On the cellular automata approach to the 1D Lorentz gas

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Abstract. The one-dimensional stochastic Lorentz gas is studied in continuous space and in the cellular automata approach. It is shown that the cellular automata method leads to extra oscillations of velocity autocorrelation. The oscillations arise as a result of multiple reflections. The differences between the models become unimportant when the product of the concentration of scatterers and the probability of reflection is small.

1. Introduction

Cellular automata (CA) models have found wide application in physics (Wolfram 1986a). They are regular arrays of variables, each of which can take discrete values and the evolution of CA is defined by some local rules. It has been claimed that CA can potentially serve as models for continuum systems such as fluids (Wolfram 1986b).

In this paper we shall discuss the properties of the Lorentz gas. The model describes the motion of non-interacting light particles. They can be scattered on heavy (fixed) centres which are randomly distributed in space. The speed of light particle is constant but its velocity direction changes when the particle hits a scattering centre. In discrete (lattice) Lorentz models (Ernst and Binder 1988) velocity directions are determined by the geometry of the lattice. Hence a discrete Lorentz gas can be considered as a cellular automaton (Oleksy and Pękalski 1990).

The discussion of the Lorentz gas is limited here to the one-dimensional case, because we want to make a comparison between the discrete and continuous versions and to find when these models are equivalent. On the other hand, the 1D Lorentz model is the simplest non-trivial example which cannot be properly described in the Boltzmann approximation and the memory effects lead to power decay of the velocity autocorrelation function (Grassberger 1980, van Beijeren 1982).

2. The discrete (CA) model

We will consider the stochastic Lorentz gas in one-dimensional discrete space. The model consists of a single particle (or number of non-interacting particles) and fixed point-like scatterers which randomly occupy a fraction ρ of sites of the lattice. A particle moves from site to site with unit speed. If it meets a scatterer, then its direction of motion can be changed with probability of reflection p or can remain unchanged with probability of transmission $q = 1 - p$. The directions of velocity are denoted by 1 and -1.

Now we calculate the probability, $N_{\pm 1}(t)$, that a particle at time t is moving in the direction ± 1. In order to do this we must calculate the probability of an arbitrary trajectory which ends at time t with appropriate direction of the velocity. A trajectory can be represented by a set $\{l_1, l_2, l_3, \ldots\}$ of distances between successive scatterings. The probability, P_s, of finding two nearest centres which are s steps apart is

$$P_s = \rho(1-\rho)^{s-1}. \tag{1}$$

In this paper we use the following approximation. It is assumed that the probability of an arbitrary trajectory is the product of probabilities of scattering between neighbouring centres, irrespective of the number of backward scattering between these two centres. Hence the memory effects are taken into account, but they are limited to nearest scatterers. As an example, let us calculate the probability of the trajectory $\{m, l\}$—the particle meets a scatterer at times 0 and m and on both occasions is transmitted. The probability that the particle meets the third scatterer at time $t = m + l$ is equal to $q\rho(1-\rho)^{m-1}q\rho(1-\rho)^{l-1}\rho$ or $\rho q P_m q P_l$. As a second example, let us take the trajectory which is similar to the one above except that the particle is reflected at time $t = m + l$ and returns to the starting point at $t = 2m + 2l$. Now we must take into account the memory effect—the particle after reflection moves in the way it did before reflection. In our approximation the memory effect is limited to the nearest scatterers (to the path l in the example). Hence we obtain for the second trajectory the $\rho q^3 p P_m^2 P_l$, whereas the exact result is equal to $\rho q^3 p P_m P_l$. In the case when a particle is trapped between two scatterers separated by a distance r and it is k-times reflected, the probability of the event is equal $\rho p^k P_r$.

