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Numerical Study of a *D*-Dimensional Periodic Lorentz Gas with Universal Properties

Jean-Philippe Bouchaud[1] **and Pierre Le Doussal**[2]

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We give the results of a numerical study of the motion of a point particle in a d-dimensional array of spherical scatterers (Sinai's billiard without horizon). We find a simple universal law for the Lyapounov exponent (as a function of d) and a stretched exponential decay for the velocity autocorrelation as a function of the number of collisions. The diffusion seems to be anomalous in this problem. Ergodicity is used to predict the shape of the probability distribution of long free paths. Physical interpretations or clues are proposed.

KEY WORDS: Billiards; diffusion; correlations; Lyapounov exponents.

1. INTRODUCTION

This paper contains numerical results concerning the periodic Lorentz gas, as well as some physical interpretations and conjectures. This system is a d-dimensional array of fixed spherical scatterers (of radius R) in which a classical point particle travels and undergoes specular reflections. We choose the particle velocity to be 1. We also choose a cubical lattice with a lattice spacing equal to 2. The geometry of this billiard (in two dimensions) is shown in Fig. 1. The range of values considered for R is $0 \leqslant R \leqslant \sqrt{d}$. It is important to notice that for $R < 1$, this billiard is without horizon, i.e., the length of free paths is unbounded. When $R \geqslant 1$ the spheres overlap and when $R \geqslant (d-1)^{1/2}$, the particle is trapped in a region bounded by 2^d

[1] Laboratoire de Spectroscopie Hertzienne, École Normale Supérieure: 24, Rue Lhomond 75231 Paris Cedex, France (Laboratoire Propre du Centre National de la Recherche Scientifique, associé à l'École Normale Supérieure et à l'Université de Paris Sud).

[2] Laboratoire de Physique Théorique, École Normale Supérieure: 24, Rue Lhomond 75231 Paris Cedex, France (Laboratoire Associé au CNRS).

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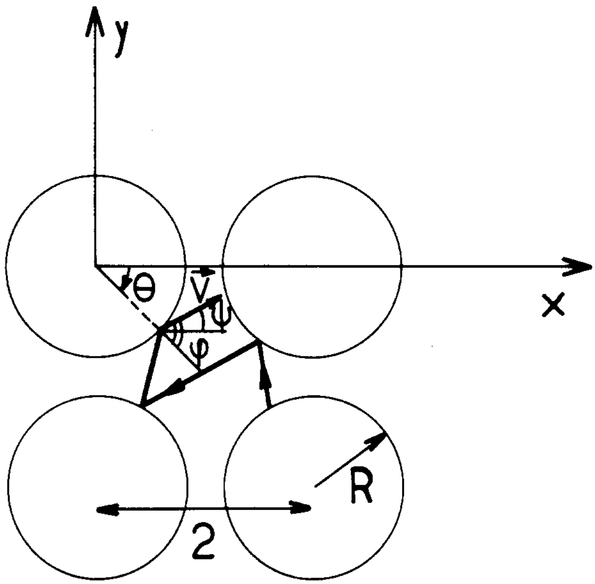

Fig. 1. The geometry of the system studied here, and the definition of the notations used below.

pieces of spheres, with an intricate geometry. Throughout we will call $\mu = |R-1|$.

The system is known to be ergodic in two dimensions, and seems experimentally to be ergodic in higher dimensions. Ergodicity means that there exists an invariant asymptotic measure $d\omega$ over the phase space such that the mean value of any physical observable over a trajectory converges towards its ergodic mean value for almost all trajectories. For example, in two dimensions, the invariant measure on the three-dimensional phase space of constant energy is $d\omega = dx\, dy\, d\psi$. The trace of this measure on the two-dimensional Poincaré section (defined by the intersection of the flow with the circles) is $d\rho = \frac{1}{2}|\cos\varphi|\, d\theta$ (see Fig. 1).

We shall assume that averages over computed trajectories are the same as over real trajectories, as was extensively studied in Ref. 1. This property is assumed here to hold also in higher dimensions.

Despite its very simple definition, and its deterministic character, the periodic Lorentz gas is an extremely chaotic system where it is impossible to make any long range prediction concerning a single trajectory. In order to give an idea, let us say that if one calculates with a computer, using double precision (16 digits), two trajectories with initial conditions differing only their last digit one would find that after a few ($\simeq 10$) collisions with the spheres these trajectories are far apart.

So, this is intrinsically a system that can only be studied under a statistical point of view. It shares this property with complicated systems (with many degrees of freedom) which are within the scope of statistical physics. Simple in its formulation, free from any *ab initio* disorder, does this model exhibit some universal (as function of d) behavior? This paper shows that it is actually the case (at least numerically) and the simplicity of the model allows us to hope that the laws stated here could be derived exactly. We studied four statistical observables, which are the simplest one could think to define here. Each one is associated with an important physical process which is of interest in much more general systems. These are as follows.

(i) The collision process, associated with the pressure of the "gas" consisting of many independent particles. We measure it with the probability distribution of free path of length s: $N(s)$, linked with σ (the number of collisions with the scatterers per unit time, or the inverse of the mean free path) by the formula

$$\sigma = \frac{1}{\int sN(s)\,ds} \tag{1.1}$$

which only holds if the system is ergodic.

The pressure is naturally connected to σ by

$$p = 2N_p\langle \cos \varphi \rangle \sigma / N_s S \tag{1.2}$$

where S is the total area of the boundary of a scatterer. N_p denotes the number of moving particles and N_s the number of scatterers.

The probability distribution of finding a particle on a free path of length s at any given time is $M(s)$, related to $N(s)$ through $M(s) \backsim sN(s)$.

(ii) Loss of information on the position of the particle. It can be measured here by the Lyapounov exponent λ, which is associated with the divergence of two nearby trajectories. It has, for $d = 2$, a precise information theory meaning via the Kolmogorov entropy. It is the minimal rate of information one has to gain from measurements to keep knowledge of the particle's position within a given precision.

(iii) The relaxation process, illustrated by the velocity autocorrelation function (VACF) decay which is associated with the statistical loss of memory on initial conditions. It has no known rigorous link with the Lyapounov exponent, and if such a link exists, it must be a very subtle one (cf. Section 4).

(iv) The self-generated diffusion process, which was shown to be Brownian in two dimensions with a diffusion coefficient D in the case of a billiard with finite horizon.[8] This result has to be slightly modified here.

In each paragraph we focus on a specific observable. We first describe experimental results, then give our interpretation.

2. THE RATE OF COLLISION WITH THE SPHERES

We used for all our calculations a VAX/VMS coupled to an array processor FPS-164, using double precision (16 digits). Each trajectory was calculated for 10^5 to 2×10^7 collisions, depending on the rate of convergence.

