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Abstract. In cellular automaton fluids, where binary collision laws admit reflections, the Stosszahl ansatz and the Boltzmann equation are no longer valid at low densities. This is proven for a class of Lorentz gas models, defined on cubic lattices, for which the diffusion coefficient is calculated from a self-consistent ring kinetic equation or effective medium theory. The calculated results are in excellent agreement with results from molecular dynamics simulations over the whole density interval.

1. Introduction

Intuitively one might expect that the Boltzmann equation gives a correct kinetic description of transport properties in lattice gases at sufficient dilution, at least for dimensionality d larger than two. However, this is in general not the case, as we found in recent computer simulations [1]. The primary goal of this paper is to provide a theoretical explanation of these observations using kinetic theory. A secondary goal is to demonstrate that, also in the context of cellular automaton (CA) fluids, the systematic many-body methods developed in kinetic theory offer a means to understand and explicitly calculate non-equilibrium properties in cases where the simple probabilistic arguments of the Stosszahl ansatz fail completely at low densities and the Boltzmann equation breaks down.

In existing simulations of cellular automaton fluids [2] the measured transport properties could be explained quantitatively—within acceptable error bars—by the Boltzmann equation. The agreement holds not only at low and high density (because of particle-hole symmetry), but surprisingly also at intermediate densities. It holds for viscosities [2] and tagged particle diffusion [3, 4], both in CA fluids with deterministic and with stochastic collision dynamics. Similar quantitative agreement was found in lattice versions of the Lorentz gas [5, 6]. Even the mode-coupling calculations by Kadanoff *et al* [7] of the logarithmic size dependence of the viscosities in the two-dimensional FHP-lattice gases [2] do not yield substantial deviations from Boltzmann for the typical system sizes used in the simulations.

The essential feature shared by these lattice gases is the *absence of backscattering* (reversal of velocities in binary collisions), at least at low densities where triple collisions are rare. (Triple collisions give 'backscattering' of third order in the density.) In a single-component CA fluid of indistinguishable unlabelled particles with momentum conserving collision rules (such as HPP [8] or FHP models [2]) backscattering is an ill defined concept. However, in tagged particle systems and Lorentz gases, one can follow the complete trajectory of a tagged particle and investigate the lack or presence

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of backscattering. In computer simulations on such models it appears that very large or very small deviations from the Boltzmann prediction occur, depending on the presence or absence of backscattering.

To investigate this problem one needs to develop a systematic kinetic theory for CA fluids that enables one to calculate systematically higher-order density corrections to the Boltzmann equation. We further want to avoid the difficulties, inherent to two-dimensional fluid-type models, in which transport coefficients are proportional to the logarithm of the system size. In order to do so we have chosen a simple CA fluid, namely a lattice Lorentz gas, where the scatterers are fixed to the sites of a square lattice. We will use stochastic collision rules, defined through the three probabilities α, β, γ with the normalisation $\alpha+\beta+2\gamma=1$, where α is the transmission probability, β the reflection or backscattering probability and γ the deflection probability in an orthogonal direction. By varying these parameters one may possibly fine-tune to certain exceptional features of the lattice models; backscattering is one of them. This model has been studied before by Okamura *et al* [9] using the Boltzmann approximation of uncorrelated collisions.

There exist many lattice Lorentz models with deterministic rules, only a few of which are mentioned. Binder [5, 10] has performed computer simulations on a model where the moving particle turns right/left upon collision with a scatterer at even/odd times. At low densities there is qualitative agreement with the Boltzmann equation. Ruijgrok and Cohen [6] performed simulations on a model, where a random fraction of sites is occupied by fixed deflecting mirrors, located at angle $\pm\pi/2$ with equal probability. Simulations and Boltzmann results agree quite well at all densities. There is no backscattering in these models [5, 6].

Another closely related Lorentz lattice gas was introduced by Gunn and Ortuño [11]. In their model a fraction of sites, $P(0)=1-c$, does not contain scatterers, whereas the remaining fractions $P(\pi/2)$, $P(-\pi/2)$ and $P(\pi)$ are filled by right-turning, left-turning and backscatterers, respectively.

It is well known in the literature [12–14] that the possibility of backscattering and retracing trajectories may create long-time memory effects that can change the (low-density) Boltzmann value of the diffusion coefficient by a substantial fraction. This is the case in a 1D gas of hard rods [12] or in a wind-tree model where tree corners are cut off [13]. Strong backscattering can even make the diffusion coefficient vanish, as is the case in the Ehrenfest wind-tree model with overlapping trees [14]. Similar things happen in lattice gas models or cellular automaton fluids.

Kinetic theory is the standard tool to investigate such problems. As the first step one has to estimate the relative importance of different collision sequences in the coupled limit of small density of scatterers c and of large time t, where t is typically of the order of the mean free time, $t_{\mathrm{mf}}\sim 1/c$. The methods for estimating c and t dependence of the phase space associated with uncorrelated collisions, rings, repeated and nested rings, orbiting events, non-ring sequences, etc, is exactly the same as used by Hauge and Cohen [14] in their analysis of Ehrenfest's wind-tree model. We simply summarise the results in figure 1 in order to show which diagrams have to be resummed in a systematic low density theory of $\mathcal{O}(1)$ and $\mathcal{O}(c)$ respectively.

In models without backscattering the only $\mathcal{O}(1)$ contributions come from uncorrelated collisions, summed by the Boltzmann equation. However, in models *with* backscattering one not only has to sum uncorrelated collisions, but also rings and repeated rings in order to be consistent to lowest order in the density. This shows the *breakdown of the Boltzmann equation* for such models.