Taking into account the contribution from all possible trajectories to $N_{\pm 1}(t)$, we obtain the following expression

$$N_{\pm 1}(t+1) = (1-\rho)^{t+1} N_{\pm 1}(0) + \sum_{k=1}^{t+1} p^k N_{\pm(-1)^k}(0) W_k(t+1)$$

$$+ q \sum_{k=0}^{t} p^k \sum_{m=0}^{t-k} \rho N_{\pm(-1)^k}(m) C_k(t-m) \tag{2}$$

where

$$C_k(t) = (1-\rho)^{[t/(k+1)]} - (1-\rho)^{[t/k]} \tag{3}$$

$$W_k(t+1) = U_{k+1}(t+1) + U_{k-1}(t) - 2U_k(t+1) - \rho(1-\rho)^{[t/(k-1)]} \tag{4}$$

$$U_k(t) = \{k - \rho(t - k[t/k])\}(1-\rho)^{[t/k]} \tag{5}$$

and $[x]$ denotes the integer part of x.

The derivation of equation (2) is presented in the appendix. The first term in (2) describes the free motion of a particle. The second term represents the motion of a particle between nearest scatterers during time $t+1$ and the particle is (multiply) reflected. These two terms are exact. The last term in (2) represents the contribution from all remaining trajectories, in which probabilities are calculated in an approximate way. It is worth noting that $N_1(t) + N_{-1}(t) = 1$.

The velocity autocorrelation function (VAF) is usually defined as

$$\Phi(t) = \langle v(0)v(t) \rangle \tag{6}$$

where $\langle \ldots \rangle$ means averaging over configurations of scatterers. In our case (unit speed), choosing $N_1(0) = 1$ we can express the VAF as $\Phi(t) = N_1(t) - N_{-1}(t)$. Taking (2) into

account we obtain

$$\Phi(t+1) = (1-\rho)^{t+1} + \sum_{k=1}^{t+1} (-1)^k p^k W_k(t+1) + q \sum_{k=0}^{t} (-1)^k p^k \sum_{m=0}^{t-k} \rho C_k(t-m)\Phi(m). \quad (7)$$

The expression for the VAF is exact for $p = 1$.

3. Computer simulations

In order to confirm the behaviour of the VAF described by (7), we performed computer simulations of the 1D Lorentz gas in the same way as Grassberger (Grassberger 1980) but in discrete space. In each run we chose randomly, with probability $\rho = 0.1$, the position of the scatterers. Then the particle started from the origin and its direction of motion was observed in 20 units of mean free time, $t_{mf} = 1/\rho p$. The system was large enough that particles never reached its boundary. The number of runs was 2×10^5 and errors were of order 10^{-3}.

The simulations were performed for $p = 1$, 0.85 and 0.75 for two reasons. The theory presented above is exact for $p = 1$ and it seems to be a good approximation for p near 1. The second reason is that the effects we want to discuss are better seen for p in this range. The results of the simulations (open circles) and solutions of (7) (full circles) presented in figure 1 show a good qualitative agreement. In the simulation as well as in the theory, two features of the VAF are seen: (i) long oscillations—minima for τ near 2 and maxima for τ near 6, (ii) short oscillations ('teeth'), superimposed on the long oscillations, which become larger and sharper as p approaches 1. We will show later that the 'teeth' are not present in VAF of the continuous model, so they come from the discreteness of the space, not from the approximation.

4. The continuous model

Instead of deriving an equation for the VAF in the continuous model, we get it as the limit of (7) for $\rho \to 0$. First, the time is expressed in mean free time units $\tau = t/t_{mf}$, then the integer part $[\tau/\rho]$ is replaced by τ/ρ and Σ_t is replaced by $t_{mf} \int d\tau$. Hence the following equation is obtained:

$$\phi(\tau) = e^{-\tau/p} + \sum_{k=1}^{\infty} (-1)^k p^k w(\tau/p) + \frac{q}{p} \sum_{k=0}^{\infty} (-1)^k p^k \int_0^{\tau} d\sigma\, c_k\left(\frac{\tau-\sigma}{p}\right) \phi(\sigma) \quad (8)$$

where

$$w_k(x) = (k+1) e^{-x/(k+1)} + (k-1) e^{-x/(k-1)} - 2k e^{-x/k} \quad (9)$$

$$c_k(x) = e^{-x/(k+1)} - e^{-x/k}. \quad (10)$$

Let us note that for $p = 1$ equation (8) becomes the same as that derived by Grassberger (1980) for this limiting case.