2.1. Rate of Collision

The asymptotic measure allows us to calculate σ in any dimension, with the help of a kinetic theory of gases argument:

$$\sigma = \frac{\int d\rho \text{ (unnormalized)}}{\int d\omega \text{ (unnormalized)}} \tag{2.1}$$

The explicit formula is simple for $R \leqslant 1$: σ is the cross section of the hyperspheres divided by the total accessible volume (which can be seen as a normalization to one particle per unit volume):

$$\sigma_d = \frac{V(d-1)}{2^d - V(d)} \quad \text{with} \quad \frac{2\pi^{d/2} R^d}{d\Gamma(d/2)} = V(d) \tag{2.2}$$

We can obtain the pressure by inserting (2.1) into (1.2). We find

$$p = \frac{1}{d\Omega} \tag{2.3}$$

where Ω is the total accessible volume per cell [$2^d - V(d)$ for $R \leqslant 1$]. We thus for recover the perfect gas law as it should be for a gas of independent particles.

This system has been proven to be ergodic in two dimensions, and we checked numerically that formula (2.2) is very well obeyed. A convergence better than 1% is obtained alter roughly 10^6 collisions. Formula (2.2) still gives the observed σ in three dimensions, thus in agreement with the belief that the system remains ergodic in three dimensions. We only have indications about ergodicity in higher dimensions as will be further discussed in Section 4.3.

2.2. Distribution of Path Length.

Calling s the length of a free path between two successives collisions, $N(s)$ represents the probability density of having a path of length s. It is normalized as

$$1 = \int N(s)\, ds$$

In Ref. 2 we discuss the behavior of $N(s)$ for small s when R is close to 1 (in two dimensions): in particular, we find that, for $R = 1$ $N(s)$ diverges like $s^{-1/2}$ for small s.

We are interested here in the large-s behavior of $N(s)$. It is clear that when $R > (d-1)^{1/2}$, $N(s) = 0$ if $s > s_{max}$. It is possible to derive the asymptotic behavior of $N(s)$ in two dimensions if R is close to 1. Let us call "windows" the directions along which the paths can be as long as one wants. If $R \lesssim 1$, the only windows are long the axis of the square lattice (cf. Fig. 2). In this case, using the asymptotic measure (assumed to be reached), we have for large s

$$N(s)\, ds \propto (1-R) \int \cos\varphi\, d\varphi\, d\theta$$

$$\simeq (1-R)\, ds \int_{-1/s}^{\theta - 1/s} \left(\theta' + \frac{1}{s}\right) \frac{1}{s^2}\, d\theta'$$

$$\text{with} \quad 1 - \cos\theta = \frac{\theta^2}{2} = \frac{1}{s^2} s$$

$$= \frac{1-R}{s^3}\, ds$$

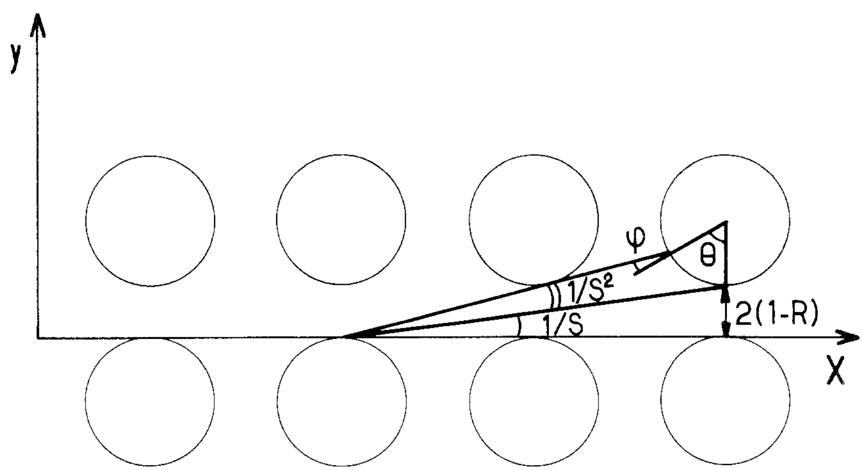

Fig. 2. One of the windows along which a particle can escape.

We have checked numerically that $N(s)$ behaves like s^{-3} plus higher-order terms for $R=0.9$.

When R decreases, new windows appear, and the same argument can be applied for each window, replacing $1-R$ by the width of the window. The total asymptotic behavior of $N(s)$ remains s^{-3} but only for s larger and larger as R decreases (one must have $s \gg R^{-1}$). When $1 \ll s \ll R^{-1}$ the impact does not have to be tangential (the small $\cos \varphi$ factor disappears) and thus the law is expected to be rather $s^{-2.5}$. This will be of importance in Section 3.

A last remark can be made: suppose that in Fig. 2 the arc of circles are replaced by curves having locally a structure $y = x^n$ along the window ($n=2$ for the circles). For a lattice of such scatterers the same argument would lead to the same decay in $N(s)$ which is thus independent of the shape of the scatterers.

3. THE LYAPOUNOV EXPONENT

3.1. Definition

This system falls into the category of dispersed billiards which are known to be K systems (Sinai[3] at least for two dimensions). It means that two nearby trajectories diverge exponentially with time and one can define a strictly positive Lyapounov exponent for the flow F^T, by

$$\lambda_t = \lim_{T \to \infty} \frac{1}{T} \log \|DF^T(x) \cdot \mathbf{e}\| \tag{3.1}$$

where $\|\cdots\|$ is the vector norm and $DF^T(x)$ is the differential of the flow F^T at point x. λ_t exists for almost every tangent vector $\mathbf{e}$ at point x and does not depend on x nor on $\mathbf{e}$, as explained in Refs. 4 and 5. Numerically we use the technique described in Ref. 5. We average over a trajectory the increase in distance of two nearby trajectories between T and $T+\tau$. τ is a (small enough) numerical parameter on which λ_t does not depend.

Another Lyapounov exponent λ_k, relative to the Poincaré section, can be defined by a formula analogous to (3.1) replacing T by the number of collisions K. It is known that a "mean field" formula relates (in two dimensions λ_t to λ_k: from Abramov's formula and Pesin's theorem we have $\lambda_t = \sigma \lambda_k$, supposing that the invariant measure is reached. We calculate λ_t and use this formula to obtain λ_k.

In d dimension ($d > 2$) the phase space is of dimension $2d-1$, and the differential of the flow DF^T possesses $d-1$ eigenvalues of modulus higher than 1. This is why the numerical convergence of (3.1) is not very good in high dimension for small R. For a finite waiting time the calculated Lyapounov exponent is less than the real one, because the chosen direction **e** not only "feels" the highest eigenvalue but all the eigenvalues of modulus >1. But in two dimensions, the convergence is very good, for all R.

