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Decay of Correlations in the Regular Lorentz Gas

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The regular Lorentz gas on triangular lattice is studied numerically and analytically. The velocity correlation function is shown to decay exponentially in the number of collisions with a decay rate which vanishes as the scatterers approach close packing. The crossover to power law decay at close packing is described by a scaling function.

KEY WORDS: Lorentz gas; velocity correlation functions; billiards; dynamical systems.

1. INTRODUCTION

In this note we present a numerical study of the decay of the velocity correlation function in the regular Lorentz model and provide a simple analysis of our results. In the Lorentz model a single point particle obeying classical dynamics moves in an array of immobile scatterers. In the present study the particle moves on the plane and the scatterers are disks on a triangular lattice as shown in Fig. 1. The disks have unit radius and the particles move with constant velocity and unit speed between elastic collisions with the disks. The paramater W measures the distance of closest approach between neighboring scatterers and completely characterizes the system. We study W in the range $0 < W < W_1$, where $W_1 = 0.3094$. In this range the particle moves in an infinite region but has a finite horizon in the sense that the maximum free path is bounded from above. When $W < 0$, the particle moves in a finite region and the model is known as a billiard model whereas when $W > W_1$ there is an infinite horizon.

Regular Lorentz models play an important role in our understanding of transport phenomena. They are simple enough to admit rigorous

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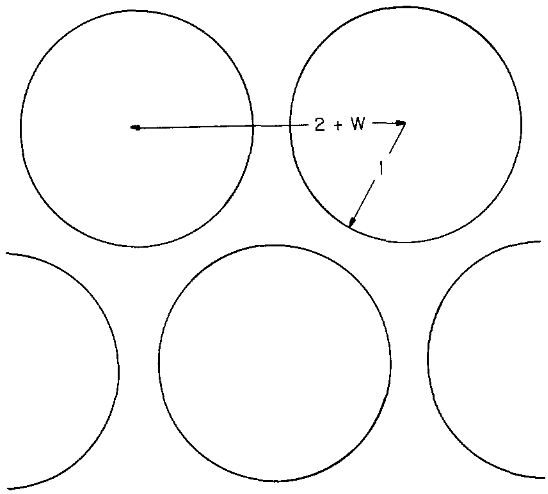


Fig. 1. Scatterers in the regular Lorentz gas have radius one and lie on a triangular lattice with lattice constant $2+W$.

mathematical analysis and complex enough to display realistic transport properties. In recent years there has been considerable interest in these models. Bunimovich and Sinai[1] showed that the regular Lorentz model described above for $0<W<W_1$ is a K-system and that the average particle motion is diffusive. Machta and Zwanzig[2] showed that this diffusive motion can be described for small W as a random walk between trapping regions formed between three disks. Machta[3] studied the $W=0$ billiard and Bouchaud and Le Doussal[4] studied the equivalent billiard on a square lattice. In both cases the velocity correlation function (VCF) was found to decay like $1/n$, where n is the number of collisions. In Ref. 3 this slow decay of correlations was attributed to particle motion near the points of tangential contact of the disks. Power law decay of the VCF also occurs in the regular Lorentz model when the horizon is infinite[5] ($W>W_1$ for the triangular lattice and for any positive separation between the disks for the square lattice) and, in general, in chaotic dynamical systems with integrable segments.[6] The VCF as a function of time rather than collision number has also been investigated for regular Lorentz models.[2,4,7] In cases where the free paths of the particle may be either arbitrarily large or arbitrarily small, the VCF as a function of collision number and time behave in qualitatively different ways. We emphasize that the present discussion is concerned solely with the VCF as a function of collision number.

