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# Transport Properties, Lyapunov Exponents, and Entropy per Unit Time

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For dynamical systems of large spatial extension giving rise to transport phenomena, like the Lorentz gas, we establish a relationship between the transport coefficient and the difference between the positive Lyapunov exponent and the Kolmogorov-Sinai entropy per unit time, characterizing the fractal and chaotic repeller of trapped trajectories. Consequences for nonequilibrium statistical mechanics are discussed.

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Randomness is a property shared by both conservative and dissipative dynamical systems. Recently, an extensive amount of work has been devoted to this fundamental property and, in particular, to the mechanisms by which it can be generated from deterministic evolution laws governed by differential equations or mappings.[1-3] Dynamical randomness is characterized by a positive Kolmogorov-Sinai (KS) entropy per unti time, $h_{\rm KS}$, giving the data-accumulation rate necessary to follow the deterministic time evolution and to recover the continuous trajectory of the system from the recorded data.[1,2] In closed dynamical systems, such as strange attractors or defocusing billiards, it is known that dynamical randomness has its origin in sensitivity to initial conditions, which is characterized by the Lyapunov exponents $\{\lambda_i\}$.[1,2] More precisely, according to Pesin's theorem,[2,4] a direct relationship is established in the form

$$h_{\rm KS}=\sum_{\lambda_i>0}\lambda_i\,. \tag{1}$$

On the other hand, deterministic dynamical systems are known to give rise to transport properties like diffusion.[5] We shall be concerned in the present Letter with dynamical systems of infinite spatial extension where particle diffusion is possible in real space. Examples of such systems are the coupled turbulent cells of the Couette-Taylor flow[6] or theoretical models like the Lorentz gas[7-9] or coupled one-dimensional maps[10] where the diffusion coefficient reflects the random walk performed by the individual particles (assumed to be independent) in the system,

$$\mathcal{D}=\lim_{t\to\infty}\langle (x_t-x_0)^2\rangle/2t\,. \tag{2}$$

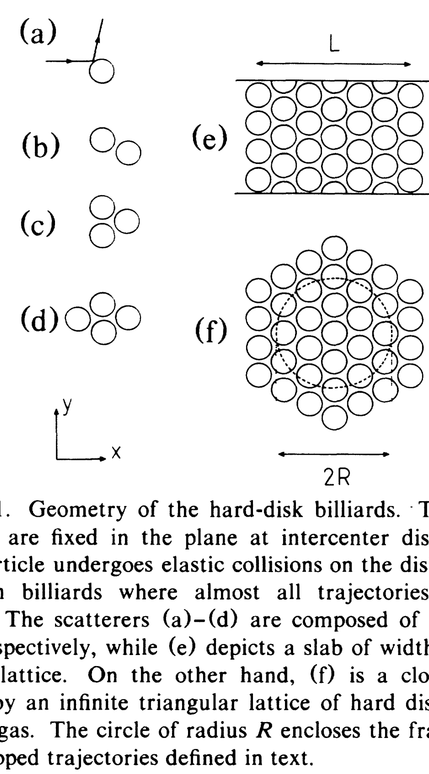


FIG. 1. Geometry of the hard-disk billiards. The disks of radius $a$ are fixed in the plane at intercenter distance $r$. A point particle undergoes elastic collisions on the disks. (a)–(e) are open billiards where almost all trajectories escape to infinity. The scatterers (a)–(d) are composed of one to four disks, respectively, while (e) depicts a slab of width $L$ in a triangular lattice. On the other hand, (f) is a closed billiard formed by an infinite triangular lattice of hard disks, i.e., the Lorentz gas. The circle of radius $R$ encloses the fractal repeller of trapped trajectories defined in text.

As proved for the Lorentz gas by scaling-limit methods,[7,9] the projection $x_t$ of the position of the particle along an axis is driven over large scale by Gaussian dynamical fluctuations according to

$$\lim_{t\to\infty} \mathrm{Prob}\{x_t - x_0 < u(2\mathcal{D}t)^{1/2}\} = (2\pi)^{-1/2}\int_{-\infty}^{u} e^{-s^2/2}ds\,. \quad (3)$$

Despite the probabilistic nature of such a property, it is natural to conjecture that there should be an intimate relation between the aforementioned randomness and the small-scale motion of the particle. The purpose of this Letter is to establish a direct connection between these properties for a class of diffusion processes in dynamical systems with few degrees of freedom.