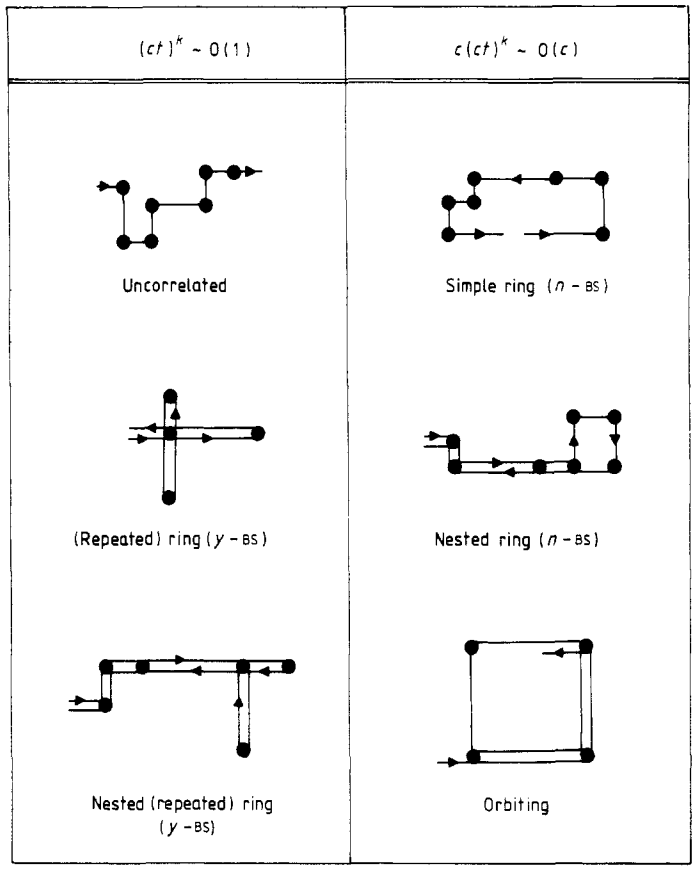

Figure 1. Examples of collision sequences that contribute to order 1 (left) or to order c (right).

In this paper we develop a method that, for lattice gases with backscattering, resums in one stroke a large class of $\mathcal{O}(1)$-diagrams. The method is essentially an effective medium approach.

The paper is organised as follows: the model is defined in § 2, where also the equation for the time evolution of the probability distribution is constructed. Time correlation functions and transport coefficients are introduced in § 3 and calculated in § 4 in the Boltzmann approximation. Section 5 contains the effective medium theory, which is solved numerically and compared with computer simulations in § 6. The analytic solution at small density of scatterers is studied in § 7, while § 8 treats low- and high-density corrections to the diffusion coefficient. Conclusions and results are summarised in § 9 and technical details are given in two appendices.

2. Chapman–Kolmogorov equation

We consider a Lorentz gas on a d-dimensional cubic lattice [1, 10] with N sites, unit lattice distance and a fraction c of sites—chosen at random—occupied by scatterers. A particle moves at times $t = 0, 1, 2, \ldots$ with unit speed from site to site. Its trajectories

are straight lines until the particle hits a scatterer, where it will be scattered into one of the lattice directions with probabilities depending on the incident velocities.

Let $p(n, i, t)$ be the probability in a given configuration of scatterers that the moving particle is at site n and *arrives* there with 'velocity' i (i.e. comes from lattice site $n - e_i$). Here velocity variables $i, j, \ldots$ take the values $i, j = 1, 2, \ldots, 2d \bmod(2d)$ and refer respectively to the lattice directions $e_x, e_y, \ldots, e_d, e_{-x}, e_{-y}, \ldots, e_{-d}$. The microscopic or fluctuating density of scatterers is described by the random variable c_n taking on the values

$$c_n = \begin{cases} 1 & \text{with probability } c \\ 0 & \text{with probability } 1-c. \end{cases} \tag{2.1}$$

The distribution function for the moving particle is $\langle p(n, i, t)\rangle$, where $\langle \ldots \rangle$ denotes an average over the configuration of scatterers, i.e. an average over all c_n with weight function (2.1).

If all $c_n = 1$, the moving particle performs a random walk with correlated jumps [15, 9]. For $c < 1$ the model represents a lattice version of the Lorentz gas. The scattering laws are further specified by introducing a transmission probability α, a reflection probability β and a deflection probability γ for any orthogonal direction with normalisation

$$\alpha + \beta + 2(d-1)\gamma = 1. \tag{2.2}$$

We write this in the form of a $2d \times 2d$ transition matrix

$$W_{ij} = \begin{pmatrix} \alpha\gamma\gamma \ldots \beta\gamma\gamma \ldots \\ \gamma\alpha\gamma \ldots \gamma\beta\gamma \ldots \\ \gamma\gamma\alpha \ldots \gamma\gamma\beta \ldots \\ \ldots\ldots\ldots\ldots \\ \beta\gamma\gamma \ldots \alpha\gamma\gamma \ldots \\ \gamma\beta\gamma \ldots \gamma\alpha\gamma \ldots \\ \gamma\gamma\beta \ldots \gamma\gamma\alpha \ldots \\ \ldots\ldots\ldots\ldots \end{pmatrix} \tag{2.3}$$

with $\Sigma_j W_{ji} = \Sigma_i W_{ji} = 1$.

If all sites are occupied by scatterers, i.e. all $c_n = 1$, one simply constructs the Chapman–Kolmogorov (CK) equation for the probability distribution [16], namely

$$\begin{aligned} p(n + e_i, i, t+1) &= \sum_j W_{ij} p(n, j, t) \\ &= \alpha p(n, i, t) + \beta p(n, -i, t) + \gamma \sum_{j \neq \pm i} p(n, j, t) \end{aligned} \tag{2.4a}$$

or in matrix notation

$$p(t+1) = S^{-1} W p(t). \tag{2.4b}$$

Here, the probability distribution $p(t)$ is considered as a $2dN$-dimensional vector with labels (n, i), the 'free streaming operator' S, shifting the particle with phase (n, i) to $(n + e_i, i)$, is a $2dN \times 2dN$ matrix:

$$S_{ni,mj} = S_{nm}\delta_{ij} = \delta_{n+e_i,m}\delta_{ij} \tag{2.5}$$

and the transition matrix W is

$$W_{ni,mj} = \delta_{nm} W_{ij}. \tag{2.6}$$

If a site does not contain a scatterer, the particle continues in its original direction. Thus, the CK equation for the probability distribution $p(n, i, t)$ for our Lorentz model in a given realisation of scatterers $\{c_n\}$ is

$$p(n+e_i, i, t+1) = (1-c_n)p(n, i, t) + c_n \sum_j W_{ij} p(n, j, t) \tag{2.7a}$$

or, in matrix form and vector notation,

$$p(t+1) = S^{-1}(1+CT)p(t) \equiv (1-L)p(t) \tag{2.7b}$$

with

$$\begin{aligned} T &= W - 1 \\ L &= 1 - S^{-1}(1+CT) \end{aligned} \tag{2.8}$$

where T is the collision operator. The matrix of density fluctuations C is diagonal in the coordinate representation, $C_{ni,mj} = c_n \delta_{nm} \delta_{ij}$. We note that the steady-state solution of (2.7) is uniform, namely $p(n, i, \infty) = \text{constant} = (2dN)^{-1}$.