Our work is motivated by the rigorous analysis of the Lorentz model given by Bunimovich and Sinai,[1] which showed that the decay of the

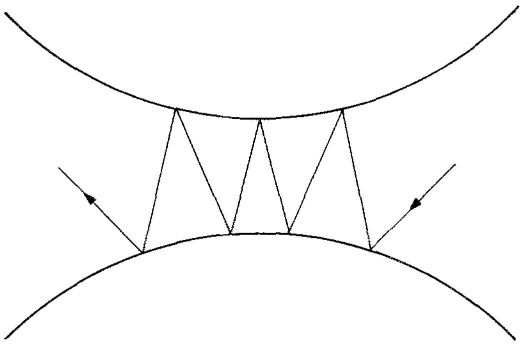


Fig. 2. An example of a particle trajectory in the vertex between two scatterers.

velocity correlation function, $C(n)$, as a function of the number of collisions is bounded, for large, n, by

$$|C(n)| \leqslant e^{-n^{\gamma}}, \qquad n \to \infty \tag{1}$$

where the exponent γ lies in the range $0<\gamma<1$. Bunimovich and Sinai were unable to establish the value of γ. Our numerical work and qualitative analysis supports the hypothesis that the VCF decays as an ordinary exponential ($\gamma = 1$) with decay rate $\lambda = W + (W^2 + 2W)^{1/2}$. We also find a crossover function which shows how the VCF goes over to power law behavior as $W \to 0$. Our results are in contrast with numerical studies[8] of the related diamond billiard in which stretched exponential decay ($\gamma < 1$) apparently holds. The diamond billiard is obtained from the regular Lorentz gas on a square lattice when $W < 0$. Stretched exponential behavior of the VCF also appears to hold for intermediate times in the Lorentz gas on a square lattice.[4]

The outline of the paper is as follows. In Section 2 we give a simple analysis of the VCF. This analysis is based on the hypothesis that the large n behavior of the VCF is dominated by long sequences of collisions of the kind shown in Fig. 2. In Section 3 we present numerical results for the VCF. The paper closes with a discussion.

2. ANALYSIS OF THE VELOCITY CORRELATION FUNCTION

The analysis of the VCF is based on the idea that its large n behavior is dominated by long sequences of collisions in a vertex. By vertex we mean any of the regions of phase space in which the position of the particle is near the line connecting the centers of two neighboring disks and the velocity is nearly parallel to this line. A sequence of collisions in a vertex is shown in Fig. 2. In each vertex there is a period two orbit which, like all periodic orbits in the Lorentz gas, is unstable. However, it is our hypothesis that the period two orbit in the vertex is less unstable than all other periodic orbits. This is because it has the shortest free paths and thus trajectories near this orbit are defocused the least by the negative curvature of the scatterers. Given this hypothesis we argue that the asymptotic behavior of the VCF is exponential with decay rate given by the largest eigenvalue of the linearized motion in the vertex. We note here that this reasoning does not apply in the presence of an infinite horizon when long sequences of nearly tangential collision are possible.

Consider a sequence of m collisions which remain in a single vertex. At each collision the velocity is nearly reversed so that the contribution of this sequence of collisions to $C(n)$ alternates in sign and is of order one for $n \leqslant m$. In order to estimate the contribution of all trajectories in a vertex to $C(n)$ we need to determine the phase space available for sequences of n or more collisions in a vertex. This is done qualitatively below and quantitatively in the Appendix.

Each collision in a vertex can be described by two angles as shown in Fig. 3. θ_m measures the angle that the velocity makes with the normal at the point of collision and α_m measures the angle between the point of collision and the line connecting the centers of the two disks forming the vertex. Elementary geometric considerations yield the following exact relation between the mth and $(m+1)$th collision in a vertex:

$$\sin \alpha_{m+1} - \sin \alpha_m = (2 + W - \cos \alpha_{m+1} - \cos \alpha_m) \tan(\theta_m + \alpha_m) \tag{2}$$

$$\theta_{m+1} - \theta_m = \alpha_{m+1} - \alpha_m \tag{3}$$

For θ_m and α_m sufficiently small this mapping can be linearized yielding

$$\begin{bmatrix} \alpha_{m+1} \\ \theta_{m+1} \end{bmatrix} - \begin{bmatrix} \alpha_m \\ \theta_m \end{bmatrix} = \begin{bmatrix} W & W \\ 2+W & W \end{bmatrix} \begin{bmatrix} \alpha_m \\ \theta_m \end{bmatrix} \tag{4}$$

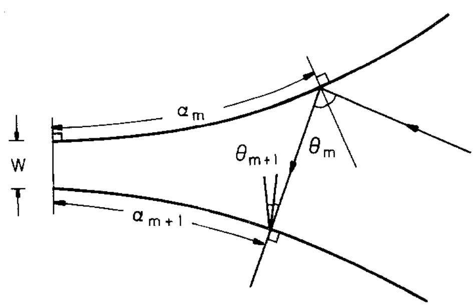


Fig. 3. Angles θ_m and α_m describe the position and velocity of the particle at each collision.

