First return map of the periodic Lorentz gas

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We obtain the first return map of the periodic Lorentz gas treated as a Sinai's billiard. By using this map we compute numerically the largest Lyapunov exponent and the velocity autocorrelation function for the triangular Lorentz gas in the high density regime.

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We consider a system of moving particles in the plane outside a periodic set of disks of radius R centered at the sites of a triangular lattice. The particles are elastically reflected on the boundary of the disks. This is the triangular periodic Lorentz gas [1,2], viewed here as a concrete example of a hyperbolic scattering billiard [3,4]. Billiard systems are Hamiltonian and preserve the Liouville measure μ [5,6].

Let $\vec{q}(t)$ and $\vec{v}(t)$ be the position and velocity of the particle at time t, with respect to a Cartesian frame at rest. We choose a Cartesian frame located at a lattice site, with an orthogonal basis $(\vec{e}_x,\vec{e}_y)$, $|\vec{e}_x|=1$, $|\vec{e}_y|=\sqrt{3}$ so that the location of the scatterers is determined by a pair $(l,m)\in\frac{1}{2}Z\times\frac{1}{2}Z$.

The value of the radius R of the scatterers may change, defining two different regimes of density. When $R\leq\sqrt{3}/4$ the path of the particle between two successive collisions is unbounded, and we call this the low density or the infinite horizon regime. When $R>\sqrt{3}/4$, the path between successive collisions becomes bounded, and this situation corresponds to the high density or finite horizon regime. If $R=\frac{1}{2}$ the scatterers just touch, the particle is trapped in a curved triangular domain, and we call this the close packing configuration of the scatterers. If $R>\frac{1}{2}$ the scatterers overlap and the particle is trapped in a curved triangular domain, but the vertices do not touch tangentially. The problem of the statistical behavior of the evolution and the asymptotics of the velocity autocorrelation function have been studied by several authors [2,7–9].

We recall here that if the time intervals τ between successive collisions are uniformily bounded (finite horizon), then the central limit theorem holds [1,4]. In the case of a triangular periodic lattice the Wigner-Seitz hexagon is the quotient space $R^2/\frac{1}{2}Z\times\frac{1}{2}Z$. If D is the interior of all disks, the configuration space is $Q=(R^2-D)/\frac{1}{2}Z\times\frac{1}{2}Z$ [1,10,11].

The sides of the hexagon are called transparent walls [12], they are crossed at least twice, then play no role in the dynamics, and their length determines the normalization factor of the invariant measure. As the velocity of the particle is a constant of motion, here taken equal to 1, the phase space of the system is the unit tangent bundle over Q,

$$\Gamma=\{y=(q_1,q_2,\theta)/(q_1,q_2)\in Q,\theta\in[0,2\pi]\} . \quad (1)$$

We denote by S_t, $t\in(-\infty,\infty)$, the flow generated by the dynamics on Γ.

Billiards systems are studied in terms of their global section [6], which is the set $\partial\Gamma^+$ of all phase points "just after collision." The set $\partial\Gamma^+$ is a union of closed two-dimensional Riemannian manifolds, usually parametrized in terms of the Birkhoff coordinates (r,ϕ) [5,11] r being the arclength along ∂Q and ϕ the angle between the incoming velocity and the local oriented tangent at the collision point $\vec{q}(r)$.

As the transparent walls play no role in the configuration space, the global section can be restricted to

$$\begin{aligned}\partial\Gamma^+&=\{x=(r,\phi)/r\in[0,2\pi R],\phi\in[0,\pi]\}\\&=[0,2\pi R]\times[0,\pi] . \quad (2)\end{aligned}$$

$\partial\Gamma^+$ is a cylindric surface with a metric $dr^2+d\phi^2$. When the flying time $\tau(x)$ is bounded (i.e., the horizon is finite), $\partial\Gamma^+$ is a global section of the phase flow S_t because almost all trajectories return to $\partial\Gamma^+$ after crossing $\partial\Gamma^+$.