There is a subtlety in the recursion relation (2.7*b*) regarding the initial condition. It is imposed by prescription of $p(n, i, 0+)$, where $p(n, i, 0+)$ specifies the *outgoing* velocity at time $t = 0+$. Consequently $p(n, i, 1) = p(n-e_i, i, 0)$ or $p(1) = S^{-1}p(0)$ (recall that for $t > 0$, $p(n, i, t)$ gives the incoming velocities). Equation (2.7*b*) applies for $t \geqslant 2$ and has the formal solution

$$\begin{aligned} p(t) &\equiv P(t)p(0) \\ &= [S^{-1}(1+CT)]^{t-1} S^{-1} p(0) = (1-L)^{t-1} S^{-1} p(0). \end{aligned} \tag{2.9}$$

Equation (2.7) applies also to the conditional probability $P(t)$, or explicitly $P_{ni,mj}(t)$, with initial condition $P(0) = 1$ or $P_{ni,mj}(0) = \delta_{nm}\delta_{ij}$. Regarding notation it will prove convenient to use a separate vector and matrix notation for $2d$-vectors and $2d \times 2d$ matrices in the velocity labels i, j only, $i, j = 1, 2, \ldots, 2d$. In this notation (i, j) labels are suppressed and the explicit dependence on position variables is indicated by subscripts. For instance, $P_{nm}(t)$ is a matrix with components $(P_{nm}(t))_{ij} = P_{ni,mj}(t)$. We will further use diagonal matrices of the form V_α $(\alpha = x, y, z, \ldots, d)$, defined as $(V_\alpha)_{ij} = (e_i)_\alpha \delta_{ij}$, where $(e_i)_\alpha$ is the αth cartesian component of the ith lattice vector e_i. Furthermore, $\exp(iqV) = \exp(\Sigma_\alpha \, iq_\alpha V_\alpha)$ and $S_{nm}(V) = \delta_{n+V,m}$ (see (2.5)), where $(f(V))_{ij} = f(e_i)\delta_{ij}$.

The $2d$-vectors will be denoted by kets and we can construct a basis from $|1\rangle$, $|V_\alpha\rangle$ and $|V_\alpha^2\rangle$ with $\alpha = x, y, z, \ldots, d$, where $(|1\rangle)_i = 1$ and $|V_\alpha^l\rangle = V_\alpha^l |1\rangle$. In addition, an inner product is introduced as

$$\langle a|b\rangle = \frac{1}{2d} \sum_i (|a\rangle)_i (|b\rangle)_i. \tag{2.10}$$

For some further properties of cubic symmetric matrices and vectors we refer to appendix 1.

We further note that the matrix $S_{nm}(V)$ is translationally invariant, as it depends only on $(n-m)$; however, the evolution operator on the RHS of (2.7*b*), i.e.

$$L_{nm} = \delta_{nm} - (S^{-1})_{nm}(1+c_m T) \tag{2.11}$$

is not translationally invariant, because it depends explicitly on m. Let A_{nm} be a translationally invariant matrix; hence it is diagonal in Fourier representation with diagonal elements

$$\hat{A}(q) = \sum_n e^{-iqn} A_{n0}. \tag{2.12}$$

The inverse transformation is

$$A_{n0} = N^{-1} \sum_{q \in 1BZ} e^{iqn} \hat{A}(q) \equiv \int_q e^{iqn} \hat{A}(q). \tag{2.13}$$

The q are reciprocal lattice vectors, located in the first Brillouin zone (1BZ). In the thermodynamic limit ($N \to \infty$), the q sum may be replaced by an integral. The integration symbol stands for

$$\int_q (\ldots) \equiv \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{d^{(d)}q}{(2\pi)^d} (\ldots). \tag{2.14}$$

3. Correlation functions

The quantities of main interest are the response function, the velocity autocorrelation function (VACF) and the diffusion coefficient. They can all be expressed in terms of the two-time probability distribution in the steady state:

$$\langle p(n, i, t; m, j, 0) \rangle = (2dN)^{-1} \langle P_{ni,mj}(t) \rangle. \tag{3.1}$$

Here the initial distribution $p(n, i, 0) = (2dN)^{-1}$ is taken to be the steady-state solution. The probability for a displacement $(n-m)$ may be obtained from (3.1) by summing over all i, j:

$$(2dN)^{-1} \sum_{ij} \langle P_{ni,mj}(t) \rangle = N^{-1} \langle 1 | P_{nm}(t) | 1 \rangle. \tag{3.2}$$

The bracket expression on the RHS of (3.2) also implies an average $\langle \ldots \rangle$ over the random variables $\{c_n\}$. Hence it depends only on $(n-m)$ because of translational invariance. The Fourier transform or the intermediate scattering function generates the moments of displacement. Similarly for the velocity autocorrelation function (VACF):

$$\varphi(t) = \frac{1}{2d} \sum_n \sum_{ij} e_{ix} e_{jx} \langle P_{ni,0j}(t+1) \rangle = \sum_n \langle V_x | P_{n0}(t+1) | V_x \rangle \tag{3.3}$$

where $\varphi(0) = 1/d$. Then the diffusion coefficient is given by the following time correlation expression [5, 17-19]:

$$D = \frac{1}{2d} + \sum_{t=1}^{\infty} \varphi(t). \tag{3.4}$$

The basic quantity in which all correlation functions can be expressed is the Laplace transform of $\langle P(t) \rangle$, referred to as the propagator. It is defined as a $2dN \times 2dN$ matrix

$$\begin{aligned} \Gamma(z) &= \sum_{t=1}^{\infty} (1+z)^{-t} \langle P(t) \rangle \\ &= \langle (z+L)^{-1} S^{-1} \rangle = \langle [(1+z)S - 1 - CT]^{-1} \rangle. \end{aligned} \tag{3.5}$$

The second equality was obtained with the help of (2.8). The dynamic structure function or response function $\mathscr{F}(q, z)$ is the Fourier-Laplace transform of (3.2). It can be expressed in terms of the propagator (3.5) as

$$\mathscr{F}(q, z) = \sum_{t=1}^{\infty} \sum_{n} (1+z)^{-t} \, \mathrm{e}^{-\mathrm{i}qn} \langle 1 | P_{n0}(t) | 1 \rangle = \langle 1 | \hat{\Gamma}(q, z) | 1 \rangle \tag{3.6}$$

where the Fourier representation (2.12) of Γ has been used. Similarly, the Laplace transform of the VACF becomes, on account of (3.2) and (3.5):

$$\Phi(z) = \sum_{t=1}^{\infty} (1+z)^{-t} \varphi(t-1) = \langle V_x | \hat{\Gamma}(0, z) | V_x \rangle. \tag{3.7}$$

The present analysis of the probability distribution and time correlation functions shows that the correlated random walk on a disordered lattice can be formulated as a standard kinetic theory problem for a Lorentz gas. In the next sections we exploit these similarities by using the Boltzmann equation and the self-consistent ring equation to calculate correlation functions and transport properties.