Introducing the Laplace transform

$$\psi(z) = \int_0^{\infty} d\tau\, e^{-\tau z}\phi(\tau) \quad (11)$$

we can solve (8)

$$\psi(z) = -(1+p)^2 \sum_{m=1}^{\infty} (-1)^m p^m \frac{m^2}{1+zpm} \left(1 + \frac{1-p^2}{p} \sum_{m=1}^{\infty} (-1)^m p^m \frac{m}{1+zpm}\right)^{-1}. \quad (12)$$
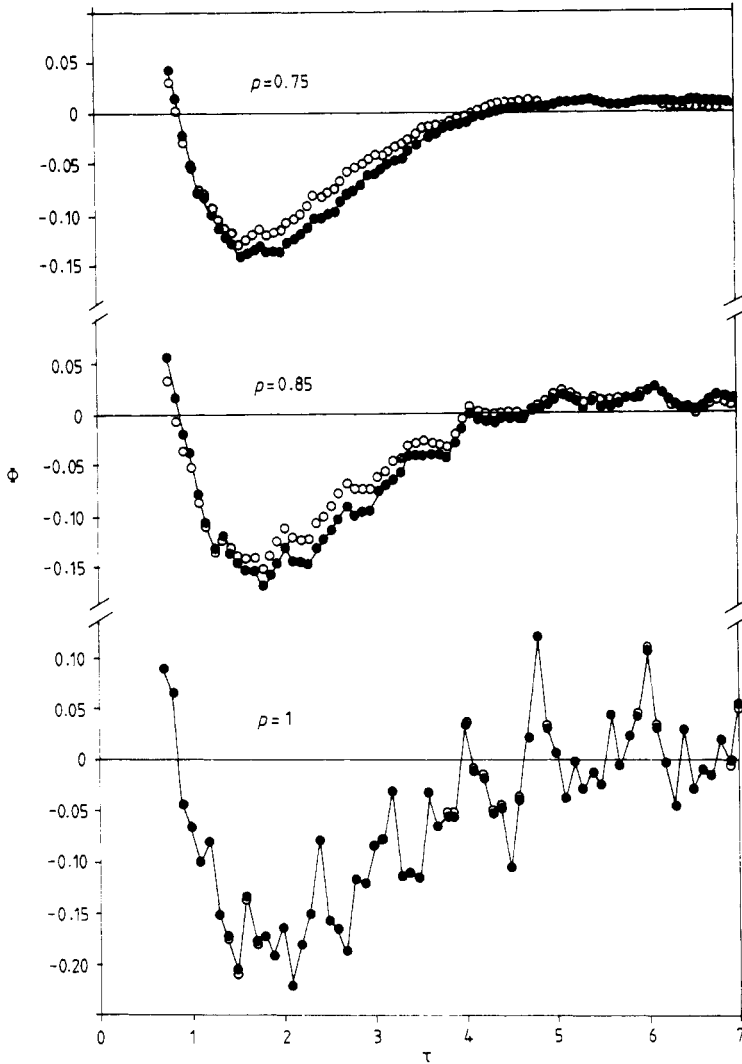
Figure 1. Time dependence of the velocity autocorrelation function of the discrete model for reflection probabilities $p = 0.75$, 0.85 and 1. Full circles represent the predictions of theory, open circles plot the computer simulation, in which errors are smaller than the diameter of the circle.

For small p, $\psi(z) = 1/(z+2) + O(p^2)$, the inverse transform

$$\phi(\tau) = e^{-2\tau} + O(p^2) \tag{13}$$

is the same as the VAF in the Boltzmann approximation.

