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1992 J. Phys. A: Math. Gen. 25 1093

(http://iopscience.iop.org/0305-4470/25/5/017)

J. Phys. A: Math. Gen. 25 (1992) 1093–1103. Printed in the UK

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Received 29 July 1991

Abstract. We investigate the properties of a model in which a particle moves on a square lattice with a fraction of the sites randomly occupied by stationary scatterers. Between two successive collisions with the scatterers, the particle performs random walk. The velocity autocorrelation function, measured by the computer moment propagation method, has an algebraic long-time tail although for some model parameters it decays very slowly at large time. We discuss the diffusion process in such a model calculating the diffusion coefficient in the Boltzmann and effective medium approximations. It is shown that correlated collisions play an important role in the description of diffusion for an intermediate density of scatterers.

1. Introduction

In Lorentz gases non-interacting particles move through randomly placed scatterers. Recent investigations [1–4] have shown that the lattice version of the Lorentz gas is an interesting example of a lattice gas for which the Boltzmann equation is inadequate. For example the diffusion coefficient, in models admitting reflection collisions, may deviate by more than 100% from the Boltzmann prediction [4]. This deviation is a consequence of the strongly correlated collisions occurring in the gas, which are not taken into account in the Boltzmann approximation. Moreover, the long-time behaviour of the velocity autocorrelation function (VAF) is characterized by algebraic decay, whereas the Boltzmann equation predicts exponential decay. Frenkel with his collaborators [5, 6] has developed a very accurate computer simulation technique, called moment propagation, which allows direct measurement of the VAF in cellular automata lattice gases with stochastic collision rules. Their measurements of the VAF for the 2D lattice Lorentz gases show the t^{-2} algebraic tail. In the square lattice they observed a fast $[(-1)^t]$ oscillation of the VAF.

In a previous paper [7] we considered a Lorentz lattice gas (LLG) with particles interacting through elastic collisions. The collisions between particles led to unusual behaviour in the diffusion coefficient as a function of particle density; it exhibited a maximum in the low particle density range. The increase in the diffusion coefficient with particle density can be understood as a de-correlation of the particle–scatterer collision by elastic particle–particle collisions. Moreover, we observed that the difference between the computer simulation diffusion coefficient and the Boltzmann prediction decreased for the intermediate particle density. In this paper we are interested in the problem of diffusion in the LLG in which the interacting particles have a high particle density. We want to know whether the correlated collisions are also important in the description of diffusion in a dense lattice gas.

In order to study diffusion in the high particle density limit we will introduce a simple one-particle model, which will be called a random Lorentz model (RLM). It will be shown that the RLM can also describe a random walk, a correlated random walk and the site percolation problem.

Applying the moment-propagation computer method to the RLM we shall discuss the properties of the VAF. It will be shown that the RLM exhibits a new type of long-time behaviour in the VAF.

Comparing the diffusion coefficient measured in the computer simulation with the Boltzmann prediction we will discuss the influence of the randomness of scatterers on diffusion in the RLM. Ernst and van Velzen [1] have shown that the diffusion coefficient of a LLG calculated in the effective medium approximation (EMA) is in excellent agreement with the computer simulation result for the whole scatterer density range. In this paper we shall also calculate the diffusion coefficient of the RLM in the EMA and by comparison with computer simulation results, the limitation of the EMA will be discussed.

2. The model

In the LLG with interaction a particle collides both with scatterers and other particles [7]. Diffusion of a tagged particle in such a model can be reduced to a strictly one-particle problem in two limiting cases:

(i) the low particle density limit where the problem is equivalent to diffusion in a ballistic LLG; and

(ii) the high particle density limit where the problem corresponds to diffusion in the RLM.

Case (i) has been widely investigated [1, 3, 4] and seems to be well understood. The latter we shall introduce and discuss in this paper.

