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1991 J. Phys. A: Math. Gen. 24 L751

(http://iopscience.iop.org/0305-4470/24/13/009)

J. Phys. A: Math. Gen. 24 (1991) L751–L755. Printed in the UK

LETTER TO THE EDITOR

Diffusion coefficient increases with density in a lattice-gas model

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Received 27 March 1991

Abstract. We report computer simulations of the diffusion coefficient in a two-dimensional lattice Lorentz gas with interacting particles. The simulations show that the diffusion coefficient has a maximum as a function of the particle density in models with strongly correlated particle-scatterer collisions.

Unusual behaviour of the diffusion coefficient has been revealed in molecular-dynamics simulations of a hard ellipsoid liquid crystal [1]. One of the two diffusion coefficients in the nematic-liquid-crystal phase increases with density, reaches a maximum and then decreases. In the lattice-gas models of atomic fluids the diffusion coefficient monotonically decreases with density [2–4] and computer simulation data agree very well with the Enskog diffusion coefficient [2]. In this letter we introduce the simplest model—superposition of a lattice Lorentz gas and a cellular automata lattice gas—which describes an increase of the diffusion coefficient. We study density dependence of the diffusion coefficient both by the molecular-dynamics method and analytically within the Boltzmann approximation.

The model consists of particles moving with constant speed on the square lattice in discrete time steps. At every time step particles are only allowed to be situated at lattice sites with velocities specified by the set of nearest-neighbour lattice vectors: $\boldsymbol{e}_1=(1,0)$, $\boldsymbol{e}_2=(0,-1)$, $\boldsymbol{e}_3=(-1,0)$, $\boldsymbol{e}_4=(0,1)$. Two particles cannot occupy the same site with the same velocity. The particles are characterized by density per link $d=M/(4V)$ where M, V are numbers of particles and sites, respectively.

The N fixed scatterers are randomly placed at lattice sites with probability (density of scatterers) $\rho=N/V$. If a particle hits a scatterer its velocity direction changes. The scattering rules are stochastic and characterized by the transition matrix

$$\mathbb{P}=\begin{pmatrix}\alpha & \gamma & \beta & \gamma\\ \gamma & \alpha & \gamma & \beta\\ \beta & \gamma & \alpha & \gamma\\ \gamma & \beta & \gamma & \alpha\end{pmatrix} \tag{1}$$

where α, β and γ are probabilities of transmission, reflection and deflection in an orthogonal direction, respectively. They obey the normalization condition $\alpha+\beta+2\gamma=1$.

0305-4470/91/130751+05$03.50

The dynamics of the system consists of two steps.

(1) *Propagation.* All particles move at one time step: each particle is shifted from initial position $\boldsymbol{r}$ to neighbouring site $\boldsymbol{r}+\boldsymbol{e}_i$ along its velocity direction $\boldsymbol{e}_i$.

(2) *Collision.* Particles at all sites undergo collisions.

(i) *Particle–scatterer collision* as described above when the scatterer is present at a site. If more than one particle hits the same scatterer at the same time then the particles cannot be scattered independently because of the assumption that only one particle can occupy one link. In such a case we choose the following rule: velocities of all particles at the site with a scatterer are simultaneously reflected with probability β, transmitted with probability α and deflected with probability γ.

(ii) *Particle–particle collision* if there is no scatterer at a site occupied by two or more particles. In order to study the diffusion process we consider all particles to be distinguishable. The particle–particle collision rules are stochastic with *equal probabilities* for the output configurations, similarly as in a model for self-diffusion [3]. Two-particle collision rules are presented in figure 1. The post-collision configurations from figure 1(a) are chosen with probability $\frac{1}{4}$ and those from figure 1(b) with probability $\frac{1}{2}$. In the case of three-particle and four-particle collisions the output configurations are obtained from permutations of an input configuration.