The diffusion coefficient, D_c, is obtained from the VAF as

$$D_c = \int_0^\infty dt\, \phi(t). \tag{14}$$

It is easy to see that D_c is proportional to $\psi(0)$. Hence we obtain
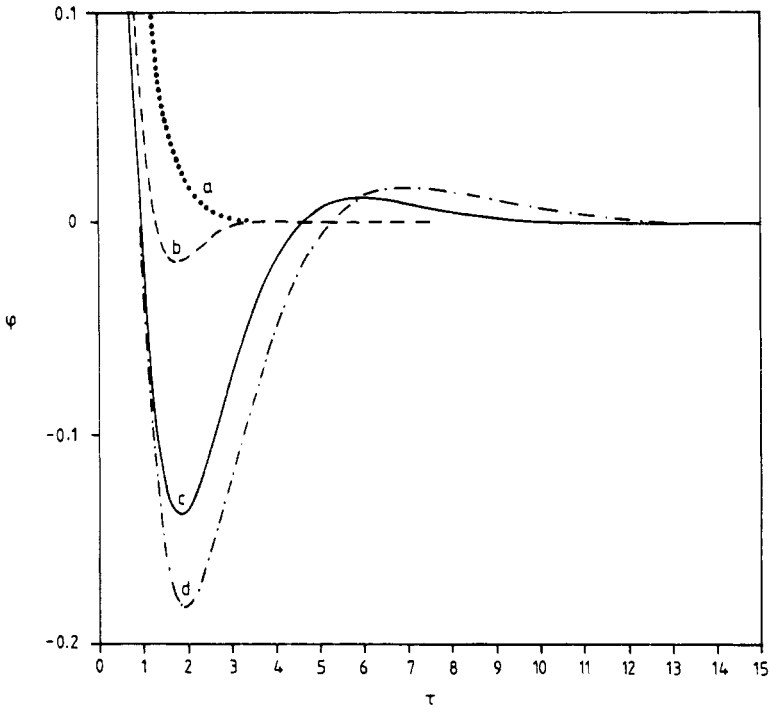
$$D_c = (1-p)D_0 \tag{15}$$

Figure 2. Time dependence of the velocity autocorrelation function of the continuous model for several reflection probabilities: $p = 0$ (a), $p = 0.25$ (b), $p = 0.75$ (c) and $p = 1$ (d).

where D_0 is the diffusion constant calculated for the VAF in the Boltzmann approximation, equation (13). The equation (15) for D_c is exact (Grassberger 1980)[†].

In figure 2 we present the VAF, obtained by a numerical solution of (8) for several values of p. The VAF decays in an oscillatory way. With decreasing p the oscillations become shorter and more strongly damped, and they disappear as p approaches 0.

5. A comparison between the discrete model and the continuous model

From figure 1 and figure 2 we see that the VAF of the discrete model has extra oscillations ('teeth') in comparison with the VAF of the continuous model. These teeth are created by the discreteness of the model, because the same approximation was applied to both versions of the Lorentz gas. Moreover, the teeth are also observed in results of computer simulations of the 1D discrete Lorentz gas (see figure 1). The magnitude of the teeth decreases strongly with decreasing p. In figure 3 we present the difference between the discrete VAF, Φ, and the continuous one, ϕ, for $p = 0.85$ and for two concentrations of scatterers $\rho = 0.1$ and $\rho = 0.025$. For $\rho = 0.1$ (upper curve) the difference is comparable with the VAF for $\tau > 4$. Decreasing ρ four times (lower curve) leads to a reduction of the difference by nearly one order of magnitude. So in this case the discrete VAF can be considered as a good approximation to the continuous one.