A RLM consists of a lattice with a fraction of sites, c, randomly occupied by stationary scatterers. Particles move from a site to a neighbouring one in a unit time step. If the particle is on a site without a scatterer, it will go to one of the nearest neighbours with equal probability. In other words the particle performs a random walk. On a site occupied by a scatterer, the particle is scattered as in a stochastic Lorentz gas [1, 4]. This means that change of direction of motion at a site with a scatterer is described by a transition matrix. In this paper we consider a RLM on a square lattice. The transition rates are the following: α is the probability of transmission, β is the probability of reflection and γ is the probability of deflection in an orthogonal direction. They satisfy the normalization condition: $\alpha+\beta+2\gamma=1$. It is worth emphasizing the difference between the LLG and the RLM. In both models a particle is scattered upon collision with scatterer. In the LLG between two successive collisions the particle moves freely along a straight line connecting two scatterers whereas in the RLM the particle performs a random walk in the time between two successive collisions with scatterers.

There are four special (limiting) problems which can also be described by the RLM:

(i) random walk on uniform lattice ($c=0$ or $\alpha=\beta=\gamma=0.25$);

(ii) correlated random walk ($c=1$);

(iii) site percolation problem ($\beta = 1, \alpha = \gamma = 0$); and

(iv) LLG with isotropic scatterers with density $c' = 1 - c$ ($\alpha = 1, \beta = \gamma = 0$).

The site percolation problem in the RLM will be discussed in more detail in sections 4 and 5.

3. The Chapman–Kolmogorov equation

In this section we derive the equation of the motion, the Chapman–Kolmogorov equation, for the RLM. Let $p(r, i, t)$ denote the probability that, in a given configuration of scatterers, the particle at time t is at site r with velocity e_i. Assuming the lattice constant and time step to be equal to one, the velocity of the particle is one of the four lattice vectors

$$e_i = (\cos(\pi i/2), \sin(\pi i/2)) \qquad i = 0, 1, 2, 3. \tag{3.1}$$

The Chapman–Kolmogorov (CK) equation can be written in the following way

$$\begin{aligned} p(\boldsymbol{r} + e_i, i, t+1) = {} & (1 - c_{\boldsymbol{r}})\tfrac{1}{4} \sum_j p(\boldsymbol{r}, j, t) \\ & + c_{\boldsymbol{r}}\{\alpha p(\boldsymbol{r}, i, t) + \gamma p(\boldsymbol{r}, i \oplus 1, t) + \beta p(\boldsymbol{r}, i \oplus 2, t) + \gamma p(\boldsymbol{r}, i \oplus 3, t)\} \end{aligned} \tag{3.2}$$

where $\oplus$ denotes addition mod 4. The first term on the right-hand side describes the contribution from the random walk (site without scatterer) and the last term takes into account the collision of the particle with a scatterer.

The fluctuation in the scatterer density is described by introducing independent random variables:

$$c_{\mathrm{r}} = \begin{cases} 1 & \text{with probability } c \\ 0 & \text{with probability } 1 - c. \end{cases} \tag{3.3}$$

It is convenient to rewrite the CK equation (3.2) in matrix form. Introducing $4N$ vectors and $4N \times 4N$ matrices and block indices (rj), the CK equation can be written

$$p(t+1) = S^{-1}[B + CT]p(t) \tag{3.4}$$

where S is the translation operator

$$S_{ri,qj} = \delta_{r+e_i,q}\delta_{ij} \tag{3.5}$$

B is the random walk matrix

$$B_{ri,qj} = \tfrac{1}{4}\delta_{rq} \tag{3.6}$$

C is the matrix of scatterer density fluctuation

$$C_{ri,qj} = c_r \delta_{r,q}\delta_{ij} \tag{3.7}$$

and T is the particle–scatterer collision matrix

$$T_{ri,qj} = \delta_{r,q} U_{ij} \tag{3.8}$$

with

$$U_{ij} = (\alpha - \tfrac{1}{4})\delta_{ij} + (\gamma - \tfrac{1}{4})(\delta_{i,j\oplus 1} + \delta_{i,j\oplus 3}) + (\beta - \tfrac{1}{4})\delta_{i,j\oplus 2}. \tag{3.9}$$

It is worth noting that in the CK equation for the LLG [1] the matrix B is replaced by a unit matrix and the collision operator T has slightly different components.

We are interested in finding the VAF and the diffusion coefficient. The VAF is defined as

$$\Phi(t) = \langle v_x(0) v_x(t) \rangle \tag{3.10}$$

where $v_x(t)$ denotes the x-component of the particle velocity at time t and $\langle \ldots \rangle$ means the average over all possible paths and different configurations of scatterers.

