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Diffusion in a Periodic Lorentz Gas

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Self-diffusion in a Lorentz gas on a triangular lattice is studied both analytically and numerically. A simple estimate for the diffusion coefficient, based on the idea of a random walk between traps, is found to be in good agreement with the numerical results.

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This Letter presents a quantitative study of the self-diffusion process in a simple dynamical system. The system in question is a Lorentz gas consisting of a single point particle moving in a triangular array of immobile disk scatterers. The point particle moves with constant velocity between elastic collisions with the disks. We take the speed of the particle and the radius of the disks to be 1 while the lattice spacing is $2+W$. The geometry is shown in Fig. 1. The separation parameter, W, completely determines the behavior of the system. At close packing, when $W=0$, the moving particle is trapped in a single triangular region formed between three disks. When $0<W<4/\sqrt{3}-2=0.3094$ the particle can wander over the entire plane but can never move further than the distance $2\sqrt{3}$ before suffering a collision. For $W>4/\sqrt{3}-2$ the particle sees an infinite horizon and may move arbitrarily far between collisions. In this paper we will study the high-density regime, defined by $0<W<4/\sqrt{3}-2$.

Bunimovich and Sinai[1,2] have obtained rigorous results for the high-density regime of this regular Lorentz model which show that it has strong ergodic properties. One of their results[2] is that the autocorrelation function of the velocity of the moving particle decays exponentially with the number of collisions. Since the time between collisions is bounded by $2\sqrt{3}$ it follows that the velocity correlation function (VCF) as a function of time is integrable and that the self-diffusion coefficient, D, exists.

In this Letter we are primarily interested in finding the dependence of D on the lattice spacing, or, equivalently, on W. First we will give a simple analytical estimate of $D(W)$ and then present the results of a numerical simulation of the model. The simple estimate is in surprising agreement with the numerical results over the entire high-density regime.

The simple analytical estimate is based on the idea that, at high densities, the exact motion of the particle can be replaced by a random walk

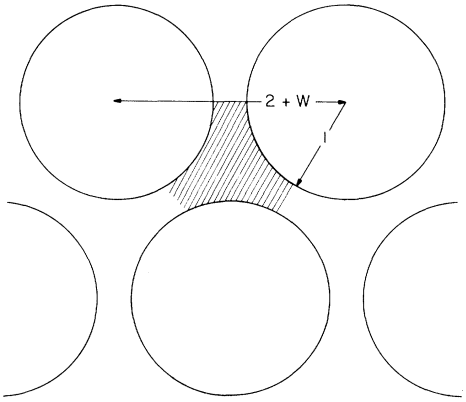

FIG. 1. The geometry of the scatterers in the periodic Lorentz gas. The cross-hatching indicates a single triangular trapping region.

between triangular trapping regions. A single such trapping region is shown by cross-hatching in Fig. 1. The assumption implicit in this estimate is that the sequence of traps visited is a Markov process. This assumption should become accurate for small W when the particle usually bounces a large number of times in each trap.

One corollary of the work of Bunimovich and Sinai is that the motion of the particle in the high-density periodic Lorentz gas is ergodic. This fact allows us to calculate exactly the average residence time, τ, in a trapping region. The average rate, τ^{-1}, at which a particle leaves a given trap is determined by the fraction of phase space available for exiting from the trap. The total volume of phase space associated with a single trap is simply $2\pi A$ where A is the area of the trap. (The factor 2π is the measure of the velocity space.) The portion of this phase space from which a particle escapes from the trap in a time less than Δt has a volume $6W\Delta t$ since $3W$ is the total length of the three exits of the trap. The average rate for leaving a trap is thus

$$\tau^{-1} = 3W/\pi A . \tag{1}$$

Expressing the trap area A in terms of W, we obtain

$$A = \tfrac{1}{4}\sqrt{3}\,(2+W)^2 - \tfrac{1}{2}\pi \tag{2}$$

so that

$$\tau = (\pi/6W)[\tfrac{1}{2}\sqrt{3}\,(2+W)^2 - \pi] . \tag{3}$$

This value for τ is exact for all $W > 0$.

From the average trapping time τ we can obtain an estimate of the diffusion coefficient, $D(W)$, by treating the trajectory of the particle as a random walk between traps. In this approximation we suppose that each jump between traps is independent of the previous jumps. For random walks on two-dimensional isotropic lattices it is well known that

$$D = l^2/4\tau , \tag{4}$$

where l, the distance between traps, is given by

$$l = (2+W)/\sqrt{3} . \tag{5}$$

Combining Eqs. (3)–(5) we obtain the random-walk approximation to the diffusion coefficient:

$$D_{\mathrm{rw}}(W) = (W/\pi)(2+W)^2[\sqrt{3}\,(2+W)^2 - 2\pi]^{-1} . \tag{6}$$

Equation (6) can also be found by a method discussed by Zwanzig[3] in connection with the continuous-time random walk of a system between cells in configuration space. In effect, it comes from an "Eyring-like" approximation to the transition rate between cells.

