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Abnormal Diffusion in Wind-tree Lattice Gases

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Abstract. It is found numerically that a two-dimensional left-turning particle-scatterer system does not diffuse for scatterer densities slightly above one-half, or greater. For smaller densities, the diffusion coefficient is much lower than what the Boltzmann approximation predicts; this is caused by orbiting events.

An isotropic-scattering model with reflective impurities also shows deviations from the diffusion equation for various densities of isotropic and reflective scatterers, caused by retracing events.

1. Introduction

Hardy, de Pazzis and Pomeau first attempted to model fluids with cellular automata over ten years ago [1]. In the past two years we have seen a major revival of this approach [2–4]. Much effort has been spent in studying the viscosity coefficient in order to find its size dependence in two dimensions [5] or to simulate the highest possible Reynolds number [6,7]. The study of diffusion in such systems has been limited [8–11], probably because of the lack of particle identity in these models. The first study of diffusion in cellular automata models was probably that of Gates [12], in which he proved the non-existence of diffusion in certain lattice wind-tree models at high density of scatterers. The continuum wind-tree model is a four-velocity particle (wind) and square scatterers (trees) system introduced by the Ehrenfests [13] to illustrate the approach of a probability distribution to equilibrium. Along with a similar model with circular scatterers studied by Lorentz [14], the Ehrenfests's model has been very useful in identifying high-density phenomena in fluids [15]. Gates introduced five deterministic models, only one of which had point scatterers (henceforth model V). The other four were area-occupying models with different potentials between scatterers. The first simulations of lattice particle-scatterer systems [16] showed low-density diffusive behavior in a non-chiral version of Gates's model V, which will be described in the next section. Theoretical expressions for the diffusion coefficient have been obtained [17] for the analogous stochastic models, showing excellent agreement with simulations [16,18,19]. An interesting case is that of stochastic isotropic scattering. The possibility of reflection brings in a contribution from retracing trajectories which modifies directly the Boltzmann level (uncorrelated scatterers) solution. Simulations and an effective medium approximation theory show excellent agreement in this case [20]. In the present paper we go a step further, and explore high-density phenomena in lattice gases which not only reduce the diffusion coefficient, but cause it to vanish altogether. This paper proceeds as follows: in section 2 we study analytically and numerically model V of Gates. We find numerically that the threshold for abnormal diffusion is much lower than what has been proved, and that even when diffusion exists the Boltzmann level theory is inadequate. In section 3 we present numerical calculations of the mean-squared displacement ($\langle r^2 \rangle$) for a lattice particle-scatterer model where a few scatterers are purely reflective. Einstein's studies of Brownian motion [21] predict linear growth of $\langle r^2 \rangle$ for long times. For certain concentrations of scatterers this model shows abnormal diffusion (id est, slower-than-linear growth of $\langle r^2 \rangle$). All the models in this paper are formulated in the square lattice. For a study of diffusion — characterized by a second-rank tensor — the symmetry of this lattice is adequate [22]. Finally, in section 4 we discuss the results of this paper, comment on previous theoretical work, and propose deterministic particle-point scatterer systems that should also exhibit abnormal diffusion.

2. Theory and simulations for a left-turning model

Of the five models proposed by Gates, only model V consists of point particles and scatterers, in the spirit of lattice gas automata. This model is defined as follows: a particle moves from node to node at integer time steps on the square lattice. If it does not encounter a scatterer (placed randomly at the nodes with probability c), it continues along a straight line. If it encounters one, it turns left. This type of ballistic or Newtonian model is very different in spirit from a standard random walk. Gates was able to prove that for $z > 2^{16} - 1$ the system does not behave diffusively. The fugacity z is related to the density of scatterers by $c = z(1+z)^{-1}$. Therefore, the proof applies to very high densities, $c > 1 - 2^{-16}$. Simulations at such high densities are difficult to achieve. A thought-experiment for $c = 1$ is easy to perform: the particle necessarily gets locked in length-four trajectories, and indeed does not behave diffusively. The relevant questions one can ask are (1) for what range of the density of scatterers is the Boltzmann approximation of uncorrelated scatterers valid? (2) Is Gates's proof of abnormal diffusion extremely conservative?

