Journal of Statistical Physics, Vol. 70, Nos. 3/4, 1993

Diffusion in Lorentz Lattice Gas Automata with Backscattering

H. van Beijeren[1] and M. H. Ernst[1]

Received March 31, 1992; final August 20, 1992

The probability of first return to the initial interval x and the diffusion tensor $D_{\alpha\beta}$ are calculated exactly for a ballistic Lorentz gas on a Bethe lattice or Cayley tree. It consists of a moving particle and a fixed array of scatterers, located at the nodes, and the lengths of the intervals between scatterers are determined by a geometric distribution. The same values for x and $D_{\alpha\beta}$ apply also to a regular space lattice with a fraction ρ of sites occupied by a scatterer in the limit of a small concentration of scatterers. If backscattering occurs, the results are very different from the Boltzmann approximation. The theory is applied to different types of lattices and different types of scatterers having rotational or mirror symmetries.

KEY WORDS: Diffusion on Cayley trees; lattice gas automata; low-density transport coefficient; breakdown of Boltzmann approximation.

1. INTRODUCTION

Diffusion is the simplest nonequilibrium phenomenon in spatially nonuniform systems, and the Lorentz gas[1,2] is one of the simplest models to describe this phenomenon. It consists of a single moving particle, which collides with randomly placed scatterers. The model has always served as an important tool in developing and testing new theories of nonequilibrium fluids, such as the derivation of the equations of fluid dynamics and diffusion, generalized kinetic equations, the calculation of transport coefficients as a function of the density of scatterers ρ, and the study of long-time tails of Green–Kubo time correlation functions, such as the velocity correlation function.[3–6]

[1] Institute for Theoretical Physics, Princetonplein 5, P.O. Box 80006, 3508 TA Utrecht, The Netherlands.

0022-4715/93/0200-0793$07.00/0

It is therefore not a surprise that Lorentz gases are also playing an important role in the current development and understanding of cellular automata fluids. We refer to the calculation of transport coefficients,[7-13] the study of long-time tails,[14-16] anomalous diffusion,[17-19] and recurrence times.[20]

It appears that diffusion phenomena in lattice models are frequently anomalous and in general much less universal than in continuum models with or without discrete velocities. For instance, the probability distribution $P(\mathbf{r}, t)$ for the displacements of the moving particle does not always obey a diffusion equation, although its second moment may still be growing linearly with time, i.e., $\langle(\Delta r)^2\rangle \sim Dt$, so that the diffusion coefficient D would exist.[17]

Here we want to study another aspect of Lorentz gases on lattices, with yet another anomaly. If the scattering rules for the moving particle are stochastic and allow the moving particle to retrace part of its trajectory (backscattering), then the diffusion coefficient in the limit of small concentration of scatterers is not given by the Boltzmann equation. In continuous systems this effect occurs only in discrete velocity models with backscattering, such as one-dimensional systems.

The goal of the present paper is an *exact* calculation of the first return probability x and the diffusion coefficient D for a Lorentz gas on a Bethe lattice or Cayley tree, which corresponds to the correct low-density limit of the corresponding model on a regular space lattice. As it turns out, the result is very different from the Boltzmann approximation. The model consists of a collection of *identical point* scatterers placed on the nodal points of a random Bethe lattice: each scatterer has b neighbors, located in one of b fixed lattice directions with respect to the first one. The distances between neighboring scatterers are distributed independently according to a geometrical distribution $P(l) = \rho(1-\rho)^{l-1}$ with l a positive integer. In addition, there is one particle moving at constant speed among the scatterers along one of the b lattice directions. It is reflected, transmitted, or deflected with certain probabilities at each encounter with a scatterer. If the reflection probability β is vanishing, transport coefficients are exactly given by the Boltzmann equation, because the particle never returns to a scatterer already visited before. On a Bethe lattice there are no closed loops; therefore a particle can only return to a nodal point by reversing its steps, allowing for side excursions on the way back, but this is not allowed if $\beta = 0$. However, if β is nonvanishing, the moving particle may return to the initial interval.

The diffusion coefficient for this process can be calculated from the Green–Kubo expression by integrating the velocity autocorrelation function over time from 0 to ∞. The average contributions from intervals between subsequent scatterings (e.g., between the first and the second, between the second and the third scattering, etc.) can be calculated separately. It turns out that the contributions of all intervals except the one on which the particle was located initially are accounted for correctly by the solution of the Boltzmann equation. However, the initial interval has an expected length that, at low densities, is twice that of the other ones. Consequently the particle spends on average a longer time on that interval than on any other interval, and there is, apart from the Boltzmann contribution, an *extra* contribution to the diffusion coefficient for every time the moving particle returns to the initial interval. Here we shall calculate this extra contribution.

In the previous paragraph we have imposed the restrictions that the scatterers are identical and pointlike. Both restrictions are essential for the present theory to give the exact low-density limit of a Lorentz gas on a regular space lattice. In the literature several models have been considered with two or more types of point scatterers, such as random mixtures of left and right rotators[21,12] and of left- and right-turning mirrors on square[10,13] or triangular lattices.[11] The theory to be presented here does not apply to these random mixtures. In such models not only does the initial interval give a contribution, different from the Boltzmann prediction, but also each subsequent interval.

Frenkel *et al.*[23] and Ossendrijver *et al.*[24] have also considered Lorentz lattice gas cellular automata with identical scatterers of finite size with an interaction range extending to nearest neighbor lattice sites. In the low-density limit each corner of a scatterer acts as a point scatterer of a different type, the above arguments for a mixture of point scatterers apply, and no exact low-density results are known.