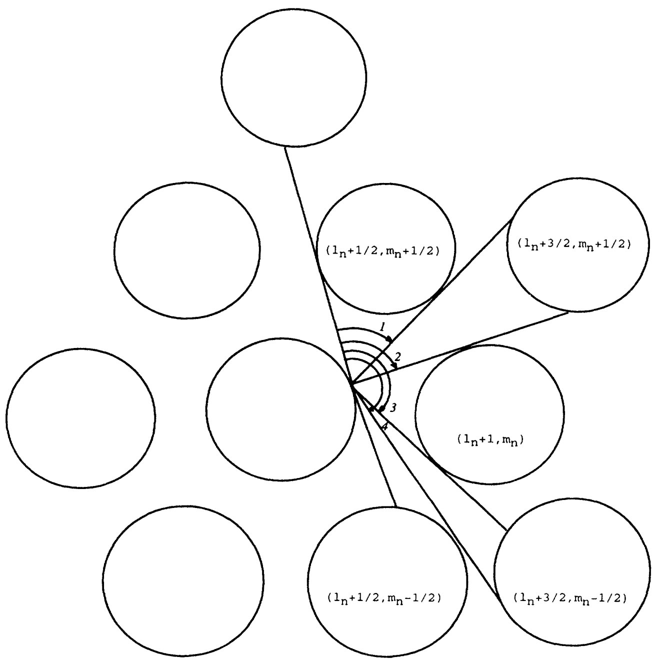

FIG. 1. Sectors that define the transfer rule.

The first return map T takes each point (r,ϕ) of the global section to the point of the next crossing. The singularities of the first return map are the points $\partial\Gamma^+$, which are tangent to the scatterers $(l,m),(l,m)\in(\frac{1}{2}Z\times\frac{1}{2}Z)$ and the preimages of tangent collisions. These points are depicted in Fig. 1.

The components $\phi_{m_1m_2}(x)$ of the set $T^{-1}(\partial(\partial\Gamma^+))$ are determined by elementary geometry to be

$$\phi_{m_1m_2}(r)=\gamma^{m_1m_2}(r)+\alpha^{m_1m_2}(r)\ , \tag{3}$$

$$\alpha^{m_1m_2}(r)=\arcsin\left\{R\left[\left[m_1-R\cos\frac{r}{R}\right]^2+\left[m_2\sqrt{3}-R\sin\frac{r}{R}\right]^2\right]^{-1/2}\right\}\ , \tag{4}$$

$$\gamma_{m_1m_2}(r)=\arctan\left|\frac{m_1\cos\frac{r}{R}+m_2\sqrt{3}\sin\frac{r}{R}-R}{m_2\sqrt{3}\cos\frac{r}{R}-m_1\sin\frac{r}{R}}\right|\ . \tag{5}$$

The singular curves are depicted in Fig. 2. The singular curves presented in Fig. 2 agree with the qualitative discussion of the singularities provided by Sinai [3].

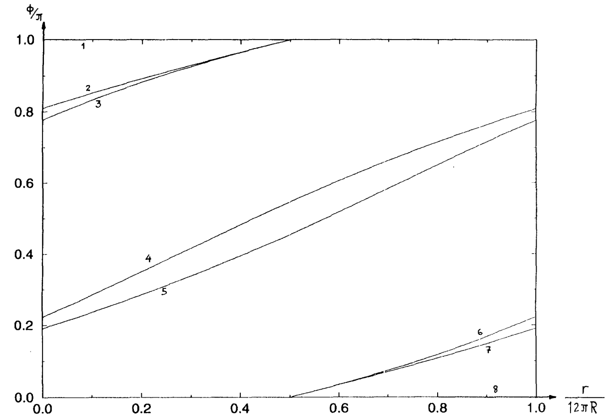

FIG. 2. Singular set determined by the functions ϕ_{m_1,m_2}.

The first return map is a diffeomorphism of the set $\partial\Gamma^+-S$, S being the set of singularities, and preserves the measure $d\nu=c_\nu\sin\phi\, dr\, d\phi$ [5,11,13], where c_ν is a normalization constant. Since the dynamics is completely deterministic, any point (q_1,q_2,θ) of the phase space Γ, $(q_1,q_2)\in Q$, $\theta\in[0,2\pi]$, is completely determined by the point $(r,\phi)\in\partial\Gamma^+$ corresponding to its last collision, and the time since that collision. This is the Ambrose-Kakutani representation of the dynamical system (Γ,S_t,μ) as the flow above the cascade T on the base space M with the help of the generating function $\tau(x)$ [6,13–15].