The mean square displacement of a particle at time t can be expressed by the VAF in the following way [8]

$$\langle X^2(t) \rangle = t \left(\Phi(0) + 2 \sum_{\tau=1}^{t-1} \Phi(\tau) \right) - 2 \sum_{\tau=1}^{t-1} \tau \Phi(\tau). \tag{3.11}$$

The diffusion coefficient

$$D = \lim_{t \to \infty} \frac{\langle X^2(t) \rangle}{2t} \tag{3.12}$$

can be calculated from the Green–Kubo formula [1] for the two-dimensional case, i.e.

$$D = \frac{1}{4} + \sum_{t=1}^{\infty} \Phi(t). \tag{3.13}$$

The VAF can be expressed by the conditional probability $P(t)$ which is defined by rewriting equation (4) in the form

$$\begin{aligned} p(t) &= P(t) p(0) \\ &= [S^{-1}(B + CT)]^{t-1} S^{-1} p(0) \end{aligned} \tag{3.14}$$

with initial condition $P(0) = 1$.

Assuming a steady state as the initial distribution $p(r, i, t = 0) = (4N)^{-1}$, the VAF can be written as

$$\Phi(t) = \sum_{r,q} \sum_{i,j} e_{ix} e_{jx} \frac{1}{4N} \langle P_{ri,qj}(t+1) \rangle \tag{3.15}$$

where $\langle \ldots \rangle$ denotes the average over random variables c_r and e_{ix}, the x-component of e_i.

It is convenient to introduce the propagator Γ [1] which is the Laplace transform of the $\langle P(t) \rangle$,

$$\begin{aligned} \Gamma(z) &= \sum_{t=1}^{\infty} (1+z)^{-t} \langle P(t) \rangle \\ &= \langle [(1+z)S - B - CT]^{-1} \rangle. \end{aligned} \tag{3.16}$$

The diffusion coefficient is related to $\Gamma(0)$ through

$$D = \tfrac{1}{4} \sum_{r} \sum_{i,j} e_{ix} e_{jx} \Gamma_{ri,0j}(0) - \tfrac{1}{4} \tag{3.17}$$

where we have used the translational invariance of Γ.

4. Velocity autocorrelation function

In this section we discuss the properties of the VAF using the results of computer simulation. The moment-propagation (MP) method allows a direct and accurate measurement of the VAF and is a million times more efficient than conventional simulation [5]. The basic idea of the MP method is the following: Let us consider a particle at time $t = 0$ at site r on the square lattice with a given configuration of scatterers. In the next time step the particle can be in any of four neighbouring sites. In the MP method we take into account all possibilities by calculating the probability for each path. Hence instead of tracing the individual particles we propagate the site probability $p(r, i, t)$ according to the dynamics of the model. In order to measure the VAF directly the site probability is weighted with the initial velocity $v_x(0)$. Denoting the 'weighted' site probability by $M(r, i, t)$, the MP method can be described by the following equations:

$$M(r, i, t+1) = \sum_j W_{ij}(r) M(r - e_j, j, t) \tag{4.1}$$

with initial value

$$M(r, i, 0) = e_{ix}. \tag{4.2}$$

The transition matrix $W(r)$ depends on the configuration of scatterers. It has transition rates equal to $\frac{1}{4}$ on sites without scatterers and α, β, γ are the elements of W on sites occupied by scatterers. The steady state is chosen as the initial one, thus the VAF for a given configuration of scatterers can be calculated from

$$\Phi_c(t) = \frac{1}{4N} \sum_{r,i} e_{ix} M(r, i, t). \tag{4.3}$$

Averaging over different configurations of scatterers we get the VAF for the RLM.

Let us first discuss the behaviour of the VAF in a simple case. It is obvious that there is no correlation between input and output velocities on a site without a scatterer. The same situation can happen on a site with a scatterer provided that the probability of transmission is equal to the probability of reflection, $\alpha = \beta$. It means that the probability that a particle will have unchanged velocity is the same as the probability that the particle velocity changes sign as a result of a collision with a scatterer. Hence their contributions to the VAF cancel out. The value of γ has no meaning because it describes scattering with a post-collisional velocity perpendicular to the pre-collisional one and it follows that the product of their x-components is equal to zero. Using these simple arguments we find that the VAF for the RLM with $\alpha = \beta$ is of the form

$$\Phi(t) = \begin{cases} \frac{1}{2} & \text{for } t = 0 \\ 0 & \text{for } t > 0. \end{cases} \tag{4.4}$$