We shall illustrate the main ideas with the two-dimensional Lorentz gas where a point particle is scattered by several hard disks of radius $a$ fixed in the plane. Scatterers with two, three, or more disks can be considered (Fig. 1). Collisions on the disks are defocusing. Nearby trajectories issued from a single point in the remote past form a front, called the horocycle,[1,2] with a curvature given by[11]

$$\kappa_u(X) = \cfrac{1}{l_0 + \cfrac{1}{-\cfrac{2}{a\cos\phi_1} + \cfrac{1}{l_1 + \cfrac{1}{-\cfrac{2}{a\cos\phi_2} + \cfrac{1}{l_2 + \cdots}}}}}\,, \quad (4)$$

where $\{l_i\}_{i=1}^{\infty}$ are the lengths of paths between the successive past collisions while $l_0$ is the length of path between the current position and the previous collision. The $\phi_i$'s are the angles between the incident velocity and the normal at each impact on the disks and they satisfy $\pi/2 \le \phi_i \le 3\pi/2$. Notice that the curvature (4) is always positive, expressing the defocusing character of the collisions on the disks. Every trajectory of the Lorentz gas is thus unstable and has a positive, a vanishing, and a negative Lyapunov exponent, $(\lambda_1, 0, -\lambda_1)$, because this billiard has two degrees of freedom and is time-reversal symmetric. We note that the magnitude of the velocity $v$ is a constant of motion so that the time spent along a path is obtained as its length multiplied by $v$. The positive Lyapunov exponent per unit time is then given by the time average of the horocycle curvature (4) multiplied by the velocity,

$$\lambda_1 = v \lim_{t\to\infty} \frac{1}{t}\int_0^t \kappa_u(X_t)dt\,. \quad (5)$$

In an unbounded (open) system such as the billiards of Figs. 1(a)-1(e), almost all trajectories escape to infinity.[12] If an ensemble of particles with the same magnitude of velocity but, otherwise, arbitrary initial conditions is placed between the disks at time zero, the number of particles still present in the vicinity of the disks after a lapse of time $t$ decays exponentially according to $N_t \sim N_0 e^{-\gamma t}$, where $\gamma$ defines the escape rate.[12] For instance, when the scatterer is composed of two disks there exists a periodic orbit trapped between the two disks, along the line joining both centers. This periodic orbit is unstable with a positive Lyapunov exponent equal to the escape rate [cf. (4) and (5)],

$$\gamma = \lambda_1 = \frac{v}{r-2a}\ln\frac{r-a+(r^2-2ar)^{1/2}}{a}\,, \quad (6)$$

where $r$ is the distance between the disk centers.

When the scatterer is composed of three disks a new and dramatic phenomenon arises. The ensemble of trajectories which are forever trapped between the disks now contains an infinite number of periodic orbits embedded in an uncountable set of nonperiodic orbits.[12,13] This so-called repeller[14] has a zero Lebesgue measure in the phase space and is thus a fractal[15] set sustaining chaotic motions. Indeed, the trajectories of the repeller and in one-to-one correspondence with a symbolic dynamics with a positive KS entropy per unit time. When a partition of the phase space into cells labeled by integers is performed any trajectory of the repeller which is observed along $n$ consecutive collisions can be represented by a string of integers $(\omega_0, \omega_1, \ldots, \omega_{n-1})$ together with the minimum time $T(\omega_0, \omega_1, \ldots, \omega_{n-1})$ to perform these $n$ consecutive particular collisions. The KS entropy is then defined by[1,2]

$$h_{\mathrm{KS}} = \sup_{\mathcal{A}} \lim_{n\to\infty} \frac{-\sum_{\omega_0,\omega_1,\ldots,\omega_{n-1}} \mathrm{Prob}(\omega_0,\omega_1,\ldots,\omega_{n-1})\ln \mathrm{Prob}(\omega_0,\omega_1,\ldots,\omega_{n-1})}{\sum_{\omega_0,\omega_1,\ldots,\omega_{n-1}} \mathrm{Prob}(\omega_0,\omega_1,\ldots,\omega_{n-1})T(\omega_0,\omega_1,\ldots,\omega_{n-1})}\,, \quad (7)$$

