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Long-time tail of the velocity-autocorrelation function in the Lorentz lattice gas

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We present numerical results for the first and second moments of the distribution of collision times of the $d=2$ Lorentz lattice gas with density q in the range 0.2–0.8. They are used to calculate the mean-square displacement $\langle X^2(T_k)\rangle$ as a function of the number of collisions k. Using an asymptotic relation the mean-square displacement $\langle X^2(t)\rangle$ as function of time is obtained from the latter quantity. As a result we are able to predict in an accurate numerical way the long-time tail of the velocity-autocorrelation function.

I. INTRODUCTION

The discovery of the algebraic decay of the *velocity-autocorrelation function* (VACF) in hard-sphere models[1] encouraged many scientists to construct even simpler fluid models.[2–5] The study of these models is motivated by the importance of the *long-time tail* of the VACF in transport theory. By means of the Green-Kubo formula it contributes to the diffusion constant and, in particular, when the decay is slower than t^{-1}, the diffusion coefficient diverges.[2]

Analytical and numerical results for the VACF are hard to obtain. One class of very simple models that has been studied intensively is the class of Lorentz gas models.[2–4] In these models a particle follows a straight path through a static environment of randomly distributed scatterers. After a collision with one of the scatterers the particle changes its direction according to some probabilistic or deterministic collision rule. It is known that the VACF in these models decays as $t^{-d/2-1}$.[2] Even in this simple model, analytical and numerical results are rare and disagree often.[6–8]

When the movement of the particle and the positions of the scatterers are constrained to lattice sites, then the model is called the Lorentz lattice gas. It is of recent interest[9–14] and is studied in the present paper in dimension $d=2$.

We numerically calculate the mean collision time $\langle\tau_k\rangle$ and the mean-square collision time $\langle\tau_k^2\rangle$, i.e., the first and second moment of the expected time that a particle spends in between the kth and the $(k+1)$st collision (the brackets $\langle\rangle$ denote the configurational average). Both quantities depend on the number of collisions k and exhibit a long-time tail $\sim A+Bk^{-1}+O(k^{-2})$. Next we show how the mean-square displacement $\langle X^2(t)\rangle$ is related to both quantities. It is used to calculate the long-time tail of the VACF.

In Sec. II we introduce the model and the numerical algorithm which we developed to calculate collision times. Section III summarizes the numerical results. In Sec. IV we discuss the relation between the distribution of collision times and the mean-square displacement. In Sec. V the VACF is discussed.

II. MODEL AND METHOD

We study the Lorentz lattice gas on a square lattice with N lattice sites and with a Bernoulli distribution of scatterers with density q (i.e., every lattice site is with probability q a scatterer, independent of the other lattice sites). A mobile particle starts at a randomly selected lattice site (this choice corresponds to the equilibrium distribution of the Lorentz lattice gas). It follows a straight trajectory in an arbitrary direction, at a speed of one step per time unit, until it meets one of the scatterers. Then it selects one of the $2d$ possible directions, with equal probability, and continues its linear motion up to the next scatterer. A somewhat more general model with different probabilities α for transmission, β for reflection, and γ for deflection in an orthogonal direction is studied in the literature.[14] For simplicity we restrict ourselves to the case of $\alpha=\beta=\gamma=\frac{1}{4}$.

The position of the mobile particle at time t (relative to its starting point which for simplicity is assumed to be the origin of the lattice) is denoted $X(t)$. The time a particle spends in between the kth and the $(k+1)$st scatterer is denoted τ_k. Averaging τ_k and τ_k^2 over all possible trajectories, all starting positions of one given configuration, and all possible configurations of scatterers leads to the first and second moment of the collision time. The averages $\langle\tau_k\rangle$ and $\langle\tau_k^2\rangle$ can be calculated very accurately.

In our numerical calculations we use the same algorithm as before in our study of what is called the *black and white* model.[15] Between two collisions the particle of the latter model moves as a random walker. In the Lorentz lattice gas the particle moves straight on in a deterministic way.