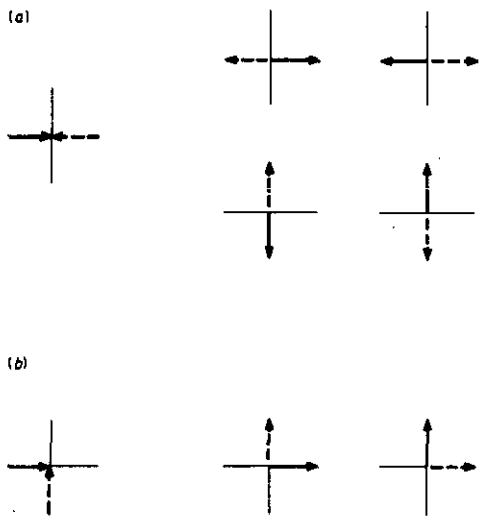

Figure 1. Examples of a two-particle head-on collision (a), right angle collision (b).

We performed simulations on a square lattice of 256×256 sites with periodic boundary conditions. The initial positions and velocities of particles were chosen randomly and stored. At sites with more than one particle (including the scatterer) the post-collision configurations of velocities were chosen randomly at each time step according to the rules. The actual position and velocity of each particle were stored in an additional array in order to keep the identity of particles. During the simulation the velocity autocorrelation function of the particle,

$$\Phi(t)=\langle \boldsymbol{v}(0)\boldsymbol{v}(t)\rangle \tag{2}$$

where $\langle \ldots \rangle$ means average over number of particles and number of configurations of scatterers, was computed. The number of independent configurations of scatterers was greater than 50. The correlations were measured for several hundred time steps and the diffusion coefficient was obtained from the Green–Kubo formula [5] for the two-dimensional case

$$D = \tfrac{1}{4} + \tfrac{1}{2} \sum_{t=1}^{\infty} \Phi(t). \tag{3}$$

The results of simulations are presented in figure 2.

Now we calculate the diffusion coefficient in the Boltzmann approximation, in which the particle–scatterer collisions as well as particle–particle collisions are considered uncorrelated. Let us consider the tagged particle in the sea of 'fluid' particles at equilibrium. Introducing $n_i(\boldsymbol{r}, t)$—the probability of finding the tagged particle at moment t and at site $\boldsymbol{r}$ with velocity $\boldsymbol{e}_i$—the equation of motion can be written in the following form

$$n_i(\boldsymbol{r}+\boldsymbol{e}_i, t+1) = \rho \sum_j P_{ij} n_j(\boldsymbol{r}, t) + (1-\rho) n_i(\boldsymbol{r}, t) + (1-\rho) \sum_j \Omega_{ij} n_j(\boldsymbol{r}, t) \tag{4}$$

where the first term on the right-hand side describes the contribution from the collision of the tagged particle with a scatterer, the second term represents free motion and the last one describes the collision of the tagged particle with the fluid particles. The Ω is a linearized particle–particle collision operator with three independent matrix elements

$$\begin{aligned} \Omega_{11} &= -\tfrac{7}{4} d(1-d)^2 - 2d^2(1-d) - \tfrac{3}{4} d^3 \\ \Omega_{12} &= \tfrac{3}{4} d(1-d)^2 + \tfrac{2}{3} d^2(1-d) + \tfrac{1}{4} d^3 \\ \Omega_{13} &= \tfrac{1}{4} d(1-d)^2 + \tfrac{2}{3} d^2(1-d) + \tfrac{1}{4} d^3. \end{aligned} \tag{5}$$

The matrix Ω has the same form as the matrix $\mathbb{P}$ (see equation (1)). Equation (4) allows us to calculate the velocity autocorrelation function of the tagged particle (1) and then the diffusion coefficient (2). Thus we obtain

$$D_{\mathrm{B}} = \frac{1}{4} \left(\frac{1+\lambda}{1-\lambda} \right) \tag{6}$$

where

$$\lambda = 1 - \rho(1-\alpha+\beta) - (1-\rho)(2d - \tfrac{4}{3} d^2 + \tfrac{1}{3} d^3). \tag{7}$$

The increase of the diffusion coefficient at small densities of particles is the most striking feature of the computer simulation result presented in figure 2. We think that this effect can be explained as a result of competitions between particle–scatterer collisions and particle–particle collisions.

In the pure Lorentz gas ($d \to 0$) only particle–scatterer collisions are present. If reflection is admitted ($\beta \neq 0$) then collisions of the particle with scatterers are strongly correlated [5, 6] and some *ring-type collisions* (collisions leading to retracing by a particle of a part of its trajectory) play an important role in the description of the diffusion process. The Boltzmann approximation does not 'notice' the ring collisions, therefore it predicts too large a diffusion coefficient. The result in the nearest scatterers approximation [6] (plotted by a cross) deviates from the Boltzmann prediction by more than 200% in the cases presented in figure 2.