3.2. Results in the Two-Dimensional Case

The $d=2$ λ_k curve is shown on Fig. 3. λ_k as a function of R is very well fitted by the following form (with α, β constants): $\lambda_k = \alpha \log \beta/R$ as predicted by Sinai.[6] Furthermore, Oono *et al.*[7] showed that $\alpha = 2$ for vanishing R. We found numerically $\alpha \simeq \beta = 2 \pm 0.2$.

Figure 4 shows the global behavior of λ_t as a function of R. λ_t is regularly growing, until $R \simeq 1$, owing to the increase of the collision rate. The interesting point is that λ_t undergoes a jump for $R=1$ (cf. Fig. 5, illustrating the good convergence of λ_t). As discussed in Ref. 2 and in Section 3.3 one probably has a $\mu^{1/2}$ law for $R<1$ (at a scale $\mu \simeq 10^{-4}$). This is very difficult to confirm experimentally. Another interesting point is the quasiconstant value of λ_t between 0.99 and 0.999, before the steep decrease very close to 1. Seen with a poorer resolution, λ_t looks like a cubic curve, of Van der Waals type, with a local maximum for $R<1$ and a local minimum for $R>1$ (cf. Fig. 4).

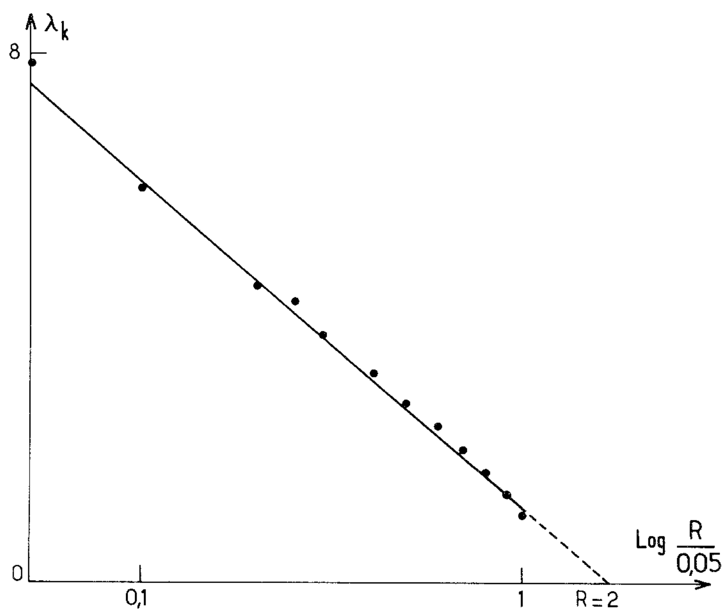

Fig. 3. λ_k vs. $\log R$ in two dimensions for $0.05 \leqslant R \leqslant 1$, in a semilogarithmic plot.

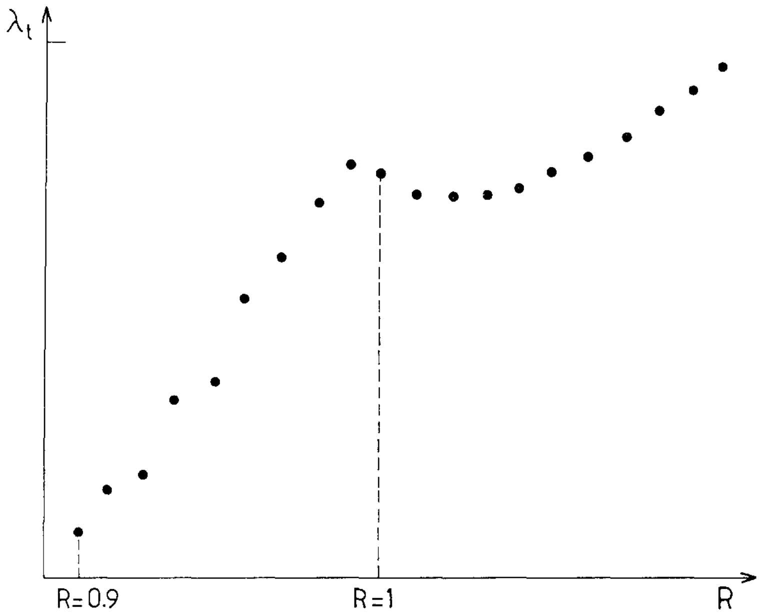

Fig. 4. λ^t vs. R at a larger scale.

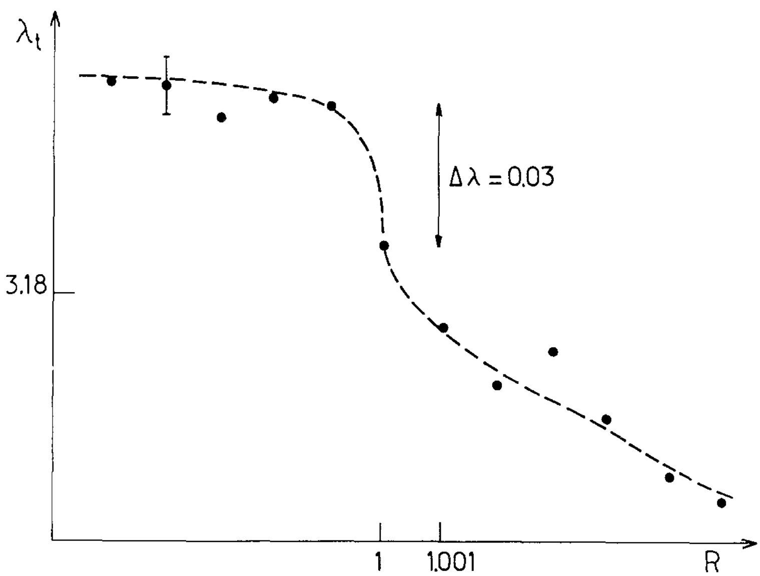

Fig. 5. λ_t vs. R for $R \simeq 1$. The plateau for $R < 1$ was confirmed by a longer run. The dashed line illustrates a possible nonanalytic behavior.