The expectation value of any observable f is

$$\langle f\rangle=\int d\mu f=\frac{1}{\nu(\tau)}\int_M d\nu(r,\phi)\int_0^{\tau(r,\phi)}dl f(r,\phi,l)\ , \tag{6}$$

where $\nu(\tau)=\langle\tau\rangle_\nu=\int_{\partial\Gamma^+}\tau(r,\phi)d\nu$. The relation between the variables θ, ν, ϕ was first found by Birkhoff [5] and extended to the most general planar billiards by Katock and Strelcyn [11]. The Strelcyn-Birkhoff implicit equation relates the above variables of the corresponding successive collision points (r,ϕ) and $(r_1,\phi_1)=T(r,\phi)$, and is given by

$$\theta=\frac{\pi}{2}+\frac{r}{2}-\phi=\frac{\pi}{2}+\frac{r_1}{2}+\phi_1 \mod(2\pi)\ . \tag{7}$$

If the particle is located at the scatterer (l,m) at the point (r,ϕ), then the particle will be found at the point (r_1,ϕ_1) on the scatterer (l_1,m_1) with

$$r_1=r-R\left[\phi-\arccos\left\{\cos\phi+\frac{1}{R}\left[\sqrt{3}(m_1-m)\sin\left[\phi-\frac{r}{R}\right]-(l_1-l)\cos\left[\phi-\frac{r}{R}\right]\right]\right\}\right]\ , \tag{8}$$

$$\phi_1=-\arccos\left\{\cos\phi-\frac{1}{R}\left[\sqrt{3}(m_1-m)\sin\left[\phi-\frac{r}{R}\right]-(l_1-l)\cos\left[\phi-\frac{r}{R}\right]\right]\right\}\ . \tag{9}$$

The location of (l_1,m_1) of the target scatterer is determined from the singularity curves [3] (see Fig. 2) as follows:

$$(l_1,m_1)=(l+\tfrac{1}{2},m+\tfrac{1}{2}) \text{ if } \phi\in[0,\phi_{1/2\,1/2}(r)] , \tag{10}$$

$$(l_1,m_1)=(l+\tfrac{3}{2},m+\tfrac{1}{2}) \text{if } \phi\in[\phi_{1/2\,1/2}(r),\phi_{3/2\,1/2}(r)] , \tag{11}$$

$$(l_1,m_1)=(l+1,m) \text{ if } \phi\in[\phi_{3/2\,1/2}(r),\phi_{10}(r)] , \tag{12}$$

$$(l_1,m_1)=(l+\tfrac{3}{2},m-\tfrac{1}{2}) \text{if } \phi\in[\phi_{10}(r),\phi_{3/2\,-1/2}(r)] , \tag{13}$$

$$(l_1,m_1)=(l+\tfrac{1}{2},m-\tfrac{1}{2}) \text{if } \phi\in[\phi_{3/2\,-1/2}(r),\pi] . \tag{14}$$

The hexagonal symmetry allows the reduction of the phase space to $[0,\pi R/6]\times[0,\pi]$.

The formulas (8) and (9) that give the first return map T are derived from the solution of the implicit Eq. (7). We derive this formula relating the parametric representation of the bounder of the scatterer with the velocity angle, which is constant between two successive collisions. The first return map T allows, for example, the computation of the velocity autocorrelation function and the Kolmogorov-Sinai (KS) entropy of the triangular Lorentz gas in the high density regime $\sqrt{3}/4<R\le\frac{1}{2}$.