For this model the Liouville equation for the probability of a particle being at node n with velocity i at time t, $p(n, e_i, t)$ is given by

$$p(n, e_i, t+1) = cp(n - e_{i-1}, e_{i-1}, t) + (1-c)p(n - e_i, e_i, t)$$

Density	D(Boltzmann)	D(Simulations)
0.1	4.75	2.18
0.2	2.25	1.01
0.5	0.75	0.205

Table 1: Density, Boltzmann-level and simulational value of the diffusion coefficient for left-turning model. Notice the deviations from the Boltzmann approximation even at low densities.

Here the e_i are unit vectors in the four directions i, which are labeled cyclically. The relevant eigenvalue of the collision operator is -1, which yields, according to the methods of [17],

$$D(c) = (2c)^{-1} - (4)^{-1}$$

We have measured the mean-squared displacement versus time for several values of scatterer density for this model. The averages have been calculated over 10^3 configurations for each value of the density. Table 1 shows the Boltzmann-level theoretical result and the simulational result for the diffusion coefficient. We see that even at very low densities the Boltzmann value is significantly higher than the simulations (which have error bars of about 10 percent). Orbiting trajectories (limit cycles) are the only possible high-density phenomenon that can account for the deviation from the Boltzmann approximation in this model.

For higher densities, we have performed a binary-tree search of the value of the density at which the system ceases to diffuse normally. This value appears to be $2^{-1} < c < 2^{-1} + 2^{-5}$, which is much lower than what Gates expected as a lower bound for diffusion.

3. Stochastic models with abnormal diffusion

Consider a two-dimensional square lattice with scatterers placed randomly at the nodes. There are two kinds of scatterers: type (1) causes a colliding particle to scatter randomly with equal probability in any of the four allowed directions. As discussed in [17,20] this model has a much lower diffusion coefficient than what the Boltzmann approximation predicts. In order to have an even more important contribution from what Hauge and Cohen [15] call retracing events, we need scatterer type (2), which reflects back the moving particle no matter which direction it comes from. As in the previous section, a particle will not change velocity as long as it does not encounter a scatterer. The reflecting scatterers model overlapping trees (reflector configurations) which are the ones that cause the diffusion coefficient to vanish in the continuum wind-tree model [15].

We have performed simulations for various densities of both types of scatterers. For each combination of densities, 30000 independent configurations were used in calculating the average mean-squared displacement ($\langle r^2 \rangle$). For long enough times, typically $400 < t < 1000$, a $\log(< r^2 >)$ vs $\log t$ plot

Density (1)+(2)	Fraction of (2)	Exponent a
0.10	0.20	0.9
0.25	0.20	0.8
0.40	0.20	0.9
0.50	0.20	0.9
0.25	0.10	1.0
0.25	0.20	0.8
0.25	0.30	0.85
0.25	0.40	0.9

Table 2: Total concentration of scatterers, fraction of reflective scatterers and algebraic exponent for the mean-squared displacement.

yields an exponent of algebraic growth, $\langle r^2 \rangle \sim t^a$. Table 2 shows the total density of scatterer types (1) plus (2) ($c = c_1 + c_2$) in column 1, the fraction of type (2) (c_2/c) in column 2 and the exponent a defined above in column 3. With an estimated uncertainty of 5%, we show clearly abnormal diffusion for several concentration values in this model.

According to Einstein's equation, the quantity $\langle r^2 \rangle / t$ should monotonically increase to a constant value for long times. Figure 1 is a plot of this quantity versus time for $c_1 + c_2 = 0.25$, $c_2/c = 0.20$. This provides further evidence for abnormal diffusion.