As mentioned already, the non-Boltzmann-contribution to the diffusion coefficient of a Lorentz gas with backscattering, caused by returns to the initial interval, is typical for *one-dimensional* models with continuous position variables.[25-27] In *higher-dimensional* models with *continuous positions and velocities* the phase space for backscattering events is *negligible* at low densities. However, in lattice gases the phase space for backscattering is a *finite fraction* of all possibilities, and kinetic theory calculations[9] have shown that the contributions from backscattering trajectories renormalize the Boltzmann value of the diffusion coefficient, even in the limit of a vanishing concentration of scatterers.

As demonstrated by Ernst *et al.*,[8] the diffusion coefficient for models on Cayley trees is in fact identical to the diffusion coefficient on the corresponding *regular lattice* in the limit of small concentration of scatterers ($\rho \to 0$), but the authors could not carry out a complete evaluation of all contributions to the diffusion coefficient in the low-density limit. In any case, the Boltzmann equation cannot be used to calculate the low-density value of the diffusion coefficients in models with backscattering. In fact, *all collision sequences on a Cayley tree* contribute to the same order in density as the uncorrelated Boltzmann collisions, whereas all closed loops, or ring collisions, *not on Cayley trees*, contribute only to higher order in the density. In ref. 9 *only a subset* of all trajectories on Cayley trees has been resummed, using an effective medium approximation. Nevertheless, the approximate transport coefficients obtained with this approximation are in excellent agreement with extensive computer simulations.

The results of the present paper (i) show that the partial resummations for the square lattice model of ref. 9 do in fact yield the exact diffusion coefficient in the low-density limit, and furthermore (ii) are valid for all Lorentz lattice gases with identical point scatterers on arbitrary d-dimensional lattices with coordination number b. In the high-density limit, where all lattice sites are occupied with scatterers, the ballistic Lorentz models reduce to random walk models, where the diffusion coefficient is known exactly. The Bethe lattice approximation also produces the exact diffusion coefficient in the high-density limit. Consequently, as it interpolates between two exact limits, it usually provides an excellent approximation for all densities.

2. LATTICE LORENTZ GAS

We first introduce a Lorentz gas on a regular d-dimensional space lattice with lattice distance c. A fraction ρ of sites, chosen at random, is occupied by a scatterer. In addition there is a single moving particle located at lattice site $\mathbf{r}$ at integer-valued times ($t = 0, 1, 2,...$). Between the times $t-1$ and t it has a constant precollision velocity $\mathbf{c}_i$ ($i = 1, 2,..., b$), where $\{\mathbf{c}_i\}$ is the set of nearest neighbor lattice vectors with $|\mathbf{c}_i| = c$ and b the coordination number of the lattice. If the moving particle hits a scatterer with incoming velocity $\mathbf{c}_j$, its outgoing velocity will be $\mathbf{c}_i$ with probability W_{ij}, normalized as $\sum_i W_{ij} = 1$.

The main interest of this paper is the diffusion tensor $D_{\alpha\beta}$, where $\alpha, \beta,... = \{x, y,..., d\}$ denote Cartesian components of tensors or vectors. It is given by the Einstein formula[2]

$$\langle \Delta x_\alpha(t)\, \Delta x_\beta(t) \rangle \simeq 2D_{\alpha\beta}\, t \tag{2.1}$$

[2] It is assumed here that there is no drift in the stationary state. If in fact there is a drift, one has to subtract $\langle \Delta x_\alpha(t) \rangle \langle \Delta x_\beta(t) \rangle$ on the left-hand side of (2.1).

which is for long times and can be transformed into a Green–Kubo formula

$$D_{\alpha\beta}=\tfrac{1}{2}\sum_{t=0}^{\infty}\{\langle v_\alpha(t)\,v_\beta(0)\rangle+\langle v_\beta(t)\,v_\alpha(0)\rangle-\langle v_\alpha v_\beta\rangle\} \tag{2.2}$$

where the subtracted term is a consequence of the discrete time variable. The fundamental quantity for calculating D is the propagator $\tilde{\Gamma}_{ij}(\mathbf{r}, t)$, defined as the conditional probability that the moving particle is at time t in the precollision state $\{\mathbf{r}, \mathbf{c}_i\}$, given that it was in the precollision state $\{\mathbf{0}, \mathbf{c}_j\}$ at the initial time $t=0$, averaged over the distribution of fixed scatterers and over the initial positions of the moving particle, keeping its initial velocity $\mathbf{c}_j$ fixed. It has the property $\tilde{\Gamma}_{ij}(\mathbf{r}, 0)=\delta_{ij}\delta(\mathbf{r}, \mathbf{o})$, where $\delta(\mathbf{r}, \mathbf{o})$ is a d-dimensional Kronecker delta function. The diffusion tensor, as given by (2.1), can be expressed as

$$D_{\alpha\beta}=\tfrac{1}{2}\sum_{ij} c_{i\alpha}(\Gamma_{ij}-\tfrac{1}{2}\delta_{ij})\,p_j c_{j\beta}+(\alpha\rightleftarrows\beta) \tag{2.3}$$

The symbol $(\alpha\rightleftarrows\beta)$ denotes a similar term with α and β interchanged and $c_{i\alpha}$ denotes a Cartesian component of the nearest neighbor lattice vector $\mathbf{c}_i$. Furthermore, p_i is the equilibrium probability of finding the velocity in direction i. It satisfies $\sum_j W_{ij}\,p_j=p_i$. In the majority of models to be considered, all directions are equally probable in the steady state, so that $p_i=1/b$. Finally, the kinetic propagator

$$\Gamma_{ij}=\sum_{t=0}^{\infty}\sum_{\mathbf{r}}\tilde{\Gamma}_{ij}(\mathbf{r}, t) \tag{2.4}$$

represents the total probability, summed over all sites of the lattice and all times ($t=0, 1, 2,\ldots$), i.e., summed over all possible trajectories.