4. The Boltzmann equation

What happens at low concentration of scatterers? If all $c_n = 0$ in (2.11), then $L = 1 - S^{-1}$ refers to free streaming. In the zero-density limit time correlations do not decay; the mean square displacement grows like t^2 and diffusion does not exist. However, if c is small but finite, then diffusive motion is observed for times $t \gg c^{-1}$, where $t_{\mathrm{mf}} \sim c^{-1}$ is the mean free time between collisions, and one expects the probability distribution $\langle p(n, i, t) \rangle$ of the moving particle to be described by a Boltzmann-type equation. In such an equation the time evolution is governed by the dynamics of the encounters of the moving particle with *different* scatterers. Only uncorrelated collisions are taken into account and all correlated collisions (returns, ring collisions) are being neglected. Thus, the average over the configurations of scatterers can simply be carried out by replacing all c_n by their average $\langle c_n \rangle = c$ or the matrix L in (2.8) and (2.11) by $\mathscr{L}^{\circ} = \langle L \rangle$. We adopt the convention of a superscript o to indicate quantities in the Boltzmann approximation. The equation of motion, resulting from this approximation is obtained from (2.7*a*) by replacing c_n by c, and reduces to the Chapman-Kolmogorov equation (2.4*a*) for a *random walk* on a uniform lattice with α, β and γ replaced by $\alpha' = 1 - c(1-\alpha)$, $\beta' = c\beta$ and $\gamma' = c\gamma$, respectively. There exists extensive literature [15, 9] on this subject, where in particular the results for the forward jump model ($\beta' = \gamma'$) [15, 20] and for the general model ($\alpha' \neq \beta' \neq \gamma'$) [9, 21] are most useful in our case.

In the next part of this section we calculate a few results in the Boltzmann approximation. A discussion of the relevance of these results is postponed till the last section.

Since the average matrix $\mathscr{L}^{\circ}_{nm} = \langle L_{nm} \rangle$ in (2.11) is translationally invariant, it is diagonalised by Fourier transformation with

$$\hat{\mathscr{L}}^{\circ}(q) = \sum_{n} \mathrm{e}^{-\mathrm{i}qn} \mathscr{L}^{\circ}_{n0} = 1 - \mathrm{e}^{-\mathrm{i}qV}[1 + cT] \tag{4.1}$$

where $\hat{S}^{-1}(q) = \exp(-\mathrm{i}qV)$ is the Fourier transform of $S^{-1}_{nm}(V) = \delta_{n-V,m}$. The propagator of the moving particle (3.5) becomes in the Boltzmann approximation:

$$\hat{G}^{\circ}(q, z) = (z + \hat{\mathscr{L}}^{\circ}(q))^{-1} \, \mathrm{e}^{-\mathrm{i}qV} = [(1+z) \, \mathrm{e}^{\mathrm{i}qV} - 1 - cT]^{-1}. \tag{4.2}$$

The calculation of $\hat{G}^\circ(q, z)$ is similar to that of the Green function in the theory of lattice dynamics of harmonic crystals [22]. The study of the spectrum of $\hat{\mathscr{L}}^0(q)$ is similar to that of the acoustical (here diffusive) and optical (here kinetic) branches of phonon (here relaxation) spectra, where the symmetries of the crystallographic point groups lead to important simplifications.

The simplifications due to cubic symmetry (see appendix 1) are most drastic when calculating quantities that only involve the long-wavelength limit of (4.1) and (4.2), in which case eigenvalues (A1.4) and (A1.5) and eigenfunctions (A1.1) and (A1.2) are known explicitly. Take, for instance, the VACF where

$$\varphi^\circ(t) = \langle V_x | (1 - \hat{\mathscr{L}}^\circ(0))^t | V_x \rangle = d^{-1}(1 - \lambda_1^\circ)^t. \tag{4.3}$$

The matrix $\hat{\mathscr{L}}^\circ(0) = -cT = c(1 - W)$ has the general cubic symmetric form discussed in appendix 1, with eigenvalues and eigenvectors given by (A1.4). Hence $|V_x\rangle$ is an eigenvector of $\hat{\mathscr{L}}^\circ(0)$ with eigenvalue λ_1°, given by

$$\lambda_1^\circ = -ct_1 = c(1 - w_1) = c(1 - \alpha + \beta) \tag{4.4}$$

where w_1 and t_1 are the $l = 1$ eigenvalues of W in (2.3) and $T = W - 1$. Summing (4.4) up to some finite limit yields a time-dependent diffusion coefficient; summing once more over t yields the detailed time dependence of the mean square displacement. The diffusion coefficient in the Boltzmann approximation follows from (3.4) and (4.3) as

$$D^\circ = (d\lambda_1^\circ)^{-1} - (2d)^{-1} = \frac{2 - c(1 - \alpha + \beta)}{2dc(1 - \alpha + \beta)}. \tag{4.5}$$

Suppose that the Boltzmann approximation indeed represents the correct low-density behaviour (which is not always the case; see § 7); then we see that the subtracted term $(2d)^{-1}$ in (4.5) is of relative $\mathscr{O}(c)$. There exist of course many more terms coming e.g. from ring and orbiting collisions [1] that also contribute to $cD(c)$ terms of $\mathscr{O}(c)$. In a systematic low-density theory the term $(2d)^{-1}$ in (4.5) should therefore be neglected.