where the supremum is taken over partitions $\mathcal{A}$ into finer and finer cells and where Prob denotes the ergodic natural invariant probability measure over the repeller. In general, the KS entropy of a repeller is not equal to the ergodic mean Lyapunov exponent given by (5). In fact, the exponential separation of nearby trajectories contributes not only to randomization on the repeller, but also to the escape from the repeller. Accordingly, the escape rate is then given by the formula[2,16]

$$\gamma = \lambda_1 - h_{KS}, \tag{8}$$

which generalizes both (1) and (6).[17] When the disks are close together and delimit a bounded domain of the plane forming a closed billiard, the escape rate vanishes and the Pesin formula (1) is recovered. On the other hand, the KS entropy is vanishing for the periodic repeller of the two-disk scatterer so that (6) follows. An inequality proved by Ruelle guarantees that (8) is always non-negative.[18] Equation (8) can thus be interpreted as saying that dynamical randomness inhibits escape from the repeller.[16]

After this survey, we turn to the case of a many-disk scatterer forming a triangular lattice of width $L$ much greater than the disk radius $a$ and the intercenter distance $r$ [Fig. 1(e)]. We assume that a point particle cannot travel through the lattice without collision, imposing the condition $r < 4a/3^{1/2}$. As for the three-disk scatterer, the set of trajectories trapped between the disks forms a fractal repeller ($\mathcal{F}_L$) characterized by a positive Lyapunov exponent $\lambda_1(\mathcal{F}_L)$ and a positive KS entropy $h_{KS}(\mathcal{F}_L)$. The escape rate of the effusion process through the borders of the scatterer of Fig. 1(e) is then given by (8). When the width $L$ of the slab is large, the effusion process is controlled by particle diffusion in the disk lattice. Now, diffusion in the Lorentz gas has been studied extensively over the last decade.[7-9] Using the scaling limit $(\varepsilon^{-1}x, \varepsilon^{-1}y, \varepsilon^{-2}t)$ with $\varepsilon \to 0$,[7] Bunimovich and Sinai[9] proved that the large-scale motion of the point particle in the Lorentz gas is diffusive in the sense of Eq. (3) with a positive and finite diffusion coefficient $\mathcal{D}$. Machta and Zwanzig gave a quantitative estimation of the diffusion coefficient as $\mathcal{D} \approx 1.97v(r - 2a)$ for a particle of velocity $v$, provided the bottleneck width $r-2a$ is small enough.[8] The probability density $f(x,y,t)$ of finding the particle near $(x,y)$ is thus governed in the scaling limit by the diffusion equation

$$\partial_t f = \mathcal{D}(\partial_x^2 + \partial_y^2) f. \tag{9}$$

Now, we can calculate the escape rate of the many-disk scatterer of Fig. 1(e) by solving (9) with the boundary conditions $f(x=0,y,t) = f(x=L,y,t) = 0$, expressing the fact that the particles escape in free motion from the borders ($x=0$ and $x=L$) of the disk lattice. In the scaling limit, the system and its repeller are uniform along the $y$ axis so that the diffusion and effusion processes are independent of the variable $y$. The solution is then

$$f(x,t) = \sum_{m=1}^{\infty} c_m e^{-\gamma_m t} \sin\left(\frac{\pi m x}{L}\right), \tag{10}$$

with $\gamma_m = \mathcal{D}(\pi m/L)^2$. The long-time decay is dominated by the smallest rate, $\gamma_1 = \mathcal{D}(\pi/L)^2$, which is to be identified with the escape rate of the repeller, $\gamma$.[12] Applying (8), we get

$$\lambda_1(\mathcal{F}_L) - h_{KS}(\mathcal{F}_L) = \mathcal{D}(\pi/L)^2 + \mathcal{O}(1/L^3), \tag{11}$$