The method for calculating Γ, to be developed below, also allows us to calculate time sums of general correlation functions, with v_x in (2.2) replaced by some function of the velocity, $Q(\mathbf{v})$. For example, $Q_{\alpha\beta}(\mathbf{v})=v_\alpha v_\beta-(1/d)\,v^2\delta_{\alpha\beta}$. The resulting expression for the time sum is given by (2.3) with c_{ix} replaced by $Q_{i\alpha\beta}\equiv Q_{\alpha\beta}(\mathbf{c}_i)$, i.e.,

$$\begin{aligned}D_Q&=\sum_{t=0}^{\infty}\langle Q_{\alpha\beta}(\mathbf{v}(t))\,Q_{\alpha\beta}(\mathbf{v}(0))\rangle-\tfrac{1}{2}\langle Q^2_{\alpha\beta}(\mathbf{v})\rangle\\&=\sum_{ij} Q_{i\alpha\beta}(\Gamma_{ij}-\tfrac{1}{2}\delta_{ij})\,p_j Q_{j\alpha\beta}\end{aligned} \tag{2.5}$$

3. LORENTZ GASES ON BETHE LATTICES

From arguments presented in the Introduction, it follows that the diffusion tensor on a regular lattice *at low densities* is given exactly by the diffusion tensor of a Bethe lattice or Cayley tree, with the same point symmetries and the same type and density of scatterers. The root of the tree is the site $\mathbf{r}=0$, which represents the initial position of the moving particle. The branch points of the tree are the scatterers. The intervals between scatterers have a length l, determined by the probability distribution $P(l)=\rho(1-\rho)^{l-1}$. The average interval length is $\bar{l}=\sum_l lP(l)=1/\rho$. The moving particle is distributed with equal probabilities over all available lattice sites. If we register the position of the moving particle at time $t+\varepsilon$ ($\varepsilon\downarrow 0$) (see Fig. 1)), its mean free path [expected length of (OB)] is $\bar{l}$, whereas the expected length of (OA) is $(\bar{l}-1)$. As a consequence, the expected length of the interval (AB) on which this particle is found initially equals $2\bar{l}-1$. To calculate Γ_{ij} we start with models without backscattering, where returns of the moving particle to the initial interval are not possible. Then the probability $W_{\bar{j}j}$ vanishes, where j and $\bar{j}$ label links respectively with the velocities $\mathbf{c}_j$ and $-\mathbf{c}_j$. The total contribution to (2.4) of all possible trajectories *without backscattering* is

$$\begin{aligned}\Gamma_{ij}&=\bar{l}\{1+W+W^2+\cdots\}_{ij}\\&=\bar{l}\left\{\frac{1}{1-W}\right\}_{ij}\end{aligned}\tag{3.1}$$

where an obvious matrix notation has been used. The individual terms in (3.1) represent the contributions of trajectories with respectively 0, 1, 2,... scatterers. The factor $\bar{l}$ accounts for the integration over all possible initial configurations of the scatterers, given a fixed initial velocity $\mathbf{c}_j$ of the moving particle. The diffusion tensor in (2.3) is then given by

$$D^0_{\alpha\beta}=\frac{1}{2}\sum_{ij}\left\{\left(\frac{\bar{l}}{1-W}\right)_{ij}-\frac{1}{2}\delta_{ij}\right\}p_jc_{j\beta}+(\alpha\rightleftarrows\beta)\tag{3.2}$$

which is the prediction of the *Boltzmann equation.*

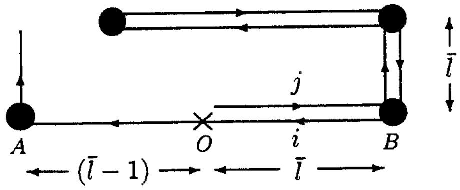

Fig. 1. Trajectory returning to the initial interval (AB), where a cross denotes the origin ($\mathbf{r}=0$), a dark circle a scattering site, and $\bar{l}=1/\rho$ is the mean free path.

Next, the possibility of backscattering will be considered, where $W_{\bar{i}i} \neq 0$. In this case the moving particle can return to intervals it has visited before. However, with the exception of the initial interval, all these intervals still have expected length $\bar{l}$ and the probability that after n scatterings the velocity of the moving particle equals $\mathbf{c}_j$ is $(W^n)_{ij}$, irrespective of whether all the scatterers encountered were different or not. As a result, (3.2) still correctly accounts for the contributions to D from all these intervals. The initial interval (AB), on the other hand, has expected length $2\bar{l}-1$, as mentioned before.