For models with $\alpha \neq \beta$ we performed a computer simulation using the MP technique on a square lattice with 255×255 sites. The results were usually averaged over 50 configurations of scatterers. We found that the behaviour of the VAF depends on the sign of $(\alpha - \beta)$. The case $\beta > \alpha$ is represented in figure 1 by the curve with full squares. The VAF is positive for even time steps and negative for odd. Such odd–even oscillations were observed in the VAF for the LLG on the square lattice [6] and in the VAF for a myopic random walk on a percolation cluster on the square lattice [9]. It has been argued that this oscillation appears due to a staggered invariant [6]. The algebraic decay of the upper and lower envelopes is well developed. Similarly as in the LLG there is no unique asymptote of the VAF of the RLM on the square lattice, i.e. the exponents of the upper and the lower envelope are different. In order to find the exponent, a simulation should be performed on a triangular lattice where the staggered invariant does not exist. The second curve in figure 1 (with open circles) represents the VAF for the case $\alpha > \beta$. The algebraic tail and odd–even oscillation are also observed. However, there is a significant difference with respect to the case represented by the first curve. In the odd–even oscillation the VAF does not change sign but there is a visible difference between the magnitudes of the odd and even time steps. For $t < 8$ the VAF is positive, at $t = 8$ it changes sign and remains negative for large t. The moment when VAF changes sign depends on model parameters.

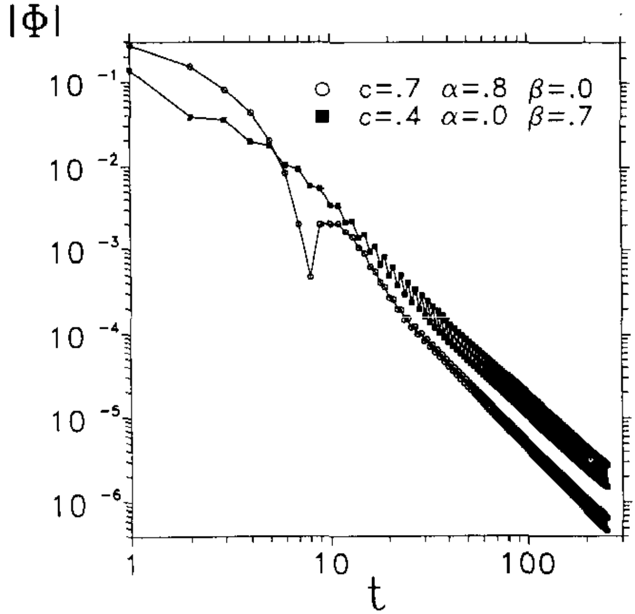

Figure 1. Log–log plot of the absolute value of the VAF as a function of time.

In figure 2 we plot the absolute value of the VAF for $\beta = 1$. In this case all scatterers play the role of reflectors. The VAF has odd–even oscillations with positive (negative) value for even (odd) times t. However the VAF decays so slowly at large time that it is very difficult to confirm this by computer simulation. The decrease in the VAF at large time is far below statistical accuracy. For example, for $c = 0.2$ the decrease in the VAF $\Phi(500) - \Phi(1000) = 6.3 \times 10^{-6}$ whereas the standard deviation of the VAF at large time is about 2.4×10^{-4}. We observed that in all the cases presented in figure 2 the absolute value of the VAF at large time ($t = 1000$) is nearly equal to $\Phi(2) = \frac{1}{2}c^2$ with an accuracy below 1%.

The case $\beta = 1$ in the RLM corresponds to a site percolation problem with percolation threshold $c = 0.407\,25$ [10]. In our model, a particle can visit each