If the lattice is completely filled with scatterers (all $c_n = 1$) then $L = 1 - S^{-1}W$ and the Lorentz gas reduces to the random walk (2.4) on a uniform lattice. The diffusion coefficient is known exactly (equation (4.5) with $c = 1$) from the theory of correlated random walks [15] on uniform lattices:

$$D = \frac{1}{d}\left[\frac{1}{\lambda_1^\circ} - \frac{1}{2}\right] = \frac{1}{2d}\,\frac{1 + \alpha - \beta}{1 - \alpha + \beta}. \tag{4.6}$$

In an almost filled lattice, i.e. at a low concentration $p = 1 - c$ of 'holes', the $\mathscr{O}(p)$ terms in (4.5) do not account for all $\mathscr{O}(p)$ corrections, as will be discussed in § 8.

5. Effective medium approximation (EMA)

The Boltzmann equation sums all uncorrelated collision sequences of the moving particle with fixed scatterers, i.e. the particle visits each scatterer at most once. In a systematic low-density theory one has to resum all $\mathscr{O}(1)$ collision events (see figure 1). For the general case of collisions with backscattering this involves not only uncorrelated collisions but, for instance, also rings, repeated and nested rings and orbiting events. In a single or repeated ring collision the particle returns respectively once or repeatedly to the same scatterer. In between two successive returns to the same scatterer the

particle collides with a set of scatterers to which it will never return afterwards. In the EMA that we will develop here, which is very similar to the self-consistent ring kinetic equations, all intermediate collision sequences are restricted to uncorrelated collisions and to nested and repeated ring collisions.

We try to perform the summation of these collisions by replacing the random matrix L in (3.5) by an effective sure matrix $\mathscr{L}$ for a uniform lattice, where the form of $\mathscr{L}$ has to be determined. In the Boltzmann approximation the random matrix L was replaced by $\mathscr{L}^0 = \langle L \rangle$ or, equivalently, the random matrix C was replaced by $\langle C \rangle = c$. In the EMA equation we try to represent the sum of all repeated ring collisions in (3.5) by a sure matrix $\mathscr{L}(z)$ with the same structure as $\langle L \rangle$, in which the collision matrix is replaced by the effective $T^e(z)$. This yields for the propagator (3.5) in EMA:

$$G(z) = (z + \mathscr{L}(z))^{-1} S^{-1} = [(1+z)S - 1 - cT^e(z)]^{-1}. \tag{5.1}$$

The procedure is completely the same as adding in the expressions for Green functions and correlation functions (3.5) a counterterm $T^e(z) - T$, to the Boltzmann $\langle L \rangle$. The method followed here is similar to Webman's derivation [23] of the effective medium approximation for random resistor networks and hopping models. Self-consistency in the sense of EMA requires the counterterm to be chosen such that all ring and repeated and nested ring terms vanish identically in a perturbation expansion of the propagator $\Gamma = \langle (z+L)^{-1} S^{-1} \rangle$ in powers of

$$\delta\mathscr{L} = \mathscr{L} - L = S^{-1}[CT - cT^e(z)] \equiv S^{-1}\delta T. \tag{5.2}$$

Once the matrix $T^e(z)$ of the effective medium is determined from this self-consistency condition, calculation of response function, VACF and diffusion coefficient in terms of $T^e(z)$ is the same as in the Boltzmann equation. The final inverse Laplace transform, back to the time variable, will of course be very complicated.

We quote for later reference the EMA value of the diffusion coefficient, which is analogous to (4.3)-(4.5)

$$D = \frac{1}{d}\left[\frac{1}{\lambda_1} - \frac{1}{2}\right]. \tag{5.3}$$

Here $\lambda_l = -ct_l^e$, where t_l^e $(l = 1, 2)$ is the l eigenvalue of the matrix $T^e(z=0)$ (see appendix 1).

We continue by expanding the resolvent $(z+L)^{-1}S^{-1}$ in (3.5) in powers of δT using (5.2). This yields

$$[(z+L)^{-1}S^{-1}]_{n0} = G_{n0} + \sum_m G_{nm}\delta T_m G_{m0} + \sum_{mm'} G_{nm}\delta T_m G_{mm'}\delta T_{m'} G_{m'0} + \ldots \tag{5.4}$$

and the matrix δT in (5.2) is diagonal in this representation. The labels m, m' on δT may refer to the same site or to different sites. We sum all intermediate sequences in (5.3) referring to the same site (repeated rings) by introducing a Θ matrix:

$$\Theta_n \equiv \delta T_n + \delta T_n G_{00}\delta T_n + \delta T_n G_{00}\delta T_n G_{00}\delta T_n + \ldots = \delta T_n (1 - R\delta T_n)^{-1} \tag{5.5}$$

with $R \equiv G_{nn} = G_{00}$ because of translational invariance. Also note that δT_n depends only on the single random variable c_n.

Combination of (5.2) and (5.4) yields for the propagator (3.5) in coordinate representation:

$$\Gamma_{n0} = G_{n0} + \sum_m G_{nm}\langle\Theta_m\rangle G_{m0} + \sum_{mm'}{}' G_{nm}\langle\Theta_m G_{mm'}\Theta_{m'}\rangle G_{m'0} + \ldots \tag{5.6}$$

with the restriction that the site labels on two consecutive Θ_m be different. As discussed below (5.1), self-consistency imposes the $2d \times 2d$ matrix condition for the effective medium [23]:

$$\langle \Theta_n \rangle = \langle \delta T_n / (1 - R\delta T_n) \rangle = 0. \tag{5.7}$$

Recall that $\delta T_n = c_n T - cT^e(z)$ on account of (5.2). This condition determines the collision matrix $T^e(z)$ of the effective medium. With the help of the relation $\langle f(c_n) \rangle = cf(1) + (1-c)f(0)$ for the quenched average, condition (5.7) can be evaluated to yield the EMA condition for self-consistency of the effective collision operator. After some algebra one finds

$$T^e = T + TRT^e - cT^e R T^e \tag{5.8}$$

where we accounted for possible non-commutability of T, T^e and R. For completeness and later reference the ring integral R is expressed using (2.13) in the Fourier transform of the propagator:

$$R(z) \equiv G_{00}(z) = \int_q \hat{G}(q, z) = \int_q [(1+z)\, e^{iqV} - 1 - cT^e(z)]^{-1}. \tag{5.9}$$

The coupled set of matrix equations (5.8), (5.9) determines the effective collision operator $T^e(z)$ and will be referred to as the *EMA equations*. Non-vanishing corrections to the EMA involve terms that contain *at least* two scatterers *and* at least two Θ referring to the same site. Expressed in the EMA propagator and the first non-vanishing correction to EMA, an expansion of the exact propagator is written as

$$\langle (z+L)^{-1} S^{-1} \rangle_{n0} = G_{n0} + \sum_{m \neq m'} G_{nm} \langle \Theta_m G_{mm'} \Theta_{m'} G_{m'm} \Theta_m G_{mm'} \Theta_{m'} \rangle G_{m'0} + \ldots . \tag{5.10}$$