The average time spent on interval (AB) by the moving particle before its first scattering is $\bar{l}$, but in subsequent returns this time equals $2\bar{l}-1$, as illustrated in Fig. 1. Obviously (3.2) accounts for $\bar{l}$ of this, but the remaining $\bar{l}-1$ have to be added separately. To do this one needs the probability R_{ij} for return to the initial interval with velocity $\mathbf{c}_i$ of a particle starting with velocity $\mathbf{c}_j$. The additional contribution to D can then be expressed as $(\bar{l}-1)\sum_{ij} \mathbf{c}_i R_{ij} p_j \mathbf{c}_j$. If X_{ij} denotes the corresponding matrix of first return probabilities to the initial interval, then R_{ij} can be expressed as

$$R_{ij} = \{X + X^2 + \cdots\}_{ij} = \{X/(1-X)\}_{ij} \tag{3.3}$$

and the diffusion tensor is

$$D_{\alpha\beta} = \frac{1}{2}\sum_{ij} c_{i\alpha} \left\{ \frac{\bar{l}}{1-W} + \frac{(\bar{l}-1)X}{1-X} - \frac{1}{2} \right\}_{ij} p_j c_{j\beta} + (\alpha \rightleftarrows \beta) \tag{3.4}$$

There is a reduction of the Boltzmann diffusion tensor D^0 in (3.2), caused by returns to the initial interval, i.e., caused by correlated collision sequences on the Bethe lattice. The probability of first return will be calculated in the next section. The result for Γ_{ij} in (3.4) can also be applied to the expression (2.5) by replacing c_i with Q_i.

4. PROBABILITY OF FIRST RETURN

On a Cayley tree the first return of the moving particle, if it occurs at all, does always occur with a velocity opposite to the initial velocity. Hence the elements of the matrix X are of the form

$$X_{ij} = x_j \delta_{\bar{i}j} \equiv x_j \mathscr{E}_{ij} \tag{4.1}$$

where x_j is the first return probability $(0 \leqslant x_j \leqslant 1)$ of a particle starting out with velocity $\mathbf{c}_j$. Combining (3.3) and (4.1), one finds

$$R_{ij} = \frac{x_j}{1 - x_{\bar{j}} x_j} \mathscr{E}_{ij} + \frac{x_{\bar{j}} x_j}{1 - x_{\bar{j}} x_j} \delta_{ij} \tag{4.2}$$

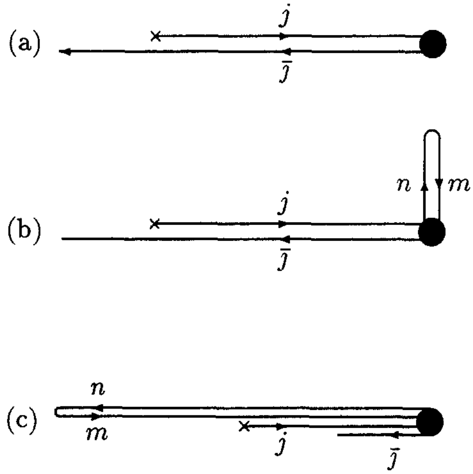

Fig. 2. Trajectories returning to the initial interval, (a) without and (b, c) with returns to a scatterer, represented by (n, m)-loops. The corresponding probability is X_{nm}.

To calculate the first return probabilities x_j, we enumerate the trajectories contributing to $R_{jj} = x_j/(1 - x_j x_j)$ in a different way, as indicated in Fig. 2. The trajectory in Fig. 2a contributes W_{jj} to R_{jj}; those in Figs. 2b and 2c contribute together $W_{jm} X_{mn} W_{nj} = (WXW)_{jj}$, etc.

Notice that also contributions from return sequences, in which the moving particle traverses the initial interval once or several times before the final return, are correctly accounted for. The total probability of return becomes

$$\begin{aligned} R_{jj} &= \{W + WXW + WXWXW + \cdots\}_{jj} \\ &= \left\{W \frac{1}{1 - XW}\right\}_{jj} \end{aligned} \tag{4.3}$$

By equating R_{jj} in (4.2) and (4.3), we obtain a set of b coupled algebraic equations from which the x_j can be solved. For Lorentz gases with high symmetry these equations simplify considerably. This will be the subject of the next section.

5. SYMMETRIC LORENTZ GASES

The results obtained in the previous sections simplify considerably if both the lattice and the transition probabilities W_{ij} exhibit rotational symmetry under appropriate rotations from $\mathbf{c}_i$ to $\mathbf{c}_j$.[3] Under these conditions the diffusion tensor reduces to a diffusion coefficient times the unit tensor and the return probability x becomes independent of the initial velocity $\mathbf{c}_i$. The b-vector c_{ix} now is an eigenvector of the matrix of transition probabilities W_{ij}, i.e., $\sum_j W_{ij} c_{jx} = w_1 c_{ix}$, where w_1 is the eigenvalue. The Boltzmann diffusion coefficient simplifies to

$$D^0 = \frac{c^2}{d}\left(\frac{\bar{l}}{1-w_1} - \frac{1}{2}\right) \tag{5.1}$$

where the relation $\sum_i c_{ix}^2 = bc^2/d$ has been used. The matrix of first return probabilities X takes the form

$$X_{ij} = x\delta_{ij} = x\mathscr{E}_{ij} \tag{5.2}$$

and the diffusion tensor (3.4) reduces to

$$D = \frac{c^2}{d}\left\{\frac{\bar{l}}{1-w_1} - \frac{(\bar{l}-1)\,x}{1+x} - \frac{1}{2}\right\} \tag{5.3}$$

where the relation $X_{ij}\mathbf{c}_j = -x\mathbf{c}_i$ has been used.