3.3. How to Isolate the Vertex Contribution

In order to isolate the vertex contribution, responsible for all the singularities around $R=1$ (Fig. 5), one could think of the following artifact. Imagine a particle trapped in a small rectangular box drawn around the vertex and compute the Lyapounov exponent for this system (cf. Fig. 6): the contribution of the vertex is then clearly enhanced. If the length w of the box is sufficiently small, the curve λ_t as a function of R should reproduce the vertex contribution for μ not too small compared to w. The curve $\lambda_t(\mu, w)$ for $w=0.05$ is shown in Fig. 7. It clearly shows that $\lambda_t(\mu, w)$ can be approximated by $\mu^{1/2}$ only if μ is not too small since $\lambda_t(0, w)$ is not strictly zero. In order to get rid of this unwanted residue and exhibit a $\mu^{1/2}$ law down to zero, one should make at the same time $w \to 0$ and $R \to 1^-$. The trouble is that in this limit the system disappears entirely! So the simplest idea is to start from a value of R very close to 1 and of w very close to zero, and parametrize (R, w) as

$$R = R_\alpha = \frac{\alpha}{1+(\alpha-1)\,R_0}\,R_0$$

$$w = w_\alpha = \frac{1}{1+(\alpha-1)\,R_0}$$

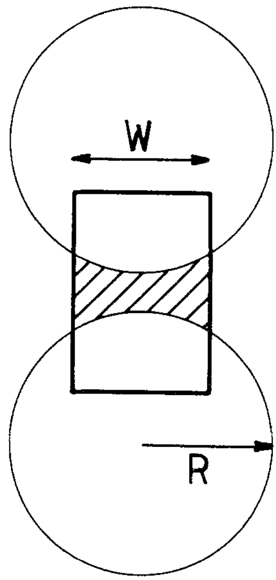

Fig. 6. The small box isolating the vertex.

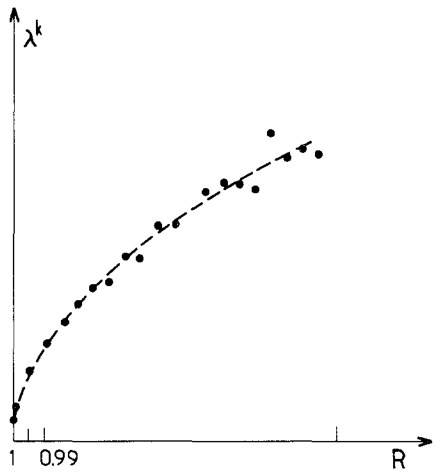

Fig. 7. $\lambda_t(\mu, w)$ for $w = 0.05$ for $\mu \leqslant 0.1$.

and let $\alpha \to \infty$. This family of little boxes can be deduced by a scaling of ratio:

$$[1 + (\alpha - 1)\, R_0]^{-1}$$

from what we will call throughout the equivalent system represented in Fig. 8, which has a constant size. This implies that λ_t for the boxes is equal to λ_t for the equivalent system multiplied by α.

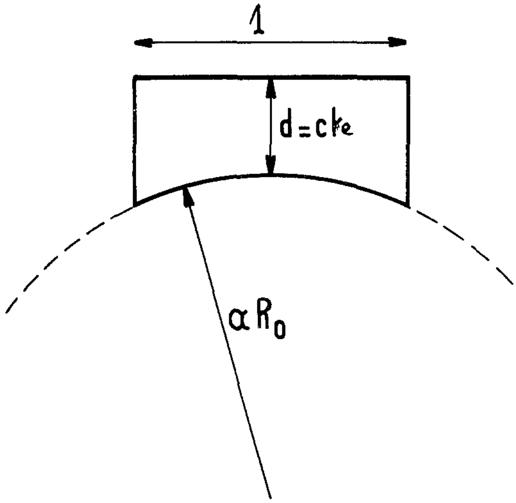

Fig. 8. The "equivalent system" which was studied for $d = 0.2$.

We have thus studied the equivalent system when $\alpha \to \infty$ (which is a rectangle in this limit). Figure 9 shows that $\lambda_t \simeq \sqrt{\alpha}$ for the family of little boxes (R_α, w_α). We then expect $\lambda_t(\mu, 1)$ to have a $\mu^{1/2}$ behavior at a small scale, as observed. The 1/2 exponent is an intermittency type of exponent, reminiscent of the fact that the Pomeau–Manneville scenario is physically realized here.[2]

The $\alpha^{-1/2}$ behavior of λ_t in the equivalent system (Fig. 8) is easy to understand if one notes that the logarithm of the eigenvalue of the linearized mapping near the unstable periodic orbit goes to zero like $(\alpha R_0)^{-1/2}$.

3.4. The *d*-Dimensional Case

The experimental results concern λ_k in dimension 2, 3, 4, 5. Figure 10 shows λ_k as a function of $\log R$ (for R between 0.3 and 1.2). Those curves are very well approximated by the following surprisingly simple form (except in the region of small R for the reason explained above):

$$\lambda_k(R) = \alpha(d) \log[\beta(d)/R] \tag{3.2}$$

with

$$\beta(d) = 2 \pm 0.2 \qquad \text{for all } d$$

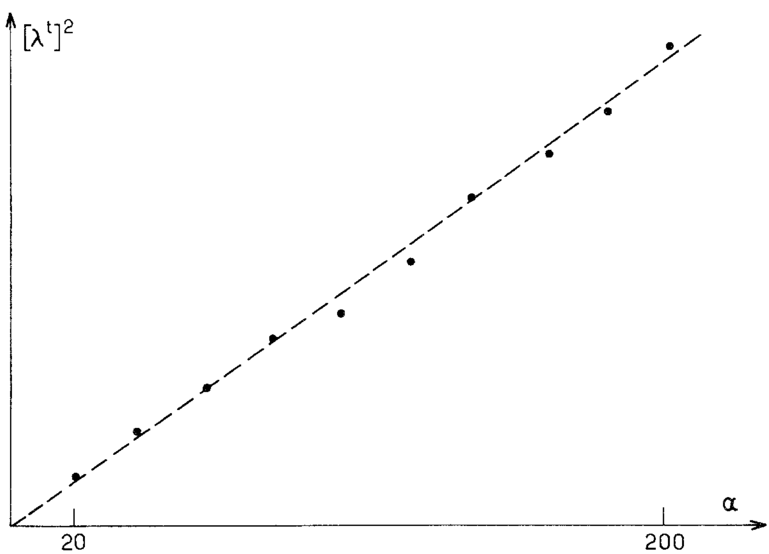

Fig. 9. λ_t^2 vs. α for the family of little "boxes."

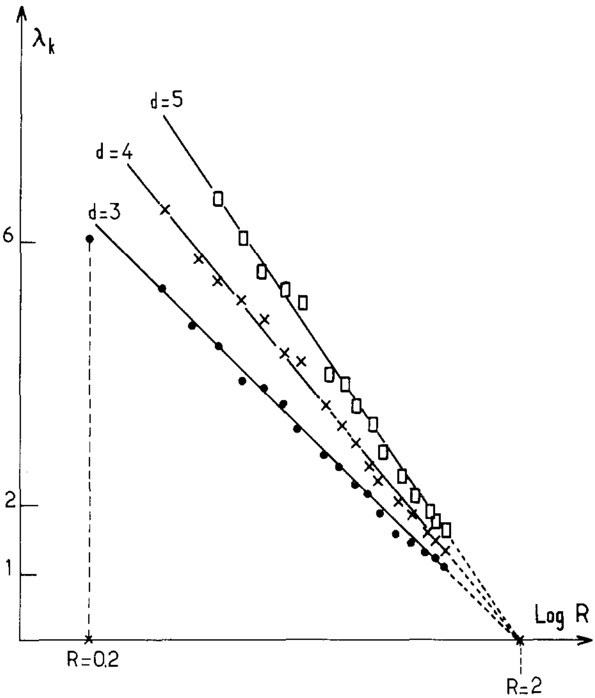

Fig. 10. λ_k vs. log R in $d=3$, 4, 5.

and

$$\alpha(2) \simeq 2$$
$$\alpha(3) \simeq 2.8$$
$$\alpha(4) \simeq 3.5$$
$$\alpha(5) \simeq 4.35$$

We notice the following:

(i) $\beta(d)$ seems to be independent of the dimension as illustrated by the common intersections at $\lambda_k = 0$ of the curves prolongated up to $R = 2$. 2 is the lattice spacing, which is the only d-independent length scale.