The only assumption used in the derivation of Eq. (6) is that jumps between trapping regions are uncorrelated with one another. Because of the strong mixing properties of scattering from surfaces of negative curvature, this assumption should hold so long as the moving particle collides several times in each trap before moving to the next trap. Thus the expected number of collisions, η, per trap residence time τ is the appropriate parameter determining the validity of the uncorrelated random-walk estimate. The average time between collisions, τ_c, can be calculated exactly in the same way as τ by replacing the length of the trap ports which appeared in the calculation of τ by the length of the walls of the trap, which is π. The result is that

$$\tau_c = \tfrac{1}{4}\sqrt{3}\,(2+W)^2 - \tfrac{1}{2}\pi \tag{7}$$

and that

$$\eta = \tau/\tau_c = \pi/3W . \tag{8}$$

In terms of η, the high-density regime is defined by

$$3.4 < \eta < \infty . \tag{9}$$

Thus we have reason to hope that the random-walk approximation will be accurate throughout the high-density regime.

We have performed computer experiments on the regular Lorentz gas to determine the VCF and its integral, the diffusion coefficient. The computer program, written in single-precision FORTRAN, initializes a single particle with a random position on the perimeter of a scatterer and a random outward velocity. It then generates the trajectory starting from that initial condition and compiles the statistics required to compute the VCF at 200 time points. After 100 000 collisions the VCF and its numerical integral are computed. This procedure was repeated five times for five different values of W and once for four other values of W including $W = 0$. Each run consumed approximately 6 min of CPU time on the University of Maryland Univac 1100/80.

The VCF for $W = 0.0$, 0.1, and 0.2 is shown in Figs. 2(a)–2(c). Table I gives the value of the diffusion coefficient obtained by numerical integration of the VCF. In each case the VCF was measured at time intervals of 0.025 and integrated out to a time of 50. Figure 3 records the

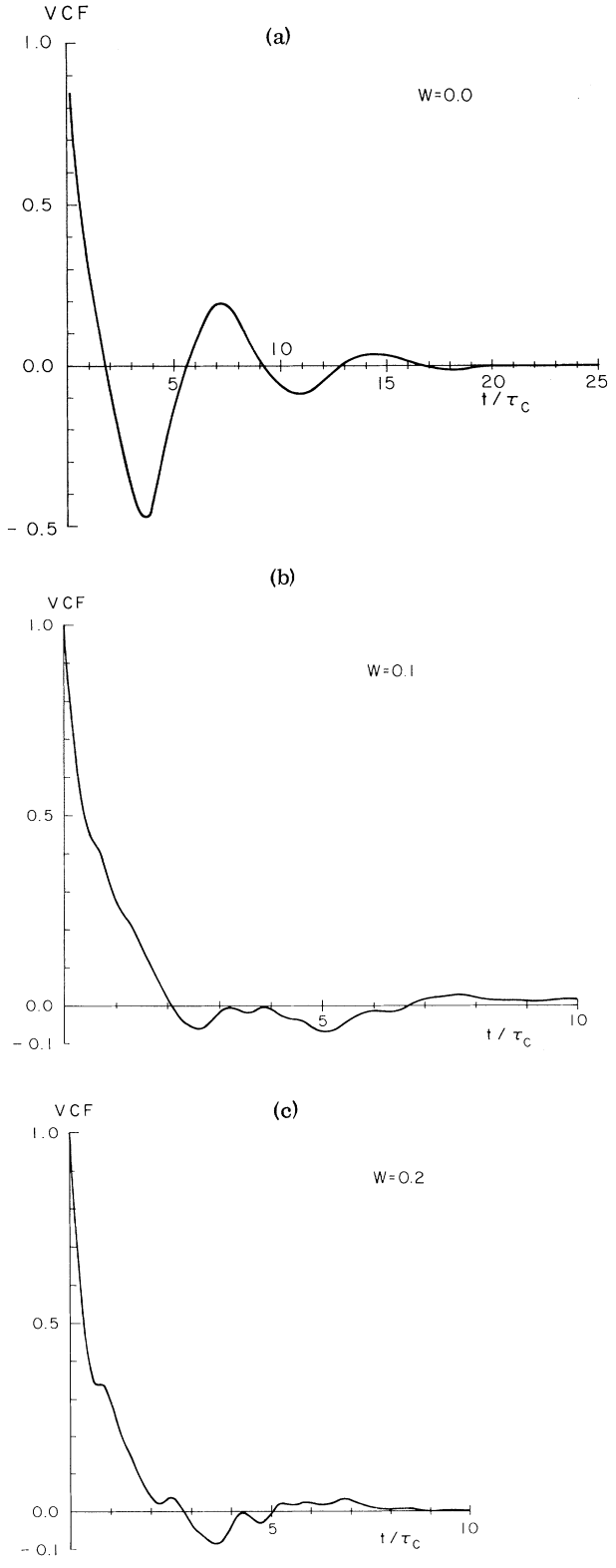

FIG. 2. The VCF for (a) $W = 0.0$, (b) $W = 0.1$, and (c) $W = 0.2$. The horizontal axis is measured in collision times.