We can describe the motion in the vertex in terms of the normal coordinates, $q^{(+)}$ and $q^{(-)}$ of the linear map. In the linear regime and for a large number, n, of collisions these coordinates behave like

$$q_n^{(\pm)} = q_0^{(\pm)} \exp(\lambda^{(\pm)} n) \tag{5}$$

where $\lambda^{(\pm)}$ are the eigenvalues of the matrix in Eq. (4),

$$\lambda^{(\pm)} = W \pm (W^2 + 2W)^{1/2} \tag{6}$$

Note that $\lambda^{(+)} > 0$, $\lambda^{(-)} < 0$ and that both vanish as $W \to 0$. In terms of the normal coordinates, the phase space available for n or more collisions in a vertex is thus independent of n in the $q^{(-)}$ direction but shrinks exponentially in the $q^{(+)}$ direction. Thus our prediction for the large n behavior of the VCF is

$$C(n) \sim (-1)^n A \exp(-\lambda n) \qquad (0 < W < W_1) \tag{7}$$

where A is a constant and hereafter we take $\lambda = \lambda^{(+)}$.

As discussed in detail by Bouchaud and Le Doussal,[9] the limit $W \to 0$ corresponds to a continuous phase transition. As the transition is approached the correlation number, $1/\lambda$, diverges and $C(n)$ decays very slowly. For $W = 0$ the linearized motion is marginally stable and cubic nonlinearities in the map, Eqs. (2) and (3), must be included for a correct treatment of the motion in the vertex. As shown in Ref. 3, this leads to power law decay of the VCF,

$$C(n) \sim (-1)^n D/n \qquad (W = 0) \tag{8}$$

Trajectories in a vertex cannot distinguish whether W is small or exactly zero unless they probe very small values of α. Since this can happen only for the longest trajectories in a vertex we expect an intermediate n power law decay for the VCF. This line of reasoning leads us to consider a scaling form for the large-n behavior of the VCF which depends on the single scale $1/\lambda$. The scaling form

$$C(n) \sim (-1)^n f(n\lambda)/n \tag{9}$$

reproduces power law decay for $W = 0$ and crosses over to exponential decay for $W > 0$ if

$$f(x) \to D \qquad x \to 0 \tag{10}$$

and

$$f(x) \sim Cxe^{-x} \qquad x \to \infty \tag{11}$$

An analytic estimate for D was obtained in Ref. 3 and, using essentially the same method, an estimate for C is made in the Appendix. The prediction is that $C = 4/\pi$ and $D = 0.7295$. The scaling form, Eq. (9), can also be obtained using the renormalization group approach of Ref. 9.