On lattices with cubic or hexagonal symmetry the b-vector $Q_i \equiv Q_{\alpha\beta}(\mathbf{c}_i)$, as defined above (2.5), is also an eigenvector of both X, with eigenvalue $+x$, and of W, with eigenvalue w_2. Consequently the expression (3.4) becomes

$$D_Q = \frac{1}{b}\sum_i Q_i Q_i \left\{\frac{\bar{l}}{1-w_2} + \frac{(\bar{l}-1)\,x}{1-x} - \frac{1}{2}\right\} \tag{5.4}$$

The overall factor $\sum_i Q_i Q_i/b$ depends on the lattice structure and equals $c^4/4$ for a square lattice and $c^4/8$ for a triangular lattice. The matrix of total return probabilities, as given by (4.2), simplifies to

$$R = \frac{x\mathscr{E}}{1-x\mathscr{E}} = \frac{x}{1-x^2}\,\mathscr{E} + \frac{x^2}{1-x^2}\,\mathbf{1} \tag{5.5}$$

and the expression (4.3) for R_{jj} is independent of j. It can be replaced by its average,

$$R_{jj} = \frac{1}{b}\sum_j R_{jj} = \frac{1}{b}\sum_{j=0}^{b}\left(\frac{\mathscr{E}W}{1-x\mathscr{E}W}\right)_{jj} = \frac{1}{b}\operatorname{Tr}\left(\frac{\mathscr{E}W}{1-x\mathscr{E}W}\right) \tag{5.6}$$

[3] In fact for the Bethe lattice it is sufficient that (i) $\sum_j c_{j\alpha}^2 = bc^2/d$, (ii) W_{jj} is independent of j, and (iii) the number of matrix elements W_{ij} with any given value is the same for each fixed i or j.

where (4.1) and (4.3) have been used to obtain the second equality. By equating R_{jj} in (5.5) and (5.6) we obtain an algebraic equation for x, i.e.,

$$\frac{x}{1-x^2}=\frac{1}{b}\operatorname{Tr}\left(\frac{\mathscr{E}W}{1-x\mathscr{E}W}\right) \tag{5.7}$$

It simplifies to

$$\frac{b}{1-x^2}=\operatorname{Tr}\frac{1}{1-x\mathscr{E}W} \tag{5.8}$$

where the physical solution satisfies $0\leqslant x\leqslant 1$. Let the b-vectors ϕ_l $(l=0, 1, 2,..., b-1)$ with components ϕ_{lj} $(j=1, 2,..., b)$ be the common eigenvectors of W, R, X, $\mathscr{E}$ with eigenvalues w_l, r_l, x_l, ε_l, respectively. The l-labels are chosen such that $W\phi_0=w_0\phi_0=\phi_0$ (normalization of transition probabilities) and such that the velocity-inversion matrix $\mathscr{E}$ has eigenvalues $\varepsilon_l=(-1)^l$, so that $r_l=\varepsilon_l x/(1+\varepsilon_l x)$. Equation (5.8) for x can be expressed in terms of eigenvalues as

$$\begin{aligned}\frac{b}{1-x^2}&=\sum_l\frac{1}{1-x\varepsilon_l w_l}\\&=\frac{1}{1-x}+\sum_{l\neq 0}^{(+)}\frac{1}{1-xw_l}+\sum_l^{(-)}\frac{1}{1+xw_l}\end{aligned} \tag{5.9}$$

The superscripts $(+)/(-)$ indicate that the l-sums are restricted to the even $(+)$ or odd $(-)$ values of l. If all eigenvalues are nondegenerate, (5.9) is an algebraic equation of degree b. Power counting shows that the degree of this polynomial equation is $(b+1)$, but it always has the solution $x=0$. In the majority of cases some eigenvalues are degenerate, which lowers the degree of the polynomial.

In Sections 6 and 7 this result will be applied to Lorentz gases on lattices with square, triangular, and other symmetries.

6. ISOTROPIC SCATTERERS

6.1. *d*-Dimensional Lattices

As a first application we consider a Lorentz gas defined on a regular d-dimensional space lattice with coordination number b and a fraction ρ of the sites occupied by scatterers. We call a scatterer *isotropic* if the transition probability is the same for every outgoing velocity channel, i.e., $W_{ij}=1/b$. This $b\times b$ transition matrix W has one eigenvalue $w_0=1$ and a $(b-1)$-fold degenerate eigenvalue $w_l = 0 (l \neq 0)$. The probability of first return x follows directly from (5.9). The result is

$$x = \frac{1}{b-1} \tag{6.1}$$

In the isotropic models the diffusion tensor is diagonal, $D_{\alpha\beta} = D\delta_{\alpha\beta}$, and the diffusion coefficient D is given by (5.3) with the mean free path $\bar{l} = 1/\rho$ and reads

$$\rho D = \frac{c^2}{d}\left[1 - \frac{1}{b} - \rho\left(\frac{1}{2} - \frac{1}{b}\right)\right] \tag{6.2}$$

For comparison we also quote the corresponding Boltzmann value in (5.3),

$$\rho D^0 = \frac{c^2}{d}\left(1 - \frac{1}{2}\rho\right) \tag{6.3}$$

Important special cases are isotropic scatterers on a *triangular* lattice ($d = 2$, $b = 6$, $c^2 = 1$) with a diffusion coefficient

$$\rho D = \frac{5}{12} - \frac{1}{6}\rho \tag{6.4}$$

or on a *hypercubic* lattice ($b = 2d$, $c^2 = 1$) with

$$\rho D = \frac{1}{2d^2}\left[2d - 1 - (d-1)\rho\right] \tag{6.5}$$

In particular for scatterers *on a line* ($d = 1$, $c^2 = 1$) this becomes

$$\rho D = \tfrac{1}{2} \tag{6.6}$$

It is *exact* for all densities[26] and differs substantially from the corresponding Boltzmann value, $\rho D^0 = 1 - \frac{1}{2}\rho$. In the limit as $\rho \to 0$, Eq. (6.2) gives the *exact* value $D = (b-1)/db\rho$ of the diffusion coefficient, which is also quite different from the Boltzmann prediction $D^0 = 1/d\rho$.