TABLE I. The diffusion coefficient as a function of W as determined from the random-walk estimate, $D_{rw}(W)$, and the computer experiment, $D_{expt}(W)$. The expected number of collisions per visit to a trap is η.

W	η	$D_{rw}(W)$	$D_{expt}(W)$
0.0	∞	0	0.0004
0.002	520	0.00387	0.0036 ± 0.0003
0.01	100	0.0180	0.017 ± 0.002
0.04	26	0.0573	0.052 ± 0.002
0.06	17	0.0760	0.069
0.1	10	0.104	0.10 ± 0.01
0.15	7.0	0.128	0.14
0.2	5.2	0.147	0.18
0.3	3.5	0.175	0.25 ± 0.01

information in Table I on a logarithmic scale and demonstrates that the theoretical estimate agrees with the numerical result rather closely over 2 orders of magnitude.

The error bars in Table I and Fig. 3 represent the spread in the values obtained in the five runs at the given values of W. We attribute this spread to averaging the VCF over a finite number of collisions (100 000) for each run and consider this to be the primary source of error in the numerical work. The error bars in the graphs of the VCF itself [Figs. 2(a)–2(c)] are slightly larger than the width of the line.

Figure 3 and Table I demonstrate that the random-walk estimate for the diffusion coefficient is in good agreement with the computer re-

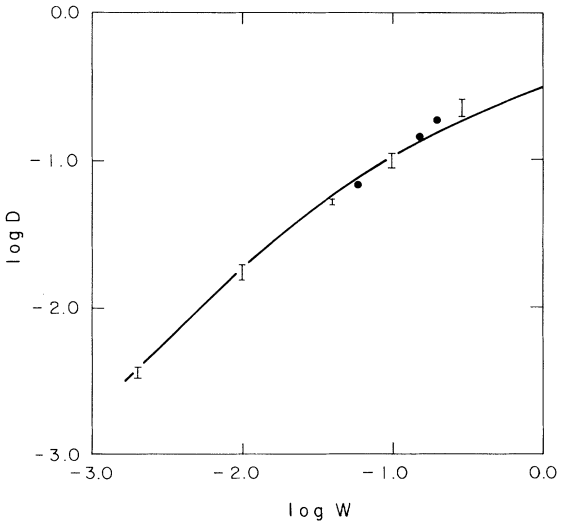

FIG. 3. The logarithm of the diffusion coefficient vs the logarithm of W. The solid line is $\log D_{rw}(W)$ and the points are $\log D_{expt}(W)$.

sults throughout the high-density regime of the periodic Lorentz gas. At the lowest two densities explored ($W = 0.2$ and $W = 0.3$) the random-walk approximation begins to underestimate the diffusion coefficient significantly. The reason for this is that, at low densities, it is possible for the moving particle to traverse a triangular trapping region without collision. On the other hand, at the highest densities explored, the random-walk estimate falls within the error bars of the computed diffusion coefficient. We conjecture that the random-walk estimate is asymptotically exact in the sense that

$$\lim_{W\to 0} \frac{D(W)}{W} = \lim_{W\to 0} \frac{D_{rw}(W)}{W} = \frac{2}{\pi(2\sqrt{3}-\pi)}, \qquad (10)$$

where $D(W)$ is the true diffusion coefficient and the number on the right-hand side of the equation is the leading coefficient in a power-series expansion of $D_{rw}(W)$.

While the random-walk approximation gives a good account of the integral of the velocity autocorrelation function we do not have any similar explanation for the rich structure of the VCF itself. It is surprising that such a simple model should exhibit such a complex VCF.

The crucial feature of the periodic Lorentz gas which allows us to map the dynamical system accurately onto a stochastic model is the fact that the trajectories are strongly mixed within each trapping region in configuration space. For this mixing to occur the traps must have the following two attributes. Firstly, their ports must be small compared to their total perimeters, and secondly, their perimeters must have convex regions from which nearby trajectories can be dispersed. A model in which the first but not the second criterion is satisfied is discussed elsewhere.[4] On the other hand, the periodicity of the Lorentz model studied here does not enter in an important way into the random-walk analysis; thus the same approximation scheme may be applicable to disordered Lorentz gases at high densities.

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