(ii) $\alpha(d)$ seems to be well fitted by the linear form

$$\alpha(d) = (3d + 2)/4 \tag{3.3}$$

it is interesting to compare this result on λ_k, which is the largest Lyapounov exponent, with a recent conjecture of Oono *et al.*[7] on the

Kolmogorov entropy of any periodic d-dimensional array of scatterers of vanishing size. Assuming Pesin formula, the Kolmogorov entropy h is equal to the sum of the positive Lyapounov exponents (up to a volume factor). Their conjecture is that

$$h \simeq -d \log R \qquad \text{for small } R \tag{3.4}$$

Our result tends to prove that for our lattice, the logarithmic form of λ_k is true for the whole range of R. If (3.4) is valid, then formulae (3.2) and (3.3) lead to the two following suggestions:

(i) Every positive Lyapounov exponent has a logarithmic dependence on R.

(ii) Using the form of $\alpha(d)$, the sum of the $(d-2)$ positive Lyapounov exponents (but the largest) is proportional to $(d-2)/4$. So one is tempted to conjecture that every nonmaximal Lyapounov exponent is equal to $\simeq 1/4 \log R/2$. This is perhaps an interesting statistical restoration of the $(d-2)$ symmetry of the problem at each collision point.

Our results on $N(s)$ allow us to discuss further the argument of Oono *et al.*[7] (3.4) is exact in two dimensions if $\langle \log s \rangle / \log \langle s \rangle \to 1$ as R goes to zero. They checked numerically that $\log\langle s \rangle - \langle \log s \rangle$ goes to 0.44 ± 0.01 as $R \to 0$. In order to understand their result, we can approximate $N(s)$ by 0 if $s \leqslant a$

$$\begin{array}{ll} s^{-\gamma} & \text{for} \quad a \leqslant s \leqslant R^{-1} \\ s^{-3} & \text{for} \quad s \geqslant R^{-1} \end{array}$$

The evaluation of $\langle s^{\varepsilon} \rangle / \langle s \rangle^{\varepsilon}$ for ε small gives

$$\begin{aligned} \Delta &= \log\langle s \rangle - \langle \log s \rangle \\ &= \log \frac{1-\gamma}{2-\gamma} + \frac{1}{1-\gamma} \qquad \text{for} \quad R \to 0 \text{ and any } a \end{aligned} \tag{3.5}$$

If we insert in this formula the geometrically expected $\gamma = 2.5$ (cf. Section 2), we find $\Delta = 0.43$. Since (3.5) varies rapidly with γ, this is a good check for γ being exactly equal to 2.5. Figure 3 of Ref. 7 shows the growth of Δ when R goes to 0, which corresponds to the passage from $\gamma = 3$ to $\gamma = 2.5$.

Formula (3.5) shows that (3.4) is no longer true if $N(s)$ goes to zero more slowly than s^{-2}.

4. THE VELOCITY AUTOCORRELATION FUNCTIONS

4.1. The $d=2$ VACF with Respect to the Number of Collisions

4.1.1. $R<1$. We have computed the average $C(n)$ over a given trajectory (starting on a sphere) of $\mathbf{v}(k)\,\mathbf{v}(k+n)$, where $\mathbf{v}(k)$ denotes the velocity after the kth collision. We found that the result does not depend on the chosen trajectory nor on the precision used. In the billiard, correlations decay very quickly, thus making numerical experiments difficult. However, by increasing the statistics to 2×10^7 collisions we obtained a well-defined curve up to $n=8$. In fact, an exact bound on $C(n)$ due to Sinai[8] for a billiard with bounded horizon (which is the case for $R>1$) and for sufficiently large n gives

$$|C(n)|\leqslant \exp[-n^{\gamma}] \qquad \text{with} \quad 0<\gamma\leqslant 1$$

This indicates that the system could be a C system for $R>1$, that is, a system for which all correlations decay exponentially. For a billiard without horizon, it has been conjectured (Bunimovitch[16]) that the decay is algebraic, as n^{-3}. Nevertheless, we found, for $R<1$, as illustrated in Fig. 11,

$$C(n)=(-1)^n\exp(-\kappa n^{\gamma}) \qquad (1<n<9) \tag{4.1}$$

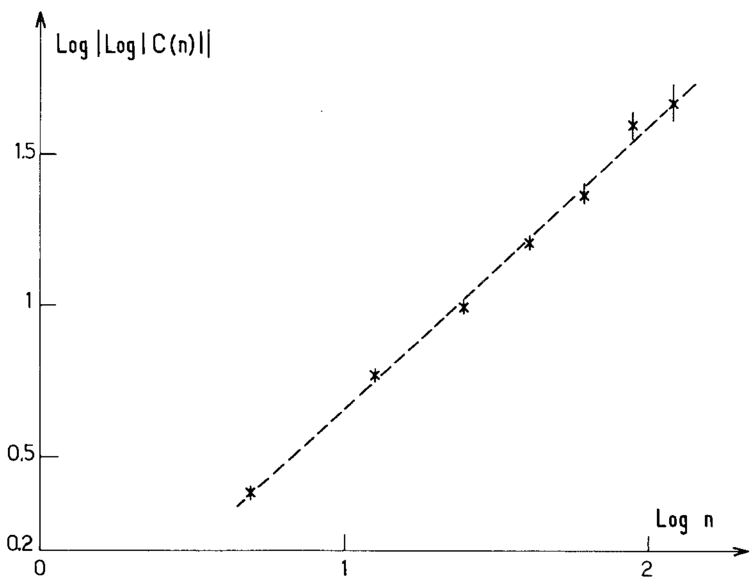

Fig. 11. $C(n)$ for $d=2$ for 2×10^7 collisions for $R=0.5$.

with $\gamma = 0.86 \pm 0.06$ (apparently independent of the radius R) and

$$\log \kappa = -0.27 \quad \text{for} \quad R = 0.5$$

$$\log \kappa = -0.2 \quad \text{for} \quad R = 0.05$$

The $C(1)$ point does not follow this law. This will be discussed later. Let us emphasize that we do not claim that (4.1) is the actual asymptotic behavior of $C(n)$. Perhaps there is a crossover region between the stretched exponential decay and an algebraic decay. But as we will discuss in the following section, this crossover could happen very late. Furthermore, as discussed in Section 4.4, the stretched exponential regime could be as important in the understanding of the system as the truly asymptotic regime.