So far our analysis was directed toward a calculation of transport coefficients in the limit as $\rho \to 0$. However, for the above Lorentz models another exact result is known, namely the high-density limit ($\rho \to 1$), where the above Lorentz models reduce to a random walk on a d-dimensional lattice with coordination number b with an exact diffusion coefficient $D = 1/2d$. Inspection of (3.4) or (5.3) shows that these equations contain, apart from the dominant terms proportional to $\bar{l}$, also a density-dependent correction term of relative $\mathcal{O}(\rho)$. Of course these correction terms do not represent the complete $\mathcal{O}(\rho)$ density correction to the diffusion coefficient on a regular lattice. Nevertheless, setting $\rho = 1$ in (3.4) or (5.3) does give the correct high-density limit. Hence, (6.2) yields the correct high- and low-density limits. As it interpolates between two correct limits, the formula is expected to yield a rather accurate prediction for all densities. This has been confirmed indeed by the computer simulations on the square lattice with isotropic scatterers, as shown in Fig. 1 of ref. 9.

As a small variation on the previous models one may exclude forward scattering, i.e., $W_{jj} = 0$, and keep all remaining outgoing states equally likely, so that $W_{ij} = 1/(b-1)$ for $i \neq j$. There is then a nondegenerate eigenvalue $w_0 = 1$, and a $(b-1)$-fold degenerate $w_l = -1/(b-1)$ for $l \neq 0$. Equation (5.8) for the probability of first return simplifies to

$$x^2 + (b-1)(b-2)\,x - b + 1 = 0 \tag{6.7}$$

The diffusion coefficient D is given by (5.3) with $w_1 = -1/(b-1)$ and x the positive root of (6.7).

6.2. Hypercubic Lattices

This name refers to the regular lattice with coordination number $b = 2d$. The model on the Bethe lattice with the same coordination number and with the same symmetry represents the corresponding low-density problem. The scattering rules are described by a transmission probability α, a reflection probability β, and a deflection probability γ for each of the remaining $2(d-1)$ directions. The normalization is

$$\alpha + \beta + 2(d-1)\,\gamma = 1 \tag{6.8}$$

The eigenvalues with the corresponding multiplicity are,

$$\begin{aligned} w_0 &= 1 && (1\times) \\ w_1 &= a - \beta && (d\times) \\ w_2 &= \alpha + \beta - 2\gamma && ((d-1)\times) \end{aligned} \tag{6.9}$$

Equation (5.9) then reduces to

$$\frac{2d-1-x}{1-x^2} = \frac{d-1}{1-xw_2} + \frac{d}{1+xw_1} \tag{6.10}$$

The solution of (6.10) should be inserted in (5.3) to obtain D for general cubic lattices.

7. SCATTERERS WITH ROTATIONAL SYMMETRY

7.1. Triangular Lattice

Here a scatterer will rotate the velocity direction of the moving particle over an angle $n\pi/3$ with $n=0, 1,..., 5$ with probabilities as defined in Fig. 3 and normalized as

$$\alpha+\beta+\gamma_R+\gamma_L+\delta_R+\delta_L=1 \tag{7.1}$$

Let the matrix $\mathscr{D}$ be the 6-dimensional representation of the clockwise rotation over an angle of $\pi/3$, where $\mathscr{D}_{ij}=\delta_{i+1,j}$. The matrix of transition probabilities for this model reads then

$$W=\alpha\mathbf{1}+\beta\mathscr{D}^3+\delta_R\mathscr{D}+\delta_L\mathscr{D}^5+\gamma_R\mathscr{D}^2+\gamma_L\mathscr{D}^4 \tag{7.2}$$

The transition probability W is invariant under inversion, i.e., $W\mathscr{E}=\mathscr{E}W$, or under rotations, $W\to\mathscr{D}^nW\mathscr{D}^{-n}$. Consequently $D_{xy}=-D_{yx}$. In addition, $D_{\alpha\beta}$ is symmetric because of (2.2), hence $D_{xy}=0$ and $D_{\alpha\beta}=D\delta_{\alpha\beta}$. For later reference we formulate this in a somewhat more general fashion, i.e., for matrices representing rotations over multiples of $2\pi/b$. Let ϕ_l $(l=0, 1, 2,..., b-1)$ with components ϕ_{lj} $(j=1, 2,..., b)$ be the eigenvectors of the rotation matrix $\mathscr{D}$; then

$$\begin{aligned}(\mathscr{D}\phi_l)_j&=\phi_{l,j+1}\equiv d_l\phi_{lj}\\ d_l&=\exp(2l\pi\hat{\imath}/b)\equiv\theta^l\\ \phi_{lj}&=\exp[2l(j-1)\pi\hat{\imath}/b]=\theta^{l(j-1)}\end{aligned} \tag{7.3}$$

where d_l are the eigenvalues and $\theta=\exp(\pi\hat{\imath}/3)=\frac{1}{2}(1+\hat{\imath}\sqrt{3})$, where $b=6$ in the triangular lattice. The corresponding eigenvalues w_l $(l=0, 1,..., 5)$ can