6. Transition rates of the effective medium

To analyse the EMA equations (5.7) we observe that $T^e(z)$ and $R(z)$ are cubic symmetric matrices of the form (2.3) (see also (A1.4)), containing for general d-values three independent elements with known eigenvalues and eigenvectors (A1.4). However, among the elements of $T^e(z)$ there are only two independent ones by conservation of probability, i.e. $T^e(z)|1\rangle = 0$ or $\Sigma_j T^e_{ij}(z) = 0$, as follows from (5.8) and $T|1\rangle = 0$. Therefore the EMA matrix condition (5.7) imposes two independent conditions. This is an extension of the standard EMA as used in the theory of random resistor networks [24] where the effective medium approximation introduces only a single effective transition rate.

For calculating diffusion coefficients it is sufficient to study only the limit $z \to 0$ of (5.1). We will restrict ourselves to this limit in actual calculations. Denoting the eigenvalues of R, T and T^e by r_l, t_l and t^e_l ($l = 0, 1, 2$) respectively, we obtain the following relation between the eigenvalues:

$$t^e_l = t_l + r_l t_l t^e_l - c r_l (t^e_l)^2. \tag{6.1}$$

Before solving this equation it is convenient to express (6.1) in terms of the relaxation constants, defined as

$$\lambda_l = -ct^e_l \qquad \tau_l = 1 - w_l = -t_l \qquad l = 1, 2. \tag{6.2a}$$

We have already seen that $T^e|1\rangle = 0$ or $\lambda_0 = 0$. We further express τ_l in terms of the primary parameters α, β, γ using the expressions (A1.4) for the eigenvalues w_l of the cubic symmetric matrix W in (2.3). This yields:

$$\begin{aligned} \tau_0 &= 0 \\ \tau_1 &= 1-\alpha+\beta \qquad = 2\beta+2\gamma \\ \tau_2 &= 1-\alpha-\beta+2\gamma = 4\gamma. \end{aligned} \tag{6.2b}$$

The EMA equation (6.1) reduces then to $r\lambda^2-(1+r\tau)\lambda+c\tau=0$ with solution

$$\lambda_l = (2r_l)^{-1}[1+r_l\tau_l-[(1+r_l\tau_l)^2-4cr_l\tau_l]^{1/2}]. \tag{6.3}$$

The unknown relaxation constants λ_l of the effective medium depend on the eigenvalues r_l of the ring matrix R in (5.9), in which the effective collision operator T^e appears itself again, or equivalently its eigenvalues λ_1 and λ_2. So $r_l = r_l(\lambda_1, \lambda_2)$, which in combination with (6.3) yields two coupled equations from which λ_1 and λ_2 can be solved.

As the next step we calculate $r_l = r_l(\lambda_1, \lambda_2)$. As the right and left eigenvectors are known (see (A1.3)-(A1.5)), the eigenvalues can be expressed as

$$r_l = \langle\tilde{\psi}_{lx}|R|\psi_{lx}\rangle = \langle\tilde{\psi}_{ly}|R|\psi_{ly}\rangle = \int_q \langle\tilde{\psi}_{lx}|A_l\rangle \tag{6.4}$$

where $|A_l\rangle$ satisfies $(l=1,2)$

$$\{e^{iqV}-1-cT^e\}|A_l\rangle = |\psi_{lx}\rangle. \tag{6.5}$$

From here on we restrict ourselves to the two-dimensional case. For details on the calculation of the eigenvalues r_l we refer to appendix 2. The results are

$$r_l(\lambda_1, \lambda_2) = \frac{A_l-2B_l}{E-2F} + \frac{(B_lE-A_lF)}{(E-2F)F}J \tag{6.6}$$

where A_l, B_l, E and F are polynomial functions of λ_1 and λ_2:

$$\begin{aligned} A_1 &= -\tfrac{1}{2}(1-\tfrac{1}{2}\lambda_1)(1-\tfrac{1}{2}\lambda_2) & B_1 &= \tfrac{1}{16}\lambda_2(1-\lambda_1) \\ A_2 &= -\tfrac{1}{2}(1-\tfrac{1}{2}\lambda_1)^2 & B_2 &= \tfrac{1}{8}\lambda_1(1-\tfrac{1}{2}\lambda_1) \\ E &= (1-\tfrac{1}{2}\lambda_1)^2(1-\tfrac{1}{2}\lambda_2) & F &= \tfrac{1}{8}\lambda_1\lambda_2(1-\tfrac{1}{2}\lambda_1) \end{aligned} \tag{6.7}$$

and J is given by

$$J = \begin{cases} \delta\left(1+\dfrac{2}{\pi}\tan^{-1}\tfrac{1}{2}(\delta^{-1}-\delta)\right) & \text{for} \quad \delta^2>0 \\ \dfrac{2}{\pi}\eta\ln\dfrac{\eta+1}{\eta-1} & \text{for} \quad \delta^2=-\eta^2<0 \end{cases} \tag{6.8}$$

with $\delta^2 = F/(E-F)$. (See also (A2.5) and (A2.10).)

Summarising our EMA analysis, (6.6)-(6.8) give the eigenvalues r_l $(l=1,2)$ of the ring matrix R as an explicit function $r_l(\lambda_1, \lambda_2)$ of the (unknown) eigenvalues $\lambda_l = -ct_l^e$ of the EMA collision matrix T^e. The EMA equation (6.3) gives an independent expression for λ_l as a function of r_l. Combination of (6.6) and (6.3) yields a set of coupled transcendental equations from which λ_l or, equivalently, r_l can be solved. Equations (6.3) and (6.6) are equivalent to the EMA equations (5.8) and (5.9). Once the λ_l are determined, (5.3) gives the EMA value of the diffusion coefficient $D = (2\lambda_1)^{-1}-\frac{1}{4}$ as a function of the density of scatterers c.