4. Conclusions

We have measured the mean squared displacement for two particle-scatterer lattice models. In a left-turning model there is no diffusion for a density of scatterers $c > 1/2$. The only theoretical lower bound for abnormal diffusion so far was calculated by Gates, $c = 1 - 2^{-16}$. We calculate the diffusion coefficient in the Boltzmann approximation. Simulational values are much lower than theoretical ones, even at low densities. For the first time we see orbiting events [15] affecting the diffusion process.

In stochastic particle-scatterer systems the possibility of retracing trajectories is known to lower [20] the diffusion coefficient obtained by the Boltzmann approximation. The inclusion of purely reflective impurities disrupts the diffusion process completely. Numerical values of the algebraic exponent of growth for the mean-squared displacement are reported in this paper.

In Gates's left-turning model the fact that the particle always turns the same way is essential to prove abnormal diffusion. In stochastic and deterministic chiral models [16–20] the orbiting events are not so important. For example, in a deterministic odd time-left deflection, even time-right deflection model, the limit cycle distribution decays roughly as $t^{-4/3}$; furthermore, after 800 time steps no more than 3 percent of all particles have become locked in orbiting events; this does not even contribute to the dominant term of the diffusion coefficient [18].

In the new stochastic models with reflective impurities we find nonlinear

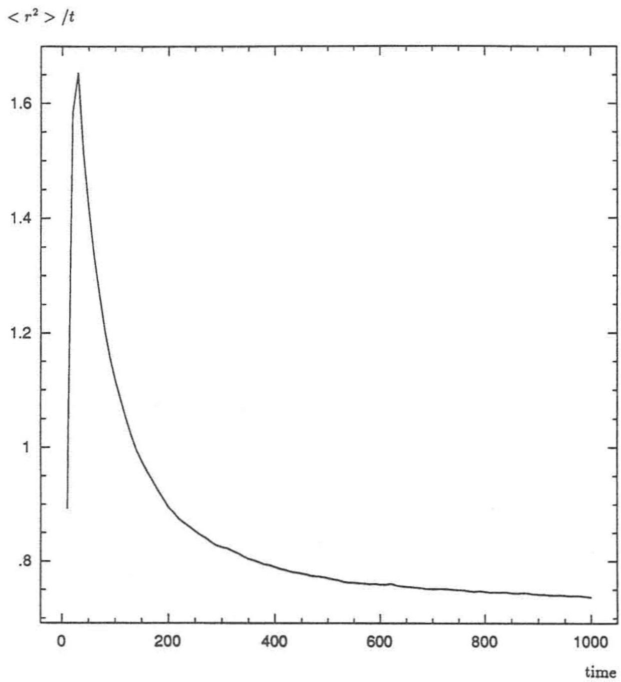

Figure 1: $< r^2 > /t$ vs time for the model in section 3, $c = 0.25$, $c_2/c = 0.2$. Normal diffusion would correspond to a monotonic increase to a constant value.

growth of the mean-squared displacement. The simple theoretical approach of van Beijeren and Hauge [23] predicts an algebraic growth exponent which falls linearly with the concentration of scatterers. This dependence has been corroborated numerically [24]. We do not observe such dependence in the new models. It is unclear whether the method of reference 23 applies in this case.

It is possible to introduce reflectors in deterministic lattice systems. For example, in the "mirror models" of Ruijgrok and Cohen [19] in which scatterers placed at 45 degrees turn $\pm x$ colliding particles to $\pm y$ directions and scatterers placed at 135 degrees turn $\pm x$ colliding particles to $\pm y$ and vice versa, a configuration consisting of a 45-degree and a 135-degree scatterer side-by-side will act as a reflector to particles hitting it with a $+y$ velocity.

We hope that this paper will stimulate theoretical work in the prediction of abnormal diffusion in lattice gas models. Especially, the introduction of reflective scatterers should shed light on the behavior of the model of Boghosian and Levermore [11], in which two particles hitting a node perpendicularly are reflected straight back. We plan in the near future to study numerically deterministic models with straight-back reflectors such as those proposed in reference [25].

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