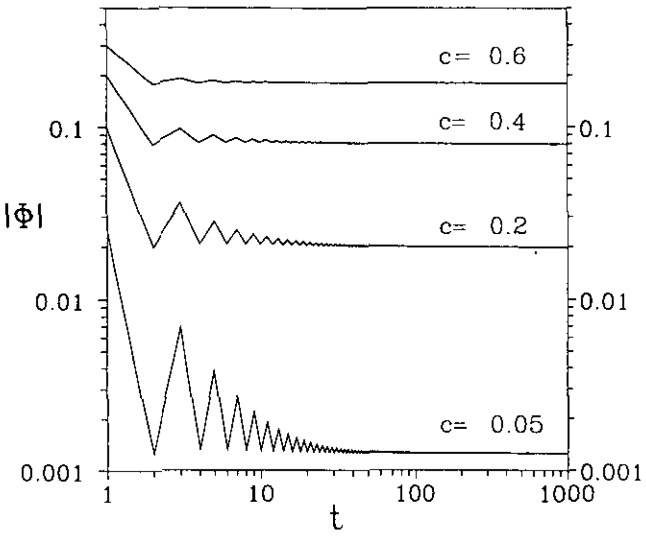

Figure 2. The same as in figure 1 for $\beta = 1$ and for several values of the scatterer density c.

site of the lattice independently of the density of scatterers c. However if a particle enters a site with a scatterer then in the next time step it must return to the previously visited site. As is seen from figure 2, the correlations persist both below and above the percolation threshold. The behaviour of the VAF for a myopic random walk on percolation cluster is different. It decays as $t^{-0.69}$ for large time [9].

5. The diffusion

As we have shown in section 3, the diffusion coefficient can be obtained from the propagator Γ. However calculating the propagator is very difficult problem. We solve this problem approximately, similarly to the case of the LLG [1], using the Boltzmann approximation and the effective medium approximation. The propagator, equation (3.16), is very similar to that for the LLG hence we omit the details concerning these approximations.

5.1. The Boltzmann approximation

In the Boltzmann approximation (BA) only uncorrelated collisions are taken into account. This means that the random variables c_r in equation (3.2) are replaced by their average values $\langle c_r \rangle = c$ and it follows that the matrix C is equal to $c\mathbf{1}$. Using the properties of cubic matrices [1] the propagator Γ can easily be calculated in the BA and the diffusion coefficient is

$$D_{\mathrm{B}} = \frac{1}{4}\frac{1 + c(\alpha - \beta)}{1 - c(\alpha - \beta)}. \tag{5.1}$$

5.2. The effective medium approximation

The EMA applied to the LLG gives a diffusion coefficient which is in very good agreement with the computer simulation result for the whole range of scatterer densities [1]. This is due to the fact that, in the EMA, a different type of ring collision is taken into account [3]. The ring-type collision leads to the particle retracing part of its trajectory; hence, this collision is particularly important in the LLG admitting reflection of the particle ($\beta \neq 0$).

In the EMA, the propagator Γ, equation (3.16), is replaced by

$$G(z) = [(1+z)S - B - cT^{e}(z)]^{-1} \tag{5.2}$$

The effective matrix $T^{e}(z)$ has the same symmetry as the matrix T and is calculated from a self-consistent equation. To derive this equation the propagator Γ was written as

$$\Gamma(z) = \langle [(1+z)S - B - cT^{e}(z) - \delta T]^{-1} \rangle \tag{5.3}$$

and is expanded in a power series of $\delta T = CT - cT^{e}(z)$. The condition for vanishing of the terms describing multiple scattering process by a single scatterer in this expansion (for details see [1]) leads to the following self-consistent matrix equation

$$\begin{aligned} T^{e} &= T + TRT^{e} - cT^{e}RT^{e} \\ R(z) &= \int_{k} [(1+z)e^{ikV} - B - cT^{e}(z)]^{-1} \end{aligned} \tag{5.4}$$

where the integration is over the Brillouin zone and V is a diagonal matrix with elements $V_{jl} = e_j \delta_{jl}$.

Solving this self-consistent equation (5.4) numerically, we find the effective matrix $T^{e}(z)$ which allows us to calculate the diffusion coefficient (3.17) with the EMA propagator G in (5.2).

5.3. Computer simulation of the diffusion coefficient

In a computer simulation we measured the VAF by the MP method and using the Green–Kubo formula (3.13) the diffusion coefficient was calculated with high accuracy, the statistical errors being well below 1%.

The results of the BA and EMA are compared with the computer simulation diffusion coefficient in figure 3. Notice that the BA gives incorrect values for D at intermediate densities of scatterers when $\alpha \neq \beta$. On the other hand, the BA predictions are exact when $c \to 0$ or $c \to 1$. The first limit corresponds to a random walk while the latter is for a correlated random walk [11]. Finally it is worth noting that in the LLG the deviation of the BA diffusion coefficient from the simulation results is largest in the low scatterer density range [1] whereas in our model the largest deviation is observed for intermediate densities (see figure 3).