The algorithm to calculate $\langle\tau_k\rangle$ is based on the following observation:

$$\langle\tau_k\rangle = N^2\langle p_i^{(1)} p_i^{(k)}\rangle , \tag{1}$$

where $p_i^{(k)}$ is the probability that scatterer i is the kth scatterer visited by the particle (the average is over all scatterers). We prove (1) by means of the identity

$$\langle\tau_k\rangle = \sum_i s_i p_i^{(k)} , \tag{2}$$

TABLE I. Mean collision time $\langle \tau_k \rangle$; fit with formula (5a) and (5b) for densities $q = 0.2$–0.8. σ is the rms error of the fit.

q	Number of configurations	Size	A'	σ	α'	β'	σ
0.8	100	200	0.0568	1.6×10^{-7}	0.0567	0.002	1.4×10^{-7}
0.7	100	200	0.0816	6×10^{-8}	0.0816	0.000	6×10^{-8}
0.6	50	300	0.105	8×10^{-7}	0.103	0.150	1.5×10^{-7}
0.5	33	350	0.127	1.9×10^{-6}	0.122	0.339	1.6×10^{-7}
0.4	50	400	0.148	1.4×10^{-6}	0.144	0.260	5×10^{-8}
0.3	50	460	0.172	2.5×10^{-6}	0.166	0.399	3×10^{-7}
0.2	33	560	0.187	4×10^{-6}	0.176	0.700	3×10^{-7}

where s_i is the average time the particle, when started at scatterer i, uses to reach the next scatterer. Since in the Lorentz lattice gas s_i and $Np_i^{(1)}$ are both identical to the distance between scatterer i and the next one (averaged over the $2d$ possible scatterers), (1) follows immediately.

We calculate the $p_i^{(k)}$'s by iteration of the master equation

$$p_i^{(k)} = \sum_j p_j^{(k-1)} P_{ji} , \tag{3}$$

where P_{ij} is the probability that scatterer j is the first scatterer visited by the particle, when started at scatterer i. The initial densities $p_i^{(1)}$ and the matrix P can be calculated iteratively in a way comparable to the exact enumeration method of Havlin *et al.*[16]

The mean-square collision times $\langle \tau_k^2 \rangle$ are calculated in a similar way. The basic formula is

$$\langle \tau_k^2 \rangle = \frac{1}{2d} \sum_{i,\alpha} s_{i,\alpha}^2 p_i^{(k)} . \tag{4}$$

Here, $s_{i,\alpha}$ is the distance between scatterer i and its neighbor in the direction α.

For details of the algorithm we refer to a forthcoming publication. The advantage of the algorithm compared to direct simulation is the automatic average over all trajectories and all starting positions of the given configuration. Because of the linear motion of the particle between the scatterers, the algorithm is highly vectorizable. As a consequence the present results are even more accurate than those for the black and white model.

III. RESULTS

We investigated configurations of the square lattice for densities q in the range 0.2–0.8, and for times up to between 100 and 200 mean collision times. We use configurations with ± 65000 scatterers which is convenient for the vectorized algorithm on a CYBER 205. With this size system the average trajectory does not cross the periodic boundaries. The results are averaged over as many configurations as needed to get the statistical error below 1%.

The results have been fitted in the asymptotic range $k = 50$–100 with

$$\langle \tau_k \rangle = q^{-1} + A' k^{-1} , \tag{5a}$$

as well as

$$\langle \tau_k \rangle = q^{-1} + \alpha' k^{-1} + \beta' k^{-2} . \tag{5b}$$

At low densities the two-parameter fit is significantly better than the one-parameter fit: the rms error σ of the former is about ten times smaller. See Table I. Similar remarks hold for $\langle \tau_k^2 \rangle$. See Table II. The fitting formulas are

$$\langle \tau_k^2 \rangle = (2-q) q^{-2} + A'' k^{-1} , \tag{6a}$$

$$\langle \tau_k^2 \rangle = (2-q) q^{-2} + \alpha'' k^{-1} + \beta'' k^{-2} . \tag{6b}$$