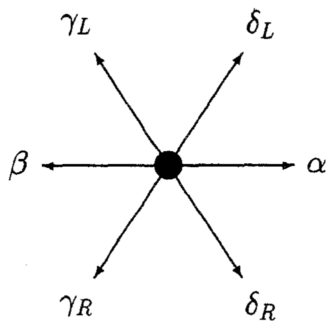

Fig. 3. Transition probabilities α, δ_R, γ_R, β, γ_L, δ_L.

be read off from (7.2) and (7.3). For instance, in the symmetric case, where $\gamma_R = \gamma_L = \gamma$ and $\delta_R = \delta_L = \delta$, one gets

$$\begin{aligned} w_0 = 1, \qquad & w_2 = w_4 = \alpha + \beta - \gamma - \delta \\ w_1 = w_5 = \alpha - \beta - \gamma + \delta, \qquad & w_3 = \alpha - \beta + 2\gamma - 2\delta \end{aligned} \tag{7.4}$$

The probability of first return follows from (5.9) and becomes in the present case

$$\frac{5-x}{1-x^2} = \frac{2}{1-xw_2} + \frac{2}{1+xw_1} + \frac{1}{1+xw_3} \tag{7.5}$$

It reduces to a cubic equation as explained below (5.9), and the physical root satisfies $0 < x < 1$. The diffusion tensor $D_{\alpha\beta} = D\delta_{\alpha\beta}$ in (2.3) is a scalar quantity. This follows directly from the fact that $c_x = \frac{1}{2}(\phi_1 + \phi_5)$ and $c_y = (2\hat{\imath})^{-1}(\phi_1 - \phi_5)$ are both eigenfunctions of the propagator W in (3.4) with eigenvalue w_1. The diffusion coefficient (5.3) then becomes

$$D = \frac{1}{2\rho}\left(\frac{1}{1-w_1} - \frac{x}{1+x} - \frac{\rho}{2}\frac{1-x}{1+x}\right) \tag{7.6}$$

where x is the physical root of (7.5). The corresponding Boltzmann value of the diffusion coefficient D^0 is obtained by setting $x = 0$ in (7.6).

In the previous examples the scatterers have rotational as well as mirror symmetries. As an illustration, we also consider a simple example of scatterers with only rotational symmetry, by setting $\gamma_L = \delta_L = 0$ and $\gamma_R = \delta_R = \gamma$. In that case the eigenvalues of the transition matrix are given by

$$\begin{aligned} w_0 = 1, \qquad & w_2 = w_4 = \alpha + \beta - \gamma \\ w_3 = \alpha - \beta, \qquad & w_1 = w_5^* = \alpha - \beta + \hat{\imath}\gamma\sqrt{3} \end{aligned} \tag{7.7}$$

The probability of first return is determined by an equation similar to (7.5) with $2/(1 + xw_1)$ replaced by $2\mathscr{R}[1/(1 + xw_1)]$, where $\mathscr{R}$ denotes the real part. The diffusion coefficient is given by (7.6) with $1/(1 - w_1)$ replaced by $\mathscr{R}[1/(1 - w_1)]$.

7.2. Square Lattice

Here we consider the square lattice analogs of the models treated in the previous subsection with transition probability α, reflection probability β, and right and left deflection probabilities γ_R and γ_L, normalized as

$$\alpha + \beta + \gamma_R + \gamma_L = 1 \tag{7.8}$$

The matrix of transition probabilities has the form

$$W = \alpha \mathbf{1} + \beta \mathscr{D}^2 + \gamma_R \mathscr{D} + \gamma_L \mathscr{D}^3 \tag{7.9}$$

where now $\mathscr{D}$ represents a rotation over $\pi/2$. The eigenfunctions and eigenvalues are given by (7.3) with $\theta = \exp(\pi \hat{\imath}/2) = \hat{\imath}$. Consequently, the eigenvalues of W are

$$\begin{aligned} w_0 &= 1, \qquad w_2 = \alpha + \beta - \gamma_R - \gamma_L \\ w_1 &= w_3^* = \alpha - \beta + \hat{\imath}(\gamma_R - \gamma_L) \end{aligned} \tag{7.10}$$

To calculate the diffusion tensor, we observe that $c_x = \frac{1}{2}(\phi_1 + \phi_3)$ and $c_y = (2\hat{\imath})^{-1}(\phi_1 - \phi_3)$ with the eigenfunctions ϕ_l given by (7.3) with $\theta = \hat{\imath}$. The diffusion tensor $D_{\alpha\beta} = D\delta_{\alpha\beta}$ is diagonal and D is given by (7.6) with $1/(1 - w_1)$ replaced by $\mathscr{R}[1/(1 - w_1)]$ and x is obtained from the equation

$$\frac{3 - x}{1 - x^2} = 2\mathscr{R} \frac{1}{1 + x w_1} + \frac{1}{1 - x w_2} \tag{7.11}$$

This concludes the applications to different lattice models.

8. DISCUSSION

For the diffusion coefficient of a particle moving on a Cayley tree with identical stochastic scatterers located at each branch point and a geometric distribution of distances between these scatterers an exact expression has been obtained. This could be identified with the low-density limit of the diffusion coefficient for a moving particle on a regular lattice with randomly distributed scatterers. The most striking conclusion is that, if backscattering is allowed, the Boltzmann equation does not give the correct low-density limit. As the model also produces the correct high-density limit (all sites occupied by scatterers) for the diffusion coefficient on the regular lattice, it usually provides very accurate approximations for intermediate densities also.