We want to emphasize that correlated collisions are important in the description of diffusion in the RLM even when scatterers do not reflect the particle ($\beta = 0$). The difference between the BA and computer simulation results is several percent (see upper curve in figure 3) and can increase up to 15% for $\alpha = 1$. Remember that this case ($\beta = 0$) in the LLG model is characterized by a very small deviation between the BA and the EMA results [1].

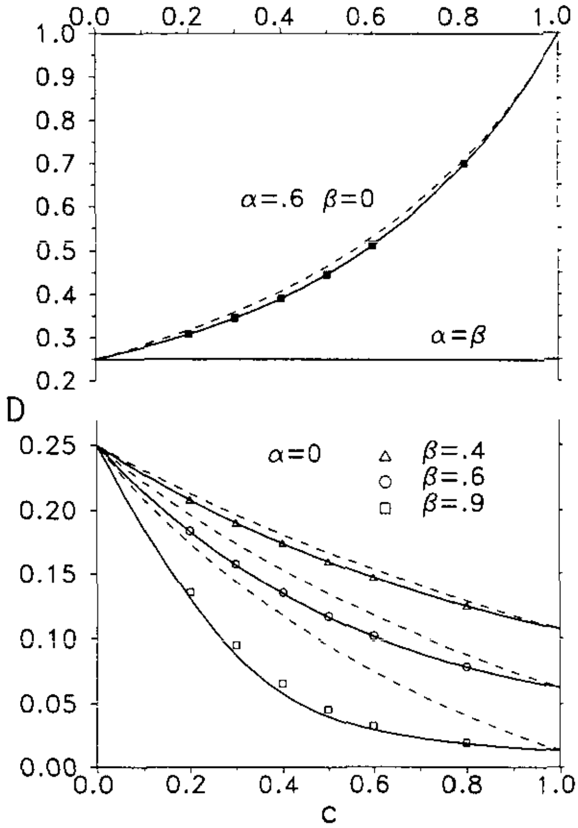

Figure 3. The diffusion coefficient as a function of scatterer density. The full (dashed) curve is the EMA (Boltzmann) prediction. Symbols denotes computer simulation MP results.

Comparing the EMA diffusion coefficient, D_{EMA} with the computer simulation result, D_{S}, we see that in most cases presented in figure 3 there is good agreement for the whole density range. Only when the probability of reflection is close to unity, does the EMA predict incorrect values for the diffusion coefficient at intermediate density. The greatest relative deviation, $\Delta = (D_{\text{S}} - D_{\text{EMA}})/D_{\text{EMA}}$, was observed for the density $c = 0.4$. As is seen in figure 4, for $\beta > 0.7$, Δ has a value greater than 1%. The breakdown of the EMA is more apparent in the case $\beta = 1$ which describes the site percolation problem. The diffusion coefficient D_{EMA} vanishes at $c = 0.3333$ (see figure 5), whereas the percolation threshold on the square lattice occurs when the density of impurities is $c = 0.40725$ [10].

The amplitude of the VAF decreases so slowly for $\beta = 1$ (see figure 2) that we cannot use the Green–Kubo formula (equation (3.13)) to calculate the diffusion coefficient by the computer MP method. Hence we calculated D as function of time, $D(t)$, dividing the mean square displacement (equation (3.11)) by $2t$. In figure 5 we plotted $D(t)$ as function of density c. The diffusion coefficient decreases with time and for $t = 10^4$ it vanishes slightly above the percolation threshold. Finally we want to emphasize that the case $\beta = 1$ provides an example in which the VAF does not decay faster than t^{-1}, but due to fast odd–even oscillations $(-1)^t$ diffusion exists.