[†] The analogue of the formula (14) in the case of the discrete model, $D_d = \sum_{t=0}^{\infty} \Phi(t)$, leads to the result $D_d = (1 - p + p\rho)/2p\rho$, which is incorrect because for $p = 1$ (when the approximation becomes exact) the D_d does not disappear.
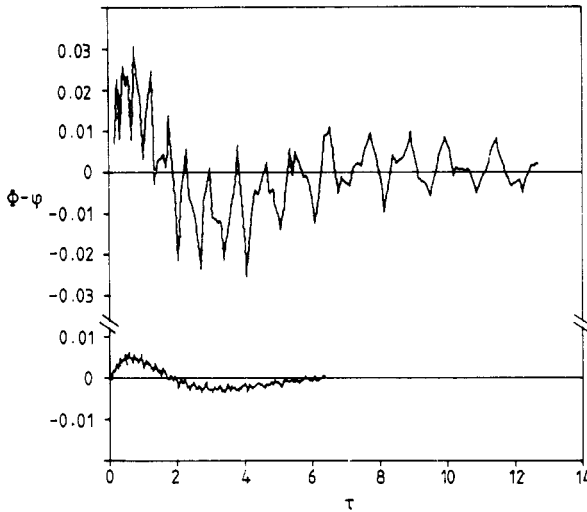
Figure 3. The difference between the VAF of the discrete model and the VAF of the continuous model as a function of time for two concentrations of scatterers: $\rho = 0.10$ (upper curve) and $\rho = 0.025$ (lower curve).

The VAF of the continuous 1D Lorentz gas can be replaced by its equivalent in the discrete model provided that the product ρp is small enough.

The common feature of both models are long oscillations of the VAF. They become longer and more damped as time increases (see figure 2). For example, the initial extrema for $p = 1$ and 0.75 are presented in table 1.

What is the origin of the oscillations? We claim that the oscillations as well as the teeth occur as a result of multiple reflections. In order to show this we use a simpler approximation than that used in section 2. Namely, the probability of successive reflections on two nearest scatterers is calculated exactly if the number of reflections is not greater than M. If it is, the probability is a product of probabilities which fulfil the above condition. It means that now the memory effects are limited to the nearest scatterers and to M reflections. The equation for the VAF of the discrete model in the approximation characterised by M, Φ_M, is of the following form:

$$\Phi_M(t+1) = (1-\rho)^{t+1} + \sum_{k=1}^{M} (-1)^k p^k W_k(t+1) + q \sum_{k=0}^{M} (-1)^k p^k \sum_{s=0}^{t-k} \rho C_k(t-s)\Phi_M(s)$$

$$+ (-p)^{M+1} \sum_{s=0}^{t-M} \rho C_M(t-s)\Phi_M(s). \tag{16}$$

We do not discuss the VAF of the continuous model. It can be obtained from (16) in the same way as (8) is obtained from (7). The behaviour of Φ_M depends strongly

Table 1. Initial extrema of the VAF for (i) $p = 1$ and (ii) 0.75.

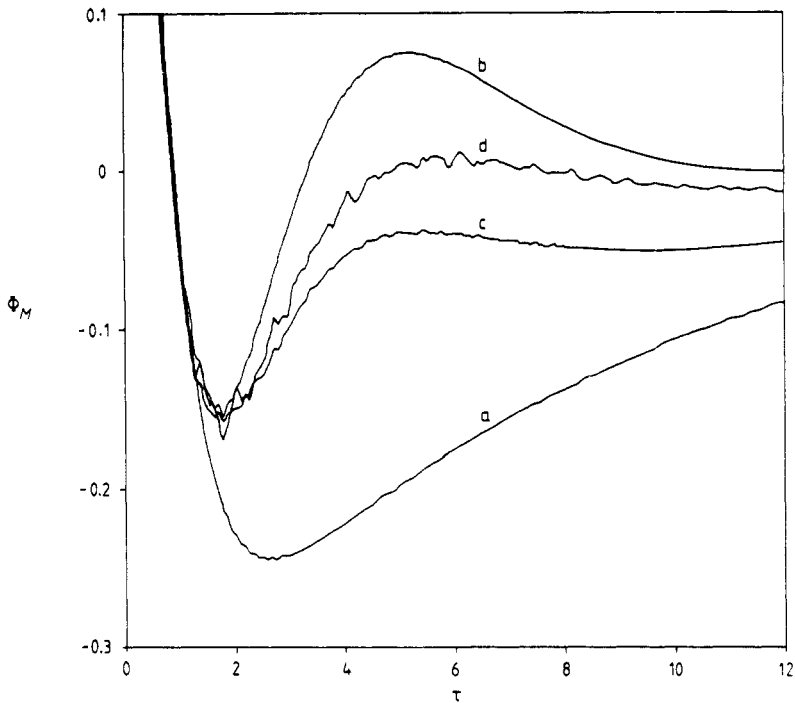| (i)	τ	1.92	7.04	15.28	26.70
	ϕ	-1.8×10^{-1}	1.7×10^{-2}	-1.2×10^{-3}	7.9×10^{-5}
(ii)	τ	1.82	5.91	12.46	21.92
	ϕ	-1.4×10^{-1}	1.2×10^{-2}	-6.1×10^{-4}	2.7×10^{-5}