IV. MEAN-SQUARE DISPLACEMENT

We start by deriving relations between collision times and total time and between collision times and mean-square displacement, respectively, First, observe that the total time T_k that a particle spends between the start and the kth visit to a scatterer satisfies

$$\langle T_k \rangle = \sum_{l=0}^{k-1} \langle \tau_l \rangle . \tag{7}$$

Indeed, one has $\tau_l = T_{l+1} - T_l$. The mean-square dis-

TABLE II. Mean-square collision time $\langle \tau_k^2 \rangle$; fit with formula (6a) and (6b).

q	Number of configurations	Size	A''	σ	α''	β''	σ
0.8	100	200	0.225	1.3×10^{-6}	0.228	−0.2	4.0×10^{-7}
0.7	100	200	0.368	6.3×10^{-7}	0.367	0.05	4.7×10^{-7}
0.6	50	300	0.592	5.8×10^{-7}	0.592	0.0	5.8×10^{-7}
0.5	33	350	0.869	3.3×10^{-6}	0.876	−0.5	6.8×10^{-7}
0.4	50	400	1.31	7.1×10^{-6}	1.29	1.2	1.7×10^{-6}
0.3	50	460	2.02	1.4×10^{-5}	1.98	2.5	1.2×10^{-6}
0.2	33	560	3.27	6.6×10^{-5}	3.10	12	5.6×10^{-6}

placement at the time of the kth collision equals

$$\langle X^2(T_k)\rangle = \left\langle \sum_n n^2 p_n(T_k) \right\rangle ,$$

where $p_n(t)$ is the probability that the particle is at site n at time t. A standard calculation leads to the result

$$\langle X^2(T_k)\rangle = \langle X^2(T_{k-1})\rangle + \langle \tau_{k-1}^2\rangle + 2\sum_n n\langle p_n(T_{k-1}) q_n\rangle , \tag{8}$$

where q_n is the local anisotropy of the distribution of scatterers

$$q_n = (1/2d)\sum_m (m-n) ,$$

with the latter summation restricted to the $2d$ scatterers m which can be reached by the particle from site n.

At intermediate densities the anisotropic contribution to $\langle X^2(T_k)\rangle$ is very small, e.g., at $q = \frac{1}{2}$ and $k \geq 4$ a numerical estimate gives absolute values smaller than 0.01 with an error of 0.02. It could possibly become important at low densities, but we did not investigate this point. We neglect it in what follows, and use the relation

$$\langle X^2(T_k)\rangle = \sum_{l=0}^{k-1} \langle \tau_l^2\rangle . \tag{9}$$

In the Boltzmann approximation the trajectory of the particle is described as a sequence of uncorrelated paths between successive collisions. In this approximation we replace $\langle \tau_k\rangle$ and $\langle \tau_k^2\rangle$ by the values q^{-1} and $(2-q)q^{-2}$, respectively. Hence one has $k = q\langle T_k\rangle$. One concludes that $\langle X^2(T_k)\rangle \simeq k(2-q)q^{-2}$. A first estimate of the diffusion constant D is then

$$D \simeq \frac{1}{2d}\frac{\langle \tau_k^2\rangle}{\langle \tau_k\rangle} \simeq \frac{2-q}{2dq}$$

(here d is the dimension of the lattice). The latter expression has been called the Boltzmann value D_B of the diffusion constant.[14]