4.1.2. Evidence for the Stretched Exponential Law. It is interesting to obtain such a law for $C(n)$ in such a simple system. In order to have a decisive test of the existence of this type of law in a billiard, we studied numerically $C(n)$ in the equivalent system defined in Section 3. We used (and of course this is very important) periodic boundary conditions which make the horizon unbounded. The interesting point of this system is that when R goes to infinity, $C(n)$ decreases very slowly: this allowed us to obtain reliable curves up to $n = 1000$. A power law is clearly ruled out (at least in this range) by Fig. 12, and Fig. 13 shows that $C(n)$ is equal to

$$\exp[-\kappa(R)\, n^{\gamma}]$$

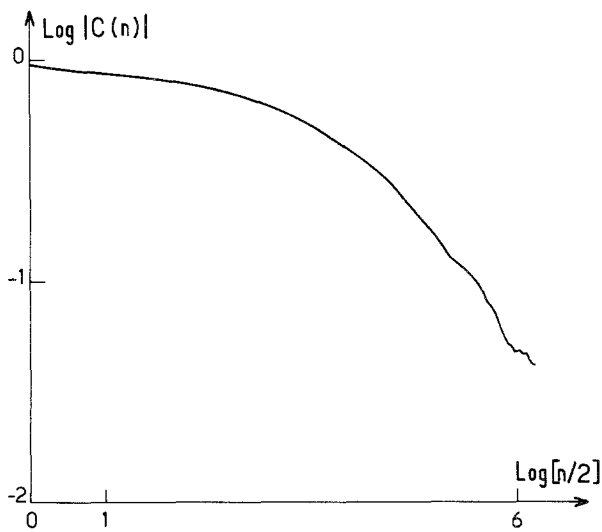

Fig. 12. $C(n)$ for the "equivalent system." This clearly rules out an algebraic decay over the time of observation. Note that the slope is always greater than -3.

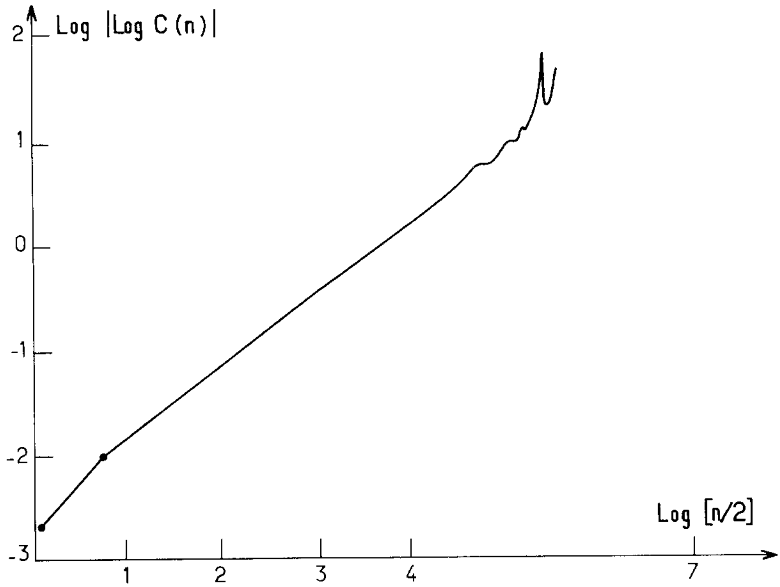

Fig. 13. The log–log curve for $C(n)$ in the equivalent system allowing to measure κ and γ. Note that $C(1)$ is not on the straight line.

with $\gamma = 0.71 \pm 0.05$ independently of R, and $\kappa(R)$ going to zero as $R \to \infty$ as R^{-z} with z of order 2 (for example, $\log \kappa(6) = -2.07$; $\log \kappa(12) = -4.28$).

4.1.3. Critical Behavior for $R = 1$. There is no rigorous result concerning the $R = 1$ case. We computed $C(n)$ for $R = 1$. Our result is compatible with a law $c(-1)^n/n$ for $n < 50$ with $c = 0.9 \pm 0.1$. This agrees with a result obtained by Machta[9] for a triangular lattice having, for $R = 1$, three vertices instead of four as in our case: According to Machta's interpretation of the $1/n$ decay, his c should differ from our's by a factor 3/4, which is approximatively true as his c is $\simeq 0.6$. Machta[9] has given a strong theoretical support for this algebraic law, by calculating the contribution to $C(n)$ of a series of successive collisions on two adjacent arcs of circles in a "vertex," where the collisions are weakly decorrelating. The transition from an exponential law to a power law decay is governed by the divergence of the correlation length ξ (in terms of the number of collisions), owing to the increasing importance of those trajectories. Note that ξ^{-1} goes to zero as $\kappa^{1/\gamma}$, so ξ may go to ∞ as $\mu^{-z/\gamma}$ with z defined above. This behavior is reminiscent of a phase transition, as for λ and, as discussed in Ref. 2, for σ.

Let us make a last remark about this algebraic law: for $R = 1$, we have a strictly positive Lyapounov exponent. Thus trajectories split exponentially, while the "relaxation process" associated to the VACF is slow. This shows that a link between the two quantities must be very subtle, if any.

4.1.4. $R > 1$. In this case, Casati *et al.*[10] found $C(n) \simeq (-1)^n \exp[-\kappa n^\gamma]$ with $\gamma \simeq 0.42$ and $\kappa = 1.4$.

It is interesting to note that γ changes by a factor $\simeq 1/2$ when R crosses 1.

In fact a correlation function different from $C(n)$ was computed in Ref. 10 but this should be irrelevant for γ.

4.2. The $d = 2$ VACF with Respect to Time

We computed $C(\Delta t) = |\langle \mathbf{v}(t)\, \mathbf{v}(t + \Delta t)\rangle|$ and found the following form: For $\Delta t \leqslant \sigma^{-1}$ (time during which the particle undergoes on average less than one collision) we have

$$C(t) \simeq \exp(-at)$$

and for $20 \gg \Delta t \gg \sigma^{-1}$ $C(t) \simeq \exp(-bt^{0.7})$. Note the 0.7 instead of 0.86 for $C(n)$. For $\Delta t \simeq 50$, Friedman *et al.*[15] found that the decay is algebraic ($\simeq 1/t$). This can now be easily understood from the s^{-2} decay of $M(s)$, as $C(t)$ behaves for large t like

$$C(t) \simeq \int_t^\infty M(s)\, ds$$

if one admits that $C(t)$ is governed by the fraction of particles which have not collided at time t.