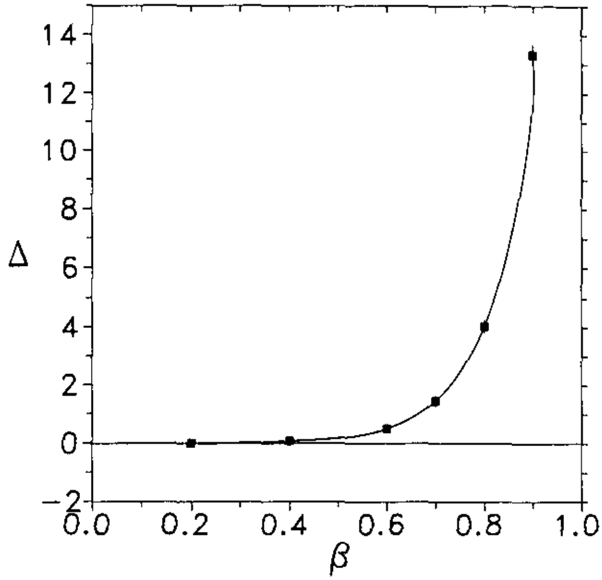

Figure 4. The relative deviation $\Delta = (D_S - D_{EMA})/D_{EMA}$ (per cent) of the computer simulation diffusion coefficient from the EMA prediction as a function of β for $\alpha = 0$ and $c = 0.4$.

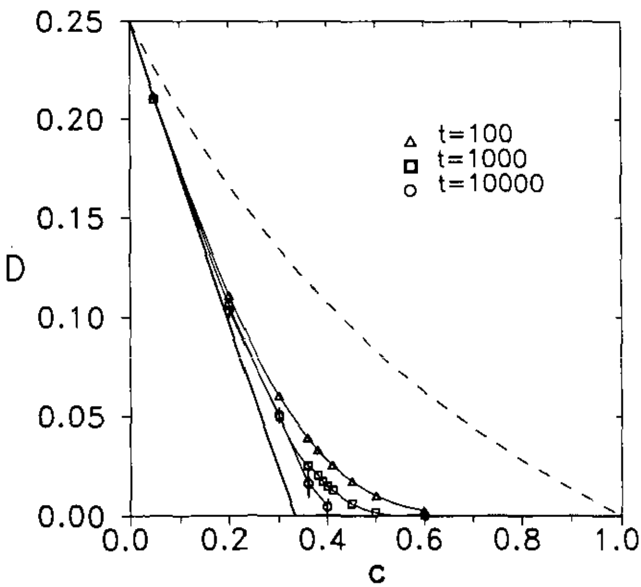

Figure 5. The diffusion coefficient as a function of scatterer density for $\beta = 1$ (site percolation problem). The full (dashed) curve is the EMA (Boltzmann) prediction. Symbols denotes computer simulation results $D(t)$ for $t = 10^2$, 10^3 and 10^4.

6. Discussion

We have investigated the RLM which corresponds to the high particle density limit of the LLG with interacting particles. We have shown that the VAF of the RLM decays algebraically at large time. In order to determine the exponent and amplitude of the decay one should investigate the RLM on a triangular lattice. The square lattice is characterized by the additional invariant (staggered density) which leads to fast odd–even oscillations in the VAF. We observed two types of odd–even oscillations which could be characterized by

(i) the difference between the magnitudes in odd and even time steps; and

(ii) the difference between the magnitudes and the difference between signs in odd and even steps.

In a special case ($\beta = 1$), when the scatterers become reflectors, the VAF decays so slowly that is difficult to confirm the decay in the computer simulation. Due to the fact that the VAF changes sign each time step, the diffusion exists. However, these two facts require a more rigorous argument to be proved. The case $\beta = 1$ is of interest for further investigation because it provides another description of the site percolation problem.

By calculating the diffusion coefficient in the BA and EMA and comparing them with computer simulation results, we pointed out that correlated collisions play an important role in the description of diffusion in the RLM at intermediate densities of scatterers. In this range the BA predicts an incorrect value for the diffusion coefficient. On the other hand the EMA predictions are in good agreement with the computer simulation results for $\beta < 0.7$. If β is close to 1 the EMA breaks down at intermediate densities of scatterers. It is worth emphasizing the difference between the RLM and the LLG. In the LLG the BA breaks down both at low and intermediate densities of scatterers. Moreover the EMA predicts the diffusion coefficient of the LLG correctly over the whole density range. In this way we have demonstrated that diffusion in a dense gas (RLM) is different from that in a rare gas (LLG).

Acknowledgment

The work one of us (CzO) was financially supported by the Polish Ministry of Education under grant P/04/268/90.

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