Figure 4. VAF for $p = 0.85$ and $\rho = 0.1$ obtained in the approximation when M multiple reflections are accounted for exactly: $M = 1$ (a), $M = 2$ (b), $M = 3$ (c) and $M = 7$ (d).

on M. It is easy to solve (16) for $M = 0$

$$\Phi_0(t) = (1 - 2p\rho)^t. \tag{17}$$

Hence, the case $M = 0$ is equivalent to the Boltzmann approximation. For $M = 1$ the function has one minimum and grows monotonically to zero for large times. The VAF has both a minimum and a maximum for $M = 2$. The number of extrema increases as M increases. Similarly, the number and magnitudes of the teeth also grow with increasing M, see figure 4. Hence the oscillations of the VAF occur if and only if the probability of multiple reflections is calculated properly.

In this way we can also explain why Grassberger (1980) obtained a VAF with only one minimum. His calculations were performed in the lowest order of p and they thus correspond to $M = 1$. However, the memory effects were not limited to the nearest scatters; thus he could obtain the power decay of the autocorrelation function.

6. The case $p = 1$

Now we want to present and discuss the unexpected behaviour of the VAF of the discrete model in the case when $p = 1$. The VAF is described by (7), which is exact in this case. The oscillations of the VAF are not damped as t goes to infinity, on the contrary they become large. Even if the concentration of scatterers is very small ($\rho = 0.005$ in figure 5) the 'teeth' appear and they grow as t increases.
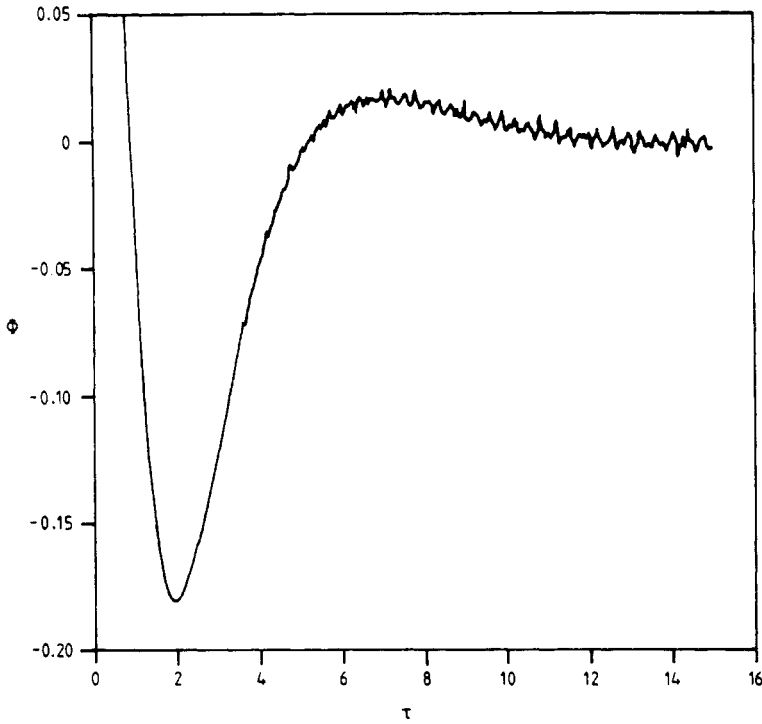
Figure 5. Time dependence of the VAF of the discrete model for $p = 1$ and $\rho = 0.005$.

