**, 793 (1993).

[6] W. Feller, *An Introduction to Probability Theory and Its Applications* (John Wiley, New York, 1957), Vol. 1, p. 360.

[7] C. Beck and D. Graudenz, Phys. Rev. A **46**, 6265 (1992).

[8] J. R. Dorfman, M. H. Ernst, and D. Jacobs, J. Stat. Phys. (to be published).

[9] D. Ruelle and J.-P. Eckmann, Rev. Mod. Phys. **57**, 617 (1985).

[10] H. van Beijeren and J. R. Dorfman, preceding Letter, Phys. Rev. Lett. **74**, 4412 (1995).