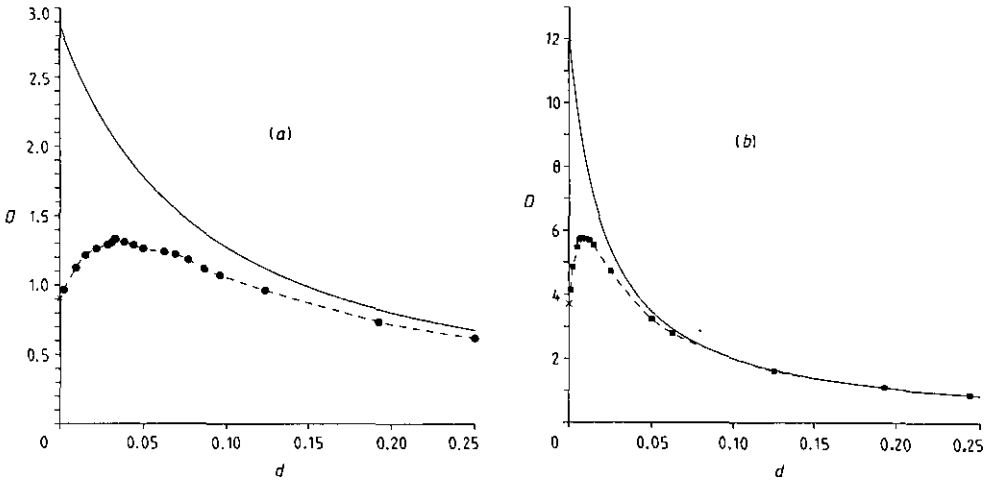

Figure 2. Diffusion coefficient as a function of density of particles per link for $\beta = 0.7$, $\alpha = \gamma = 0.1$ and for density of scatterers: (*a*) $\rho = 0.1$, (*b*) $\rho = 0.025$. The symbols denote the computer simulation result and the full curve is the Boltzmann prediction. The broken curve serves as a guide for an eye. Statistical error is smaller than size of the symbols.

Inclusion of the collisions between particles in the lattice Lorentz gas leads to lowering the number of ring collisions. We shall call this effect decorrelation of collisions. It seems to be the main reason for an increase of the diffusion coefficient at low densities of particles. Moreover, in order to observe this effect the probability of reflection, β, cannot be too small or, in other words, the particle–scatterer collisions should be correlated strongly enough. Finding the critical value β_c, below which the increase of the diffusion coefficient does not occur, is difficult in computer simulations. Lowering of β causes that the maximum of the diffusion coefficient becomes flat and it moves towards very small densities.

The effect of the decorrelation of particle–scatterer collisions can be discussed by comparison of computer simulation data with results obtained within the Boltzmann approximation. We see in figure 2(*b*) that for small density of scatterers the Boltzmann result may agree well with computer data even at small densities of particles. For the same values of probabilities α, β, γ but for a density of scatterers four times greater (see figure 2(*a*)) the Boltzmann result disagrees with computer data over the whole density range under study. The mean distance between scatterers (equal to ρ^{-1}) is smaller in the gas with $\rho = 0.1$ than in the gas with $\rho = 0.025$. Hence the appearance of a short ring collision, in which the repeated part of the trajectory is short, is more probable for $\rho = 0.1$. The decorrelation of collisions means that a particle which retraces a part of its trajectory is hit by another particle. On average it can happen if the mean free distance between particles is smaller than the length of the repeated part of the trajectory. Hence the decorrelation of collisions in a gas with $\rho = 0.1$ requires a higher density of particles than in the case with $\rho = 0.025$.

In a model without reflection ($\beta = 0$) the diffusion coefficient obtained from computer simulation decreases monotonically with density. Moreover, the computer data agree well with the Boltzmann prediction.

The diffusion in the three-dimensional version of the present model (for example on the simple cubic lattice) should possess qualitatively the same properties as the

diffusion discussed in this letter. The model on the square lattice was chosen as the simplest model to perform computer simulation.

I gratefully acknowledge the hospitality of the International Centre for Theoretical Physics in Trieste where the computer simulation was performed.

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