Before entering into a more formal discussion, we present an intuitive explanation of the effect. First, let us note that the motion of a particle is periodic for $p = 1$. If the particle is located between scatterers separated by a distance s, then at time $t = k \times 2s$, $k = 1, 2, \ldots$, it has the initial position and velocity. Of course, here we consider an ensemble of particles, so the probability that a particle is on a path of length s is equal to P_s as given in (1).

Now we show that for a concentration of scatterers, ρ, there is a time t_0 such that the VAF is greater than 0.264 (see (21)). Let us express ρ by the mean distance between scatterers l_0: $\rho = 1/l_0$. The time t_0 is chosen as the smallest common multiple of $\{2, 4, 6, \ldots, 2l_0\}$. It means that all particles placed on paths of length $1, 2, 3, \ldots, l_0$ have at time t_0 regained their initial velocities. The probability, Q, that a particle is placed on a path of length not greater than l_0 is equal to

$$Q = \sum_{s=1}^{l_0} P_s. \tag{18}$$

For any ρ, this is bounded from below,

$$Q \geqslant \frac{e-1}{e}. \tag{19}$$

The probability that the velocity of a particle at time t_0 has its initial value is greater than Q, whereas the probability that a particle has velocity opposite to the initial one is smaller than $1 - Q$. Taking into account the assumption of unit speed and the definition of the VAF, equation (6), we obtain

$$\Phi(t_0) \geqslant 2Q - 1 \tag{20}$$

or, using (19),

$$\Phi(t_0) \geq 0.264. \tag{21}$$

Furthermore, we can show that for times greater than t_0 the VAF can be greater than $\Phi(t_0)$. Let us take $t_1 = t_0(l_0 + 1)$. Hence the probability that a particle at $t = t_1$ has its initial velocity is greater than Q. It follows that $\Phi(t_1)$ can be greater than $\Phi(t_0)$.

We can draw the following conclusion. The oscillations are not damped for large time because the motion of a particle is periodic and small distances between scatterers are more probable than large ones. Thus, there are distant points on the time scale where most of the particles take initial velocity.

From a comparison between figure 1 and figure 5 we see that for smaller ρ teeth occur later and, roughly speaking, they are removed to infinity when $\rho \to 0$.

7. Discussion

We studied the 1D stochastic Lorentz gas in a CA (discrete) version as well as the continuous model in the approximation in which the memory effects, limited to the nearest scatterers, are included. The approximation is exact at $p = 1$ and, as follows from comparison between theory and computer simulation, it is very good for p near 1 (for example $p = 0.85$).

The equations for the VAF and the expression for the diffusion coefficient in both models are derived. The VAF of the continuous model decays in an oscillatory way. The oscillations become longer and more damped as time increases. The VAF of the discrete model has short oscillations, called 'teeth' in this paper, superimposed on the long oscillations. In the limiting case, $p = 1$, these short oscillations do not disappear as time goes to infinity because of the periodicity of the motion of a particle. The long as well as the short oscillations arise as results of multiple backward scatterings.

The autocorrelation functions become similar in both models when the product $p\rho$ is much smaller than $1 - p$. In other words, when the stochastic Lorentz gas can be properly described by the discrete (CA) model.

Note added in proof. The formula of the diffusion coefficient of the lattice Lorentz gas (Ernst and Binder 1989) was recently slightly modified (Ernst and van Velzen 1989) and for the one-dimensional model it can be written as $D_d = \frac{1}{2} + \sum_{t=1}^{\infty} \Phi(t)$. Hence it clarifies the problem mentioned earlier in the footnote and for the 1D Lorentz gas it gives $D_d = (1 - p)/2p\rho$. It is worth noting that the Boltzmann (Markovian) approximation gives the diffusion coefficient $D_B = (1 - p\rho)/2p\rho$ which is correct only for $\rho = 1$.