The correct value of the diffusion constant at intermediate densities is[14]

$$D = \frac{3-q}{4dq} \tag{10}$$

[the result is not exact, the low-density result is $D = (3-2q)/4dq$]. Hence the following asymptotic relation holds

$$\langle X^2(t)\rangle - \frac{t}{q} = \frac{1}{2}\left[\langle X^2(T_k)\rangle - \frac{k}{q^2}\right] + o(t) , \tag{11}$$

where the number of collisions k has to be taken so that the relation $\langle T_k\rangle = t$ holds. Apparently, the correlation effect (due to the fluctuations in the distribution of collision times, making $\langle \tau_k^2\rangle \neq \langle \tau_k\rangle^2$) is twice as large for $\langle X^2(T_k)\rangle$ as it is for $\langle X^2(t)\rangle$. We did not succeed in quantifying the leading-order corrections to Eq. (11). They are important in the calculation of the VACF and hence the results derived below should be considered with care since a potentially important correction term is not taken into account.

From (9) and (11) one obtains

$$\frac{\partial}{\partial t}\langle X^2(t)\rangle = \frac{1}{q} + \frac{1}{2}\frac{(\partial/\partial k)\langle X^2(T_k)\rangle - q^{-2}}{(\partial/\partial k)\langle T_k\rangle} \simeq \frac{1}{q} + \frac{1}{2}\frac{\langle \tau_k^2\rangle - q^2}{\langle \tau_k\rangle} , \tag{12}$$

where again the number of collisions k has to be taken such that $\langle T_k\rangle = t$.

V. THE VACF

Using the expressions (5b), (6b), and (7), and the asymptotic relation $t \simeq q^{-1}k + a' \ln k + O(1)$ there follows from (12) that

$$\frac{\partial}{\partial t}\langle X^2(t)\rangle = \frac{3-q}{2q} + \frac{1}{2q}[qa'' - (1-q)a']\frac{1}{t}\left[1 + qa'\frac{1}{t}\ln t + O\left(\frac{1}{t}\right)\right] .$$

From transport theory one has

$$\langle v(0)v(t)\rangle = \frac{1}{2}\frac{\partial^2}{\partial t^2}\langle X^2(t)\rangle .$$

Hence we obtain

$$\langle v(0)v(t)\rangle = -\frac{\gamma}{t^2} - \delta\frac{\ln t}{t^3} - O(t^{-3}) , \tag{13}$$

where $\gamma = [qa'' - (1-q)a']/4q$ and $\delta = 2qa'\gamma$. See Table III for numerical values of γ and δ. Note that at $t \sim 100$ the correction in $\ln t/t^3$ is about 0.5% of the leading-order term. We can calculate the contribution in t^{-3} as well. But these corrections are meaningless in view of our ignorance about the leading-order corrections to (11).

Direct numerical calculations[17] of the VACF show a pronounced even-odd effect: the absolute value of the correlation $\langle v(0)v(t)\rangle$ is much lower when t is even. At odd times the results of Ref. 17 for the coefficient γ coincide with ours (at densities $q = 0.6$ and $q = 0.8$ for which the results were available). We suspect that the even-odd effect is due to the anisotropic contribution which we discussed in the previous section. Indeed, consider the average anisotropy $\sum_n \langle p_n(t) q_n\rangle$, where now $p_n(t)$ is the probability that the particle is at site n, and q_n is zero if no

TABLE III. The VACF as a function of density; numerical results for the coefficients γ and δ of formula (13).

q	γ	δ
0.8	0.0535	0.0049
0.7	0.0830	0.0095
0.6	0.131	0.0162
0.5	0.189	0.0230
0.4	0.269	0.0309
0.3	0.398	0.0397
0.2	0.599	0.0422

scatterer is present at site n. We find again (by extensive numerical computation) that the average anisotropy is small, e.g., at $q=0.5$ and $t=50$ it is in absolute value of the order of 0.0015, with a large error bar. However, the sign is alternating, positive for even and negative for odd times. As a consequence, the contribution survives the double time derivative relating the VACF to the mean-square displacement. We do not know why the oscillating contribution affects only the VACF at even times. It is large compared with the value of the VACF itself, which for the given values of q and t is less than 0.0001 (as computed using the data from Table III).

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