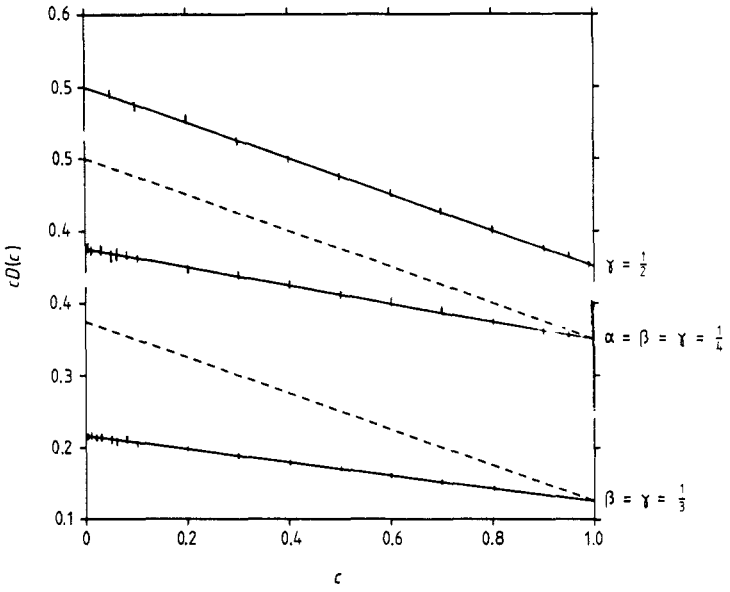

Figure 2. Results for the diffusion coefficient for some typical sets of model parameters. Full lines represent EMA results, broken lines Boltzmann approximation results. Simulations are indicated by their error bars only.

We have numerically solved the EMA equations for several values of the model parameters α, β and γ and determined the diffusion coefficient $D(c)$ as a function of the density c. The results are shown in figure 2 as full lines. We have also plotted (as broken lines) the diffusion coefficient $cD^{\circ}(c)$ in (4.5), as calculated from the uncorrelated collision (Boltzmann) approximation. The plot shows that EMA and Boltzmann results effectively coincide for a typical case without backscattering ($\gamma = \frac{1}{2}$), but it also shows that in models with backscattering there exist *large differences* between the EMA and the Boltzmann values, particularly at low densities.

To test the predictions of the EMA we have performed computer simulations for the present Lorentz model [1]. The measured diffusion coefficients are also shown in figure 2. The results obtained from simulations are in excellent agreement with the EMA results, and strongly deviate from the predictions of the Boltzmann equation in cases with backscattering. In order to understand these deviations we will study the EMA equations analytically at low and high densities. This will be done in the subsequent sections.

7. Breakdown of the Boltzmann equation

In this section we analyse the EMA equations in the limit as $c \to 0$. Here (6.3) reduces to

$$\lambda_l \simeq c\tau_l/(1 + r_l\tau_l) \qquad c \to 0 \tag{7.1}$$

and the corresponding diffusion coefficient (5.3) is, to leading order, given by

$$D \simeq (2c\tau_1)^{-1}(1 + r_1\tau_1) \qquad c \to 0 \tag{7.2}$$

where the c dependence of r_l still has to be determined. We therefore analyse the ring eigenvalues r_l in (6.6) for $c \to 0$. As λ_l is proportional to c, the dominant low-density contribution of the coefficients in (6.7) is $A \sim E \sim \mathcal{O}(1)$, $B \sim \mathcal{O}(c)$ and $F \sim \mathcal{O}(c^2)$. The parameter δ in (6.8) is $\mathcal{O}(c)$ with $\delta = (\lambda_1\lambda_2/8)^{1/2} = \mathcal{O}(c)$, and the coefficient (6.8) reduces to $J = 2\delta + \mathcal{O}(c)$. Therefore, the resulting expressions (6.6) for the ring eigenvalues r_l simplify to

$$r_1 = -\tfrac{1}{2} + \tfrac{1}{2}y^{-1} \qquad r_2 = -\tfrac{1}{2} + \tfrac{1}{2}y \qquad y^2 = 2\lambda_1/\lambda_2 \tag{7.3}$$

where terms of $\mathcal{O}(c)$ have been neglected. Calculating y from (7.1) and inserting (7.3) gives a closed quadratic equation for y with solution

$$y = (2a)^{-1}\{1 + [1 + 8ab]^{1/2}\} \tag{7.4a}$$

with

$$a = 2/\tau_1 - 1 = (\alpha + \gamma)/(\beta + \gamma) \qquad b = 2/\tau_2 - 1 = (\alpha + \beta)/2\gamma \tag{7.4b}$$

on account of (6.2b). Combining these results with (7.2) yields the effective medium approximation (EMA) or self-consistent repeated ring equation to lowest order in the concentration.

There is a peculiar cancellation of the leading terms of $\mathcal{O}(1)$ in the ring eigenvalues r_l in (7.3) if the reflection probability is vanishing ($\beta = 0$). This cancellation comes about because at low densities $\lambda_l = c\tau_l = 2l\gamma c$ ($l = 1, 2$) for $\beta = 0$, on account of (6.2). Consequently, (7.3) shows that $y = 1 + \mathcal{O}(c)$ and $r_l \sim \mathcal{O}(c)$. The *diffusion coefficient* to lowest order is given by the *Boltzmann* value $D^\circ \sim (2c\tau_1)^{-1}$ on account of (7.2). In figure 2 the diffusion coefficient is plotted as a function of the density of scatterers. Only one typical case with non-vanishing reflection probability ($\alpha = 0$, $\beta = 0$, $\gamma = \frac{1}{2}$) is shown in this plot. In general, for cases without backscattering, the Boltzmann value, cD°, determines the intercept of $cD(c)$ with the vertical axis. In the next section the slope at $c = 0$ will be calculated.

Next we consider collisions with *backscattering*, where $\beta \neq 0$. Here $y \neq 1$ for small c and the ring eigenvalues r_l in (7.3) are of $\mathcal{O}(1)$ as $c \to 0$. Consequently the low-density limit of the EMA diffusion coefficient in (7.2), $D = D^\circ(1 + r_1\tau_1)$, differs drastically from the Boltzmann prediction! The value of the correction factor D/D° can be calculated from (7.3) and (7.4) and is listed in table 1 for some typical cases. We want to stress that this is a surprising result because it shows the breakdown of the Boltzmann equation as a correct low-density kinetic theory in a two-dimensional system.