This indicates a crossover between a stretched exponential and an algebraic decay for $C(t)$.

We note the change from a stretched exponential decay for $C(t)$ for $R > 1$ (as for $C(n)$ since the free path is bounded) to an algebraic decay for $R < 1$.

4.3. $C(n)$ in d Dimensions

We studied $C(n)$ for d as high as 7.

For $d = 3$, the striking fact is that $C(n)$ is very small (< 0.08) for all n, and that $C(1)$ is strictly zero. It is difficult to obtain any curve at all.

For $d = 4$, we notice that (i) $C(n)$ is always positive and its order of magnitude is the same as in two dimensions and (ii) $C(n)$ is again of the form $\exp(-\kappa n^\gamma)$ with $\gamma = 0.83 \pm 0.05$ and $\log \kappa = 0.3$.

For $d = 5$, 6, 7, we nôte that, as d increases (cf. Fig. 14) (i) correlations are positive and for a given n, bigger as d increases; and (ii) $C(n)$ follows

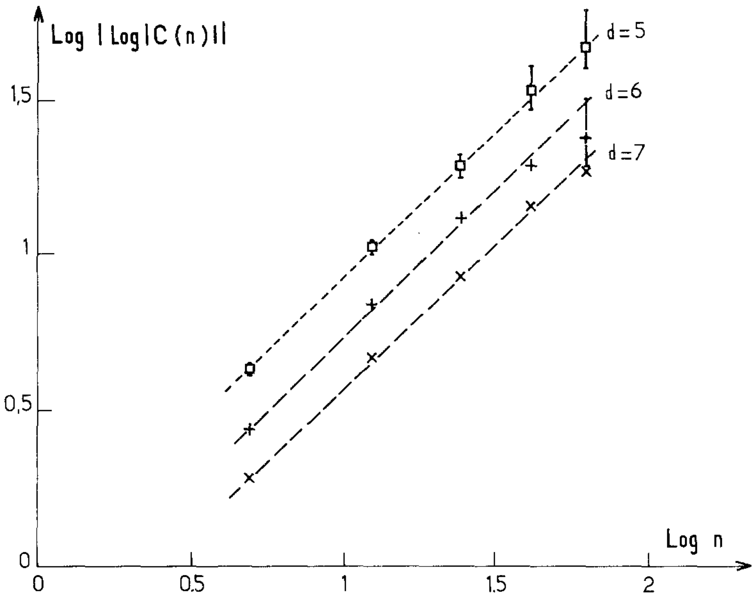

Fig. 14. $C(n)$ in dimension $d=5$, 6, 7, for, respectively, 50 000, 10 000, 5000 collisions with the sphere.

again the same law with γ getting closer to 1 and κ going to 0: $\log \kappa(5) = -0.05$, $\log \kappa(6) = -0.2$, $\log \kappa(7) = -0.4$ (within 20%).

It is easy to calculate $C(1)$, using the asymptotic measure, for any d: let φ be the deviation due to a collision. The law of distribution of φ is

$$dP(\varphi) = \frac{d-1}{2} \sin \frac{\varphi}{2} \left(\cos \frac{\varphi}{2} \right)^{d-2} d\varphi \quad \varphi \in [0, \pi]$$

thus leading to

$$\langle \cos \varphi \rangle = \frac{d-3}{d+1} = C(1)$$

This law is very well confirmed experimentally. This is a check of the ergodicity of the system in higher dimensions.

This calculation allows us to understand better the observed behavior of $C(n)$ in d dimensions:

(i) When d increases, $\langle \cos \varphi \rangle \to 1$, which means that the collisions are more and more tangential. This is due to the fact that the surface of a high-dimensional sphere is relatively very important, in the sense that the ratio surface by volume diverges as $d \to \infty$. Tangential collisions lead to a slower decay (κ goes to zero).

(ii) In two dimensions, the collisions are in great majority frontal, while in $d = 4$, they are mostly tangential. For $d = 3$, there is an exact compensation between the two effects, leading to $C(1) = 0$ and $C(n)$ negligible. Thus, it is in three dimensions that elastic collisions are the most efficient in the redistribution of velocities. This could be important for the study of the approach of equilibrium in d dimension, with $d = 3$ singled out. In high dimensions, two successive collisions usually diffuse the particle in orthogonal directions. The process then becomes Markovian. We conjecture that $\gamma \to 1$ as $d \to \infty$.

Note that $C(n)$ should be calculable for high d, using the fact that deviation angles are small. One can then convolute distribution laws for the square of the deviation angles.

4.4. Discussion of the Stretched Exponential Behavior.

Stretched exponential decay has also been obtained, for example in the William Watts relaxation model,[11] in the problem of a random walk with traps,[12] in the percolation theory,[13] and also recently in spin glasses.[17] This kind of law is beginning to be extensively discussed.[18] In particular this type of non-Markovian law can be viewed as a sum of independent Markovian relaxation process with relaxation times distributed according to a stable law (Levy or Gauss). It can also be a superposition of purely oscillatory processes as it has been shown by Mazo and Van Beijeren[19] in the case of the one-dimensional Lorentz gas. Here, successive deviations are strongly correlated by the geometry of the problem. This is associated to the following facts.

(i) γ depends on the geometry of the system: γ takes three different values for three different geometries ($R > 1$, $R < 1$, equivalent system). But γ seems to be constant, for continuous deformation of a given geometry (γ does not depend on R).

(ii) A γ different from 1 should be related with the symmetries or periodicities of the system, or more precisely, with the periodic orbits. In the billiard, periodic trajectories are dense in the phase space, and the number of periodic trajectories with period L grows exponentially with L. This superposition of periodic motions with a weight proportional to the time spent near each periodic orbit, could perhaps lead to the expected law for $C(n)$. The role of periodic orbits is clearly exhibited by the jump of γ for $R = 1$, when the most important period 2 orbit disappears.

(iii) $C(1)$ is not on the curve, because obviously there is no correlation effects for this quantity. The same remark holds for $C(\Delta t)$ when $\Delta t \leqslant \sigma^{-1}$.

5. THE DIFFUSION COEFFICIENT

5.1. Definition, Convergence, Numerical Results

We have computed a diffusion coefficient D, defined as

$$D(T) = (1/2d)\langle r^2(T)/T \rangle$$

We do not know whether the limit $D(\infty)$ exists in our case. As will be discussed there are reasons to believe that it does not exist.

Its existence has only been established in the case of bounded horizon by Bunimovich and Sinai.[8] For example, $D(\infty)$ exists in the case of the triangular lattice for a certain range of parameter (cf. Ref. 14).

When a single trajectory is observed, we find (for $R = 0.5$) the following:

(i) Above $T \simeq 300$, the curve seems to settle roughly to a linear behavior. However, a $T \log T$ behavior is not excluded.