Appendix

Here we derive (2) for the probability, $N_{\pm 1}(t + 1)$, that a particle at time $t + 1$ has its velocity pointing in the direction ± 1.

First, let us calculate the probability of the free motion, $NF_{\pm1}(t+1)$. It can be written as a product of two probabilities: (i) $N_{\pm1}(0)$, that a particle had, at $t = 0$, its velocity pointing in the direction ±1, (ii) $(1-\rho)^{t+1}$, that a particle did not encounter any scatterer in $t+1$ time steps:

$$NF_{\pm1}(t+1) = N_{\pm1}(0)(1-\rho)^{t+1}. \tag{A1}$$

Now let us calculate the probability that a particle is trapped between two nearest scatterers until time $t+1$, $NT_{\pm1}(t+1)$. The probability that a particle is trapped and reflected k times $(k = 1, 2, \ldots)$ during $t+1$ time steps and afterwards moves in the direction ±1 can be written as the product of probabilities: (i) $N_{\pm(-1)^k}(0)$, that a particle had, at $t = 0$, its velocity pointing in the direction $\pm(-1)^k$, (ii) p^k, that it was reflected k times, (iii) $\rho P_r\{r - |kr - (t+1)|\}$, that scatterers were separated by distance r (the term in the brackets $\{\ldots\}$ is the number of initial conditions for given r and k). The distance r can change from $r_{min} = 1 + [(t+1)/(k+1)]$ to $r_{max} = [t/(k-1)]$. Summing (iii) over r yields $W_k(t+1)$, (cf equation (4))

$$W_k(t+1) = \sum_{r_{min}}^{r_{max}} \rho^2(1-\rho)^{r-1}\{r - |kr - (t+1)|\}. \tag{A2}$$

Taking into account all possible numbers of reflection k during $t+1$ time steps, we obtain

$$NT_{\pm1}(t+1) = \sum_{k=1}^{t+1} p^k N_{\pm(-1)^k}(0) W_k(t+1). \tag{A3}$$

Finally we calculate, in an approximate way, the contribution from all the remaining trajectories, $NA_{\pm1}(t+1)$. Each of these can be divided into two parts in the following way. Let us assume that at moment s $(0 \leq s \leq t)$ a particle passes through a scatterer, and then remains between two nearest scatterers till the moment $t+1$. So the first part of a trajectory is an arbitrary trajectory (it represents motion of a particle between moments 0 and s), whereas the second part is limited to two nearest scatterers separated by distance r where the particle may be reflected k times $(k = 0, 1, 2 \ldots)$ between moments s and $t+1$. The probability of such a trajectory can be written as product of probabilities: (i) $q\rho N_{\pm(-1)^k}(s)$, that a particle with the velocity direction $\pm(-1)^k$ met a scatterer at moment s and was transmitted, (ii) p^k, that then it was reflected k times, (iii) P_r that the scatterers were r steps apart. The distance r may change from $r_1 = 1 + [(t-s)/(k+1)]$ to $r_2 = [(t-s)/k]$. Summing over possible numbers of reflection k, moments s and distances r, we obtain the following expression:

$$NA_{\pm1}(t+1) = q \sum_{k=0}^{t} p^k \sum_{s=0}^{t-k} \rho N_{\pm(-1)^k}(s) C_k(t-s) \tag{A4}$$

where

$$C_k(t-s) = \sum_{r_1}^{r_2} P_r \tag{A5}$$

and the result is given by (3).

The probability $N_{\pm1}(t+1)$ can be written as

$$N_{\pm1}(t+1) = NF_{\pm1}(t+1) + NT_{\pm1}(t+1) + NA_{\pm1}(t+1). \tag{A6}$$

The above equation is equivalent to (2).

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