The model can easily be extended to the case of correlated scatterers by replacing the geometrical distribution of distances between the scatterers by the distribution corresponding to the pair correlation function between the scatterers. In the low- and high-density limits this will have but a marginal effect. However, it may provide useful approximations at intermediate densities.

As mentioned already in the introduction, Ernst and van Velzen[9] calculated the diffusion coefficient of a ballistic Lorentz gas on a square lattice with stochastic scattering rules by summing a subset (self-consistent ring diagrams) of all moving particle trajectories on Cayley trees. The method is in fact an effective medium approximation. Their extensive computer simulations showed excellent agreement with the EMA results for the case of *identical point scatterers* with *stochastic scattering* laws. As it turns out, the expressions they obtained coincide with the exact expressions we derived here. In view of the excellent agreement with computer simulations, this is not entirely unexpected. Obviously the trajectories on Cayley trees that were left out of their summations do not contribute to the diffusion coefficient. It also turned out that the EMA values for the low-density diffusion coefficients no longer show excellent, but only approximate agreement with computer simulations, as soon as the scattering laws are deterministic and/or there are scatterers of different types,[13] or the scatterers have a finite size.[23,24] In that case the EMA or ring kinetic theory no longer yields the exact diffusion coefficient on a Bethe lattice.

For lattice Lorentz gases with mixtures of different types of scatterers the Bethe lattice approximation still provides the correct low-density limit of the diffusion coefficient, but its calculation is not so straightforward. If the scatterers are sufficiently isotropic, it still suffices to compute the return probabilities to the initial interval beyond the Boltzmann contribution. However, these now depend on the identities of all the other scatterers and cannot be calculated simply. Averaging over the random distribution of scatterers on the nodes of the Bethe lattice, one obtains a distribution of return probabilities. To calculate this distribution, one has to either perform a numerical summation over paths of finite span on the Bethe lattice, to obtain an approximative distribution, or solve a nonlinear set of integral equations connecting the return probabilities. Work on this is currently in progress.

REFERENCES

1. H. A. Lorentz, *Proc. R. Acad. Amsterdam* **7**:438, 585, 684 (1905).
2. P. and T. Ehrenfest, *The Conceptual Foundations to the Statistical Approach in Mechanics*, (Cornell University Press, Ithaca, New York, 1959).
3. B. J. Alder and W. E. Alley, *J. Stat. Phys.* **19**:341 (1978).
4. J. C. Lewis and J. A. Tjon, *Phys. Lett. A* **66**:349 (1978); C. Bruin, *Physica* **72**:261 (1974).
5. D. Frenkel, *Phys. Lett.* **121A**:385 (1987).
6. J. J. Brey, J. Gomez Ordoñez, and A. Santos, *Phys. Lett.* **127A**:5 (1988).
7. P. M. Binder and M. H. Ernst, *Physica A* **164**:91 (1990).
8. M. H. Ernst, G. A. van Velzen, and P. M. Binder, *Phys. Rev. A* **39**:4327 (1989).
9. M. H. Ernst and G. A. van Velzen, *J. Phys. A: Math. Gen.* **22**:4611 (1989).
10. Th. W. Ruijgrok and E. G. D. Cohen, *Phys. Lett.* **133A**:415 (1988).
11. X. P. Kong and E. G. D. Cohen, *Phys. Rev. B* **40**:4838 (1989).
12. G. A. van Velzen, *J. Phys. A: Math. Gen.* **23**:4953 (1990).

13. G. A. van Velzen, Lattice Lorentz gases, Ph.D. dissertation, University of Utrecht (1990); *J. Phys. A: Math. Gen.* **24**:787, 807 (1991).
14. M. H. Ernst and G. A. van Velzen, *J. Stat. Phys.* **57**:455 (1989).
15. P. M. Binder and D. Frenkel, *Phys. Rev. A* **42**:2463 (1990).
16. M. H. Ernst, in *Ordering Phenomena in Condensed Matter Physics*, Z. M. Galasiewicz and A. Pekalski, eds. (World Scientific, Singapore, 1991), p. 291.
17. X. P. Kong and E. G. D. Cohen, *Physica D* **47**:9 (1991).
18. E. G. D. Cohen, in *Microscopic Simulations of Complex Hydrodynamic Phenomena* (Proceedings Nato Summer School, Alghero, July 1991), M. Maréschal, ed. (World Scientific, Singapore, 1992).
19. R. M. Ziff, X. P. Kong, and E. G. D. Cohen, *Phys. Rev. A* **44**:2410 (1991).
20. L. A. Bunimovich and S. E. Troubetzkoy, Preprint, University of Bielefeld (1991).
21. J. M. F. Gunn and M. Ortuño, *J. Phys. A: Math. Gen.* **18**:L1035 (1985).
22. G. A. van Velzen, *J. Phys. A: Math. Gen.* **24**:789, 807 (1991).
23. D. Frenkel, F. van Luyn, and P. M. Binder, *Europhys. Lett.* (1992).
24. A. J. H. Ossendrijver, Diffusion in lattice Lorentz gases, M.A. thesis, University of Utrecht (1991); A. J. H. Ossendrijver, A. Santos, and M. H. Ernst, University of Utrecht (1992).
25. D. W. Jepsen, *J. Math. Phys.* **6**:405 (1965).
26. H. van Beijeren, *Rev. Mod. Phys.* **54**:195 (1982).
27. P. Grassberger, *Physica A* **103**:558 (1980).