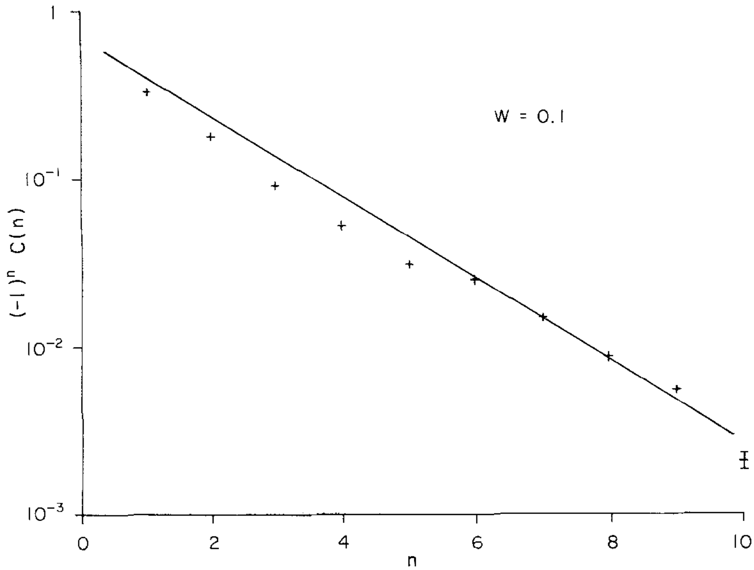
3. COMPUTER EXPERIMENT

We carried out a numerical simulation of the Lorentz gas on a triangular lattice using a CYBER 205 vector processor. We select a large number of initial points (5×10^6–3.2×10^7) chosen from the invariant measure, $d\alpha \cos\theta \, d\theta$. From each of these points, trajectories of length 30 to 50 were computed in single precision (16-digit accuracy) and the velocity correlation function was obtained by averaging. The vector architecture of the CYBER 205 was utilized by creating a vector of 10^4 points in phase space and computing trajectories originating from them in parallel.

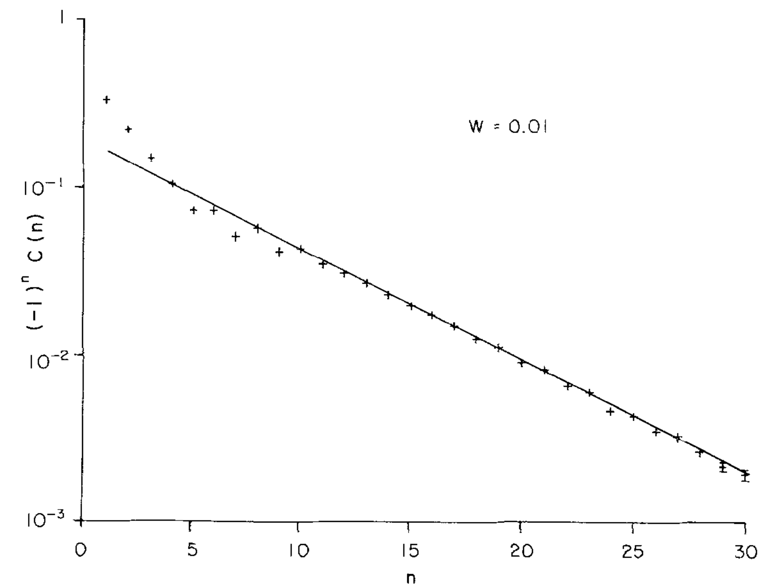
The VCF was calculated for six different values of W (0, 0.0001, 0.0005, 0.001, 0.01, and 0.1) and plotted in Figs. 4a and 4b for $W = 0.1$ and $W = 0.01$, respectively. The solid line in these figures corresponds to the predicted asymptotic decay of the VCF characterized by an exponential with decay rate λ and prefactor $(-1)^n \lambda 4/\pi$. The theory is both qualitatively and quantitatively in good agreement with the simulation for these values of W.

Figure 5 shows data for all six values of W. Guided by the scaling form of Eq. (9) we plot $(-1)^n nC(n)$ vs. λn. Since the scaling form is expected to hold only in the regime where nonvertex contributions to the VCF have decayed away, Fig. 5 shows only those points where n is greater than a value determined by visual inspection for each W. The circle on the vertical axis at 0.675 corresponds to the average of $(-1)^n nC(n)$ for $W = 0$ and $50 \leqslant n \leqslant 50$. The solid line is the predicted large $n\lambda$ behavior of the scaling function [see Eqs. (11) and (A8)] and the tick mark on the vertical axis at 0.73 is the predicted[3] $n\lambda \to 0$ limit of the scaling function. The data for all six values of W do indeed seem to lie on a single curve with the predicted large $n\lambda$ properties. On the other hand, for $n\lambda \to 0$ the observed scaling function is significantly below the theoretical limit, $D = 0.73$. It is unclear whether this is the result of an inability to probe the asymptotic regime in the computer experiment or whether it indicates that there are contributions to the asymptotic VCF not contained in the theory. For example, the present theory does not include the effect of correlations between successive visits to a vertex.