VELOCITY AUTOCORRELATION

The velocity autocorrelation function of the flow S_t is

$$C(t)=\int_\Gamma d\mu\vec{v}(S_t(r,\phi,l))\vec{v}(r,\phi,l) . \tag{15}$$

As the velocity $\vec{v}$ is constant between successive collisions we have

$$\vec{v}(r,\phi,l)=\vec{v}(r,\phi) \quad \text{for } 0<l<\tau(r,\phi) . \tag{16}$$

Therefore,

$$\vec{v}(S_t(r,\phi,l))\vec{v}(r,\phi,l)=\vec{v}(T^n(r,\phi))\vec{v}(r,\phi) \tag{17}$$

for

$$\tau(r,\phi)+\cdots+\tau(T^{n-1}(r,\phi))\le t\le\tau(r,\phi)+\cdots+\tau(T^n(r,\phi)) .$$

The velocity autocorrelation is therefore

$$C(t)=\int_{\partial\Gamma^+}d\nu\vec{v}(T^n(r,\phi))\vec{v}(r,\phi)\int_0^{\tau(r,\phi)}dl$$
$$=\int_{\partial\Gamma^+}d\nu\vec{v}(T^n(r,\phi))\vec{v}(r,\phi)\tau(r,\phi) . \tag{18}$$

Due to mixing, for large times, $t\to\infty$, we have

$$C(t)=C(n)\langle\tau\rangle_\nu , \tag{19}$$

where $C(n)=\int_{\partial\Gamma^+}d\nu\vec{v}(T^n(r,\phi))\vec{v}(r,\phi)$ is the velocity autocorrelation of the first return map.

The integral with respect to continuous time of the velocity autocorrelation function is finite only in the high density regime $\sqrt{3}/4<R\le\frac{1}{2}$. If the angles between the tangents at the break points are different from zero, which excludes the close packing case $R=\frac{1}{2}$, $C(n)$ has been shown [1,4] to be bounded subexponentially:

$$|C(n)|\le Ke^{-\alpha n^\gamma} , \tag{20}$$

where $K>0,\frac{1}{2}\le\gamma<1$ are constants and α depends upon the shape of the configuration Q. In the case of the close packing, for large time n, we have Machta's [16] estimation,

$$|C(n)|\approx\frac{A}{n} , \tag{21}$$

where A is a positive constant.

In order to verify the above estimation of $C(n)$, we computed the velocity autocorrelation function averaging over trajectories between 10^5 and 10^6 iterations of $T(r,\phi)$. In the computation, time is represented by the sequence of integers and corresponds to successive collisions. The numerical errors of the values of $C(n)$ are between 3% and 8%.

We observed that the absolute value of $C(n)$ is well fitted by the subexponential (20) [1,4], except for the close packing case (see Fig. 3). We found that the exponent γ does not depend significantly on R, being almost constant $\gamma\approx0.71\pm0.02$. This value was also found in [8]. Therefore it seems plausible to conjecture that the value $\gamma\approx0.71$ is universal for all bounded systems where the diffusion occurs.

The parameter α varies with the radius R, and as the parameter γ is constant, the transport process is characterized by the function $\alpha(R)$. A complete discussion about the diffusion in the bounded Lorentz gas and the behavior of the function $\alpha(R)$ will appear in a future work [17].

In the close packing case we found that $C(n)$ is better fitted by the algebraic law (21) proposed by Machta, with $A\cong0.45\pm0.05$, which agrees (within the numerical precision) with the numerical value obtained in [16].

ENTROPY-LYAPUNOV EXPONENT

Katock and Strelcyn have shown [11] that the presence of singularities does not prevent the application of Pesin's formula. Therefore, for our system the Kolmogorov-

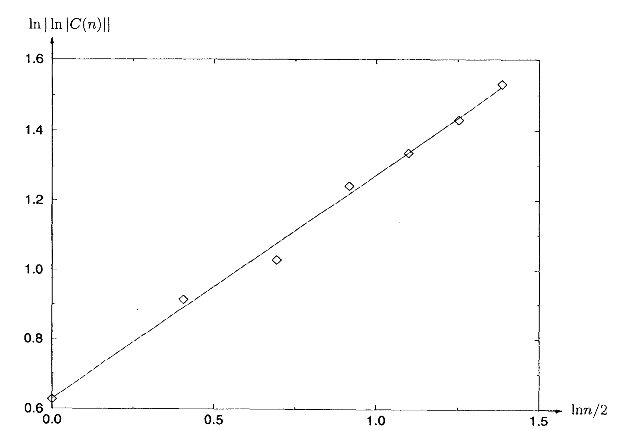

FIG. 3. Discrete velocity autocorrelation function for $R=0.45$ showing subexponential behavior.