where $\mathcal{O}(L^{-3})$ are corrections due to the finiteness of the many-disk scatterer. We observe that the difference between the Lyapunov exponent and the KS entropy of the fractal repeller ($\mathcal{F}_L$) vanishes in the limit $L \to \infty$. Indeed, for a large scatterer, the fractal repeller starts to fill the three-dimensional phase space of the flow ($\mathcal{E}$) while the escape rate decreases like $L^{-2}$. The invariant probability measure becomes the Liouville invariant measure. According to Pesin's formula (1), the Lyapunov exponent and the KS entropy are then equal to the finite and positive Lyapunov exponent $\lambda_1(\mathcal{E})$ of the closed Lorentz gas. The point is that, as Eq. (11) shows, the difference between the Lyapunov exponent and the KS entropy of the many-disk scatterer is controlled by the diffusion coefficient of the Lorentz gas. Rewriting (11), we finally obtain our main result

$$\mathcal{D} = \lim_{L\to\infty} (L/\pi)^2 [\lambda_1(\mathcal{F}_L) - h_{KS}(\mathcal{F}_L)], \tag{12}$$

which establishes a fundamental relationship between kinetic theory and ergodic theory for this class of dynamical systems of infinite spatial extension.[19]

The fractal character of the repeller has a further consequence. The classical scattering process on the many-disk scatterer is irregular and shows high sensitivity to initial conditions, a phenomenon which has been studied in several recent publications.[20] In irregular scattering, the outgoing trajectory is a very complicated function of the incoming trajectory with singularities on the fractal set of trajectories which are asymptotic to the fractal repeller. The self-similarity of the scattering functions can thus be characterized by the information dimension of the repeller that can be calculated asymptotically for large $L$ using Young's formula,[12,21]

$$D_I(\mathcal{F}_L) = 3 - \frac{2\mathcal{D}}{\lambda_1(\mathcal{E})}\left(\frac{\pi}{L}\right)^2 + \mathcal{O}\left(\frac{1}{L^3}\right). \tag{13}$$

It is striking to observe that irregular scattering is thus intimately related to a typical irreversible macroscopic process like diffusion in large open systems.

Consider now the original Lorentz gas forming a triangular lattice but covering the whole plane [Fig. 1(f)]. The dynamical system being closed, Pesin's formula applies with averaging taken over the Liouville measure. Nevertheless, it is still possible to define here a fractal set as follows. A large circle of radius $R$ ($\gg a,r$) is drawn on the lattice. The ensemble of trajectories of the Lorentz gas remaining forever inside this circle forms another fractal set ($\tilde{\mathcal{F}}_R$) of zero Liouville measure. Solving the diffusion equation (9) with the Dirichlet boundary condition on the border of the circle of radius $R$, we infer that almost all trajectories escape from the fractal $\tilde{\mathcal{F}}_R$ with a rate $\gamma = \mathcal{D}(2.40482/R)^2$, where

2.40482 is the first zero of the Bessel function $J_0(z)$. Hence, the following equation results from (8):

$$\mathcal{D} = \lim_{R\to\infty} \left( \frac{R}{2.40482} \right)^2 [\lambda_1(\tilde{\mathcal{F}}_R) - h_{KS}(\tilde{\mathcal{F}}_R)] . \quad (14)$$

This relationship between diffusion and dynamical instability is reminiscent of first-passage-time problems which are often encountered in the stochastic theory of reaction rates.[22] In a way, our results show how first-passage-time type of problems may arise in *deterministic* systems. In this way, different fractals can be constructed with different "absorbing boundaries" on the lattice corresponding to different nonequilibrium problems. Similar considerations hold for other diffusion models like the chain of baker transformations,[23] as shown elsewhere, or the random Lorentz gas.[6]

We conclude with some comments about the implications of our results for nonequilibrium statistical mechanics. It is known that the fluctuation-dissipation theorem relates the diffusion coefficient to the autocorrelation function of the velocity via the Green-Kubo integral if the system presents the ergodic property of mixing.[24] With Eqs. (12) or (14), we are now able to understand how diffusion, dynamical randomness, and sensitivity to initial conditions are interconnected. We believe that the present theory can be generalized to the hard-sphere gas where similar relationships could be established for the other transport coefficients like viscosity or heat conductivity. In this respect, microscopic simulations like molecular dynamics are likely to provide useful insight into this problem.

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