The error bars in Figs. 4a and 4b show plus and minus one standard deviation due to Monte Carlo sample size and are absent if this range is



(a)



(b)

Fig. 4. The velocity correlation function vs. collision number for two values of W, (a) $W=0.1$ and (b) $W=0.01$. The solid line is the theoretical prediction for the asymptotic behavior of the VCF.

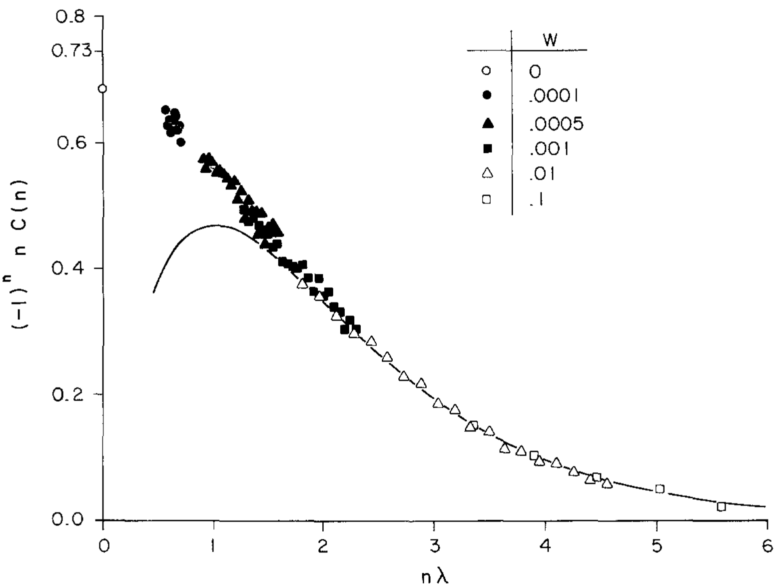


Fig. 5. The velocity correlation function vs. collision number plotted in scaled coordinates. Data from six values of W are shown. The tick mark at 0.73 is the theoretical limit as $n\lambda \to 0$ and the solid is the large $n\lambda$ prediction for the scaled VCF.

smaller than the data symbol. The error due to the finite number, N, of points sampled from phase space is easily estimated using the central limit theorem. In the computer experiment $C(n)$ is a normalized sum over the cosine of the angle ϕ, between $\hat{v}_n$ and $\hat{v}_0$. For large n, this angle is a random variable which is nearly uniformly distributed in the interval 0 to 2π so that $\cos(\phi)$ has variance 1/2 and the standard deviation of $C(n)$ is $(1/2N)^{1/2}$.

In addition to finite N errors there are round-off errors which depend upon location in phase space. Throughout most of phase space the map is strongly chaotic leading to a rapid divergence of nearby trajectories. We find that for typical initial conditions a trajectory can be extended for about 30 collisions, reversed, and then brought back to its origin. Much beyond 30 collisions the reversed trajectory is markedly different from the forward trajectory. On the other hand, for trajectories which start in the vertex the maximum reversal number is higher owing to the linearity of the map there. A more subtle difficulty stems from the algorithm itself. When the velocity is parallel to any of the nearest neighbor lattice vectors the algorithm fails and near these directions it loses accuracy. The period two orbit in the vertex is an example where the algorithm fails, and it is precisely trajectories near this orbit which lead to the long time behavior of the VCF. Fortunately, for 16-digit precision, the region in phase space where this error is large is very much smaller than the values of the VCF. Our belief is that the net effect of the round-off errors is very small and that the dominant source of error in the simulation is the finite size of the Monte Carlo sample.