Sinai entropy $h(T)$ is equal to the largest Lyapunov exponent λ. The dependence of the Lyapunov exponent of the first return map on the radius R is known only for sufficient small R (low density)

$$\lambda(R) = -2\ln(R) + O(1) , \tag{22}$$

with

$$\frac{O(R^n)}{R^n} \underset{R\to 0}{\longrightarrow} 0 .$$

This formula was derived analytically by Chernov [12] without any knowledge of the first return map T, following previous numerical calculations [8].

We investigated the dependence of the Lyapunov exponent λ in the region $\sqrt{3}/4 \le R \le 0.52$, which corresponds to the high density regime of the system. For $R > 0.52$ the numerical values of the Lyapunov exponent do not converge very well due to the small values of the curvature of the scatterers, which introduces undesirable numerical stable periodic orbits inducing unavoidable numerical errors.

As Chernov's estimation is limited to the low density regime, we use the formulas (8) and (9) for the first return map in order to compute the largest Lyapunov exponent in the high density regime. We apply the algorithm developed in [18,19] for the computation of the Lyapunov exponent, which is well adapted for the present formulation of the problem. Clearly, due to the ergodicity, we have observed the same values for λ for ν—almost all $(r,\phi)\in M$.

The values of λ converge very well, and the numerical errors are less than 0.5%. The dependence of λ versions on $\ln R$ is plotted in Fig. 4. The continuous part results from our numerical calculations and the dashed part corresponds to our conjecture about the behavior of λ in the whole domain $0 \le R \le (\sqrt{3}/3)$, based upon Chernov's result for the limit $R \to 0$ and upon the fact that $\lambda = 0$ for $R = \sqrt{3}/3$ where the trapping region defined after close packing collapses.

Our computation shows therefore that in the regime $\sqrt{3}/4 \le R \le 0.472$,

$$\lambda = -2\ln R - 1 . \tag{23}$$

Chernov's formula (22) is therefore still valid in this part of the high density regime. For $R \ge 0.472$, however, Chernov's formula is not valid because λ decreases more rapidly until its minimum value $\lambda \cong 0.32$ at the close packing point $R = \frac{1}{2}$.

Let us also remark that within the accuracy of our numerical calculations we have

$$\lambda\left[\frac{\sqrt{3}}{4}\right] = 1 - \lambda(\tfrac{1}{2}), \quad \lambda(0.472) = 0.5 . \tag{24}$$

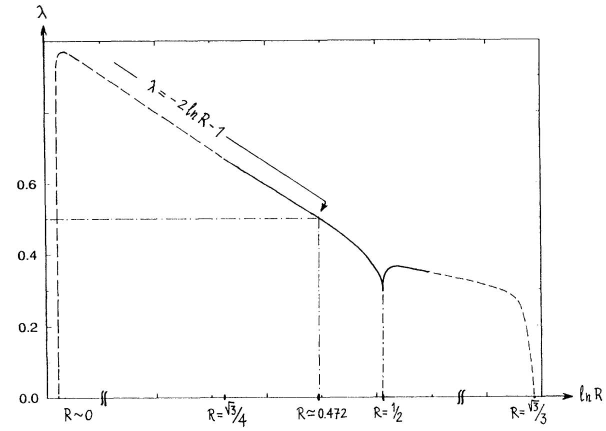

FIG. 4. Largest Lyapunov exponent. The full line corresponds to our numerical results, and the dashed line corresponds to extrapolated behavior.

The value $R \cong 0.472$ marks the end of the validity of Chernov's formula. This point looks like a critical point if the quantity $d^2\lambda/d^2(\ln R)$ is considered as an order parameter.

Concluding, using the first return map (8) and (9), we confirmed the estimations (20) and (21) for the behavior of the velocity autocorrelation function, and we conjecture that the parameter $\gamma \cong 0.71$ in (20) is a universal parameter for bounded billiards where diffusion occurs. Moreover we have computed the dependence of the Lyapunov exponent with respect to the radius R in the high density regime. We found that Chernov's formula is valid for $R \lesssim 0.472$. For $R \gtrsim 0.472$ we have a more delicate behavior, which we leave for a future study [20].

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