(ii) When different trajectories are compared one obtains very different $r^2(T)/T$.

(iii) Nevertheless, when $r^2(T)/T$ is averaged over the phase space this results in a well-defined curve $D(T, R)$ as a function of R. We obtained one curve for R very near to 1 (cf. Fig. 15) by averaging over 500 trajectories up to $T = 10\,000$. The result is that

$$D(T) \simeq \mu^{1+\eta} \qquad \text{with} \quad \eta = 0.3 \pm 0.06 \tag{5.1}$$

5.2. Discussion

From a theoretical point of view, the behavior of D as R goes to 1 is not an easy problem.

There are several arguments which could imply that $D(\infty)$ is not defined:

(i) *The VACF Behavior.* The coefficient $D(T)$ is related to the velocity autocorrelation function by the formula:

$$D = \lim_{T \to \infty} \frac{1}{2dT} \int_0^T d\tau \int_0^\tau \langle \mathbf{v}(0)\, \mathbf{v}(t) \rangle \, dt.$$

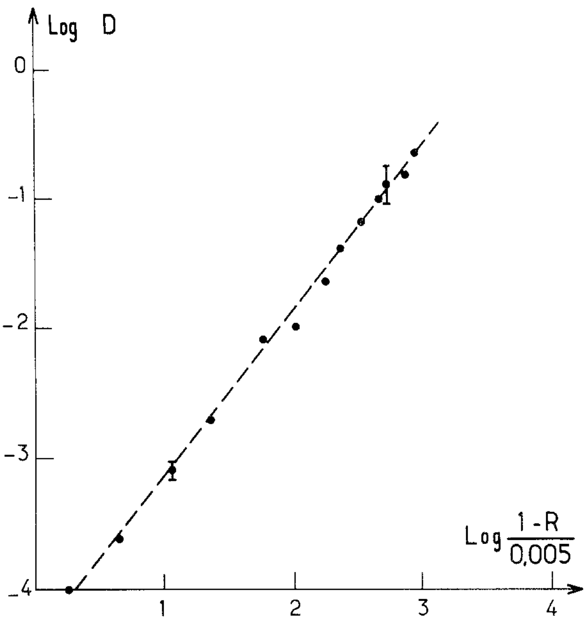

Fig. 15. Log 4. $D(T)$ as a function of $\log \mu$ for $\mu \geqslant 0.005$ and $T = 10\,000$.

If the tail $1/t$ of $C(t)$ holds true[15] this would imply that $D(T)$ behaves like $D_0 \log T$ for large T. Nevertheless, owing to the weak divergence of $D(T)$, it is not irrelevant to study $D(T)$ as a function of R for large fixed T.

(ii) *A Random Walk Model.* At first sight, one could think that for $R \simeq 1$ the particle stays trapped a long time and the direction of escape decorrelates from the entry. With this hypothesis, one can approximate the motion by a random walk between traps on a lattice with a mean waiting time T_w at every site. Experimentally we find (as expected by the ω measure) $T_w \simeq \mu^{-1}$.

If we consider the triangular symmetry case, the particle can only jump from one site to one of its nearest neighbor and we find $D(\infty)$ to be $\simeq \text{const} \times 1/T_w \simeq \mu$: this was confirmed experimentally by Machta and Zwanzig.[15]

The nonlinear μ behavior observed here for $D(T)$ with fixed T may be due to the following complications:

(a) It is not true in our case that each jump occurs between two nearest traps. More precisely, we saw that the probability of a jump of length s is given by $N(s) \simeq \mu/s^3$. Therefore $\langle s^2 \rangle$ diverges logarithmically, which could imply that $D(\infty)$ is not defined. Experimentally though, the divergence is so weak that one still obtains, for $\langle s^2 \rangle(R)$, a well-defined curve, showing the importance of finite observation time. [We expect that $D(T) \simeq \log T$.] Notice also that s^{-3} is marginal between Gaussian statistics and Levy statistics. In order to explain the value of η, a simple, but poor, scaling argument is that each jump should have a range $\mu^{1/3}$ due to the form of $N(s)$. The diffusion coefficient of such a walk is

$$D \simeq 1/T_w \times \text{range} \simeq \mu^{1.33} \text{ thus giving } \eta = 1/3$$

(b) It is not true that the direction of escape is decorrelated from the one of the entry. We find that the "forward" correlation is $\simeq 30\%$ even for $\mu = 0.001$.

(iii) *Experimental Indication.* If the law (5.1) is to be valid for very small μ (<0.005) our D will become smaller than in the triangular case, where D is linear in μ. This is surprising since this would mean that for very small μ, the diffusion is slower for an unbounded horizon [$N(s) \simeq s^{-3}$] than for a bounded horizon ($s \leqslant s_{\max}$). So, either this is true and this proves that in this problem $D(\infty)$ is meaningless (which would be an indirect proof of its nonexistence) or the law is in fact linear for very small μ but we could not check this experimentally.

Let us finally remark that it would be interesting to define an order parameter for this system by $\lim D(T)/\log T$ (if it exists) and to study its behavior as a function of μ. The diffusion coefficient is a usual order parameter for instance in percolating systems.

6. CONCLUSION AND SUMMARY

We summarize the results of this study: we have checked the ergodicity of the system by studying the rate of collisions and the velocity autocorrelation. We derived the asymptotic behavior of the distribution of path lengths. It decreases as s^{-3} (as $s^{-2.5}$ for $s < 1/R$). Those tails are important (i) for the behavior of the Kolmogorov entropy for vanishing size of scatterers: it clarifies a result obtained by Oono *et al.*[7]; (ii) for the long time behavior of the velocity autocorrelation: it confirms the experimental law obtained in Ref. 15; (iii) for the nonexistence of a diffusion coefficient.

We obtained remarkably simple logarithmic behaviors for the Lyapounov exponent as a function of R and d. We also obtained a stretched exponential decay of the velocity autocorrelation in a billiard without horizon, with a possible crossover. This law should give subtle information on the phase space of the problem. We conjecture that it becomes a pure exponential decay for $d \to \infty$.

Some points would deserve a better numerically study. These are (i) the behavior of $D(T)/\log T$ as a function of μ; (ii) the behavior of $\lim\langle r^2(n)\rangle/n$, where n is the number of collisions. This limit should exist because $C(n)$ is in any case integrable; (iii) a direct determination of z by studying $C(n)$ for R near 1; (iv) direct calculation of λ_{nonmax} in high dimension.

We find simple laws whose derivation are challenging. Many of the tools and ideas of statistical mechanics and critical phenomena seem to be relevant for this problem. Preliminary physical interpretations or clues are proposed, but much remains to be clarified. We discuss further and in more precise terms in Ref. 2 the very interesting two-dimensional $R=1$ region where we find a critical behavior with exponents which should be related to each other.

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