4. DISCUSSION

It is clear from the figures that the simple theory based on collisions in a vertex captures the main features of the observed decay of the VCF for a wide range of W and n. The theory and simulation together with Ref. 3 support the view that the asymptotic decay of the VCF is exponential for $0 < W < W_1$ and crosses over to a power law $(1/n)$ for $W = 0$. This crossover is characterized by a scaling function with the single scale $1/\lambda$. We can sharpen this picture in the form of the following two hypotheses:

(1) There exists a nontrivial function, $f(x)$, which is the limit of $(-1)^n nC(n)$ as $n \to \infty$ and $W \to 0$ holding $x = n\lambda$ fixed.

(2) The limit as $n \to \infty$ of $(-1)^n C(n) \exp(\lambda n)$ exists and is nonvanishing.

The simulation does not rule out the possibility that the true asymptotic behavior of the VCF for $0 < W < W$ is quasiexponential as permitted by the rigorous theory.[1] However, it is clear from the data that a quasiexponential component to the VCF must either have a small prefactor or an exponent [λ of Eq. (1)] close to one. It is curious that quasiexponential decay has been found in other similar billiard models.[4,8]

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APPENDIX

In this appendix we estimate the value of the prefactor C in the scaling function, Eq. (11). The method used is very similar to that employed in Ref. 3. Let $C^*(n)$ correspond to the contribution of the VCF from collision sequences which remain near a single vertex. For large n, $C^*(n)$ and $C(n)$

are presumed to be equal. We can write $C^*(n)$ as an integral over phase space

$$C^*(n) = (3/2\pi) \fint \cos\theta_0 \, d\theta_0 \, d\alpha_0 \, (-1)^n \cos[(\theta_n - \alpha_n) - (-1)^n(\theta_0 - \alpha_0)] \tag{A1}$$

In this expression the slash through the integral sign indicates that the integration is over the portion of phase space for which the sequence of collisions from 0 to n remains in a single vertex. We evaluate this integral for small W and large n and use the linear approximation, Eq. (4), to find α_n and θ_n. The integral (A1) is most easily carried out in terms of the normal coordinates, $q_n^{(+)}$ and $q_n^{(-)}$ of the linear map,

$$q_n^{(\pm)} = (1/2)[\alpha_n \pm (W/(W+2))^{1/2} \theta_n] \tag{A2}$$

Using the fact that $q_n^{(-)}$ decays exponentially in n for large n [see Eq. (5)] and that $\lambda = (2W)^{1/2}$ for small W we can write (A1) in the form

$$C^*(n) \sim (-1)^n (6/\pi\lambda) \fint dq_0^{(+)} \, dq_0^{(-)} \cos[(2/\lambda)(q_0^{(+)} - q_0^{(-)})]$$

$$\times \cos[(2/\lambda) \, q_n^{(+)} - (-1)^n (2/\lambda)(q_0^{(+)} - q_0^{(-)})] \tag{A3}$$

The integral can be further simplified by taking advantage of time reversal and reflection symmetry which allows us to restrict the region of integration to

$$0 < q_n^{(+)} < q_0^{(-)} \tag{A4}$$

if the integral is then multiplied by a factor of 8. This restriction automatically ensures that the sequence of collisions remains near a single vertex. Since $q_n^{(+)}$ grows exponentially, the inequality (A4) restricts $q_0^{(+)}$ to be much smaller than $q_0^{(-)}$ and, through (A2), yields

$$q_0^{(-)} = -2\theta_0/\lambda \tag{A5}$$

in the limit of $W \to 0$ and $n \to \infty$. Since $\theta_0 > -\pi/2$ we can now write $C^*(n)$ in the form of a definite integral

$$C^*(n) \sim (-1)^n (12/\pi) \, \lambda e^{-n\lambda} \int_0^{\pi/2} dx \int_0^x dy \cos^2(x) \cos(y) \tag{A6}$$

where we have made the change of variables $x = 2q_0^{(-)}/\lambda$ and $y = 2q_0^{(+)}e^{n\lambda}/\lambda$. This integral is easily evaluated, with the result that

$$C^*(n) \sim (-1)^n (4/\pi)\, \lambda e^{-n\lambda} \tag{A7}$$

Comparing Eq. (A7) to Eq. (11) we see that

$$C = 4/\pi \tag{A8}$$

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