For models with backscattering we also calculate the eigenvalues r_l^0 of the *simple ring matrix* R°, which is defined by (5.9) with T^e replaced by T. Then (7.3) yields for

Table 1. Comparison of Boltzmann value D°, simple ring result D_R and EMA result D for the diffusion constant, in some typical cases with non-vanishing reflection probabilities

	$cD^\circ\ (c \to 0)$	$D_R/D^\circ\ (c \to 0)$	$D/D^\circ\ (c \to 0)$
$\alpha = \beta = \gamma = \frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}(2+\sqrt{2})$	$\frac{3}{4}$
$\beta = \gamma = \frac{1}{3}$	$\frac{3}{8}$	$\frac{1}{3}(1+\sqrt{2})$	$1/\sqrt{3}$
$\beta = \frac{3}{5}$, $\gamma = \frac{1}{5}$	$\frac{5}{16}$	$\frac{3}{5}$	$\frac{1}{3}$
$\beta = \frac{4}{5}$, $\gamma = \frac{1}{10}$	$\frac{5}{18}$	$\frac{2}{5}$	$\frac{1}{10}[(9+\sqrt{41})/(3+\sqrt{41})]$

the relevant ring eigenvalue

$$r_1^0 \simeq -\frac{1}{2}+\frac{1}{2}\left(\frac{\gamma}{\beta+\gamma}\right)^{1/2} \tag{7.5}$$

to dominant order in c, and for the corresponding diffusion coefficient:

$$D_R = D^0(1+r_1^0\tau_1). \tag{7.6}$$

The values of this correction factor are also listed in table 1 for some typical values. Note that it lies roughly halfway between the Boltzmann value and the EMA value.

8. High- and low-density corrections for diffusion

In this section we consider linear corrections to the diffusion coefficient at high and low densities of scatterers. The model at $c=1$ describes a lattice uniformly filled with scatterers. The present Lorentz model (2.7) reduces to the standard random walk with correlated jumps (2.4) for which the diffusion coefficient is known *exactly*. It was given already in (4.6) and its values appear in figure 2 at $c=1$. At a high concentration of scatterers ($p=1-c$ small) the EMA equations (6.3) and (6.6) can be solved perturbatively, i.e.

$$\lambda_l \simeq \tau_l(1-p/(1-\tau_l r_l)) \qquad p\to 0 \tag{8.1}$$

and the corresponding diffusion coefficient (5.3) is

$$D \simeq (2\tau_1)^{-1}(1+p/(1-\tau_1 r_1))-\tfrac{1}{4} \qquad p\to 0. \tag{8.2}$$

Here the ring eigenvalues r_l should be evaluated at $c=1$. This can be simply achieved by replacing in (6.6)-(6.8) all λ_l by τ_l on account of (8.1), where the τ_l are given in (6.2*b*) in terms of the parameters α, β and γ. Equation (8.2) with $r_l(\lambda_1,\lambda_2)$ in (6.6) evaluated at $\lambda_l=c\tau_l$ determines the dominant high-density correction of $\mathcal{O}(p)=\mathcal{O}(1-c)$ to the diffusion coefficient (4.6) for a random walker on a lattice, almost completely filled with scatterers. In figure 2 these results determine the slopes of $cD(c)$ at $c=1$. The structure of (8.1) at a low concentration p of holes is in complete agreement with the general results for hopping models on random lattices with a low concentration of impurities [25]. The coefficient of p in λ_l has the form $-\tau_l/(1-\tau_l r_l)=-\tau_l(1+\tau_l r_l+\tau_l^2 r_l^2+\ldots)$, summing first encounter, first return, second return ... of the RW to the same impurity (being a hole in this case).

Next we consider low densities, where the EMA equations (6.3) and (6.6) can again be solved perturbatively. In order to do so, the approximation to (6.3) has to include terms of relative $\mathcal{O}(c)$.

One has to distinguish cases without backscattering ($\beta=0$) and with backscattering ($\beta\neq 0$). In the latter case we will not calculate terms of relative $\mathcal{O}(c)$, although this can be done in a straightforward manner. In the former case the contributions to λ_l and D of relative $\mathcal{O}(c)$ will be determined explicitly.

The calculations are lengthy, but straightforward. To start we only keep subleading terms in (6.6) that are of relative $\mathcal{O}(\lambda)$ and we use $J(\delta)=2\delta(1-2\delta/\pi)$ for δ small. The expressions for the ring values become

$$\begin{aligned} r_1 &= -\frac{1}{2}+\frac{1}{2}\left(\frac{\lambda_2}{2\lambda_1}\right)^{1/2}\left[1-\frac{2}{\pi}\left(\frac{\lambda_1\lambda_2}{8}\right)^{1/2}+\tfrac{1}{4}\lambda_1-\tfrac{1}{4}\lambda_2\right]+\tfrac{1}{8}\lambda_2 \\ r_2 &= -\frac{1}{2}+\frac{1}{2}\left(\frac{2\lambda_1}{\lambda_2}\right)^{1/2}\left[1-\frac{2}{\pi}\left(\frac{\lambda_1\lambda_2}{8}\right)^{1/2}-\tfrac{1}{4}\lambda_1+\tfrac{1}{4}\lambda_2\right]. \end{aligned} \tag{8.3}$$

For the case of interest here ($\beta = 0$), we recall from § 7 that the density independent terms in (8.3) cancel. So $r_l \sim \mathcal{O}(c)$. The EMA equation (6.3) yields therefore $\lambda_l = c\tau_l(1 - r_l\tau_l)$ with $\tau_l = 2l\gamma c$, consistently to the same order in the density. This yields in combination with (8.3):

$$\begin{aligned} r_1 &= \tfrac{1}{2}\gamma r_1 - \gamma r_2 + \left(\frac{1}{4} - \frac{1}{\pi}\right)\gamma c \\ r_2 &= -\tfrac{1}{2}\gamma r_1 + \gamma r_2 + \left(\frac{1}{4} - \frac{1}{\pi}\right)\gamma c \end{aligned} \tag{8.4}$$

with solution

$$\begin{aligned} r_1 &= c\left(\frac{1}{4} - \frac{1}{\pi}\right)\gamma(1 - 2\gamma)/(1 - \tfrac{3}{2}\gamma) \\ r_2 &= c\left(\frac{1}{4} - \frac{1}{\pi}\right)\gamma(1 - \gamma)/(1 - \tfrac{3}{2}\gamma). \end{aligned} \tag{8.5}$$

For Lorentz models without backscattering ($\beta = 0$) the analytic result for the EMA diffusion coefficient (5.3), to relative $\mathcal{O}(c)$ included, is

$$D = (1 + 2\gamma r_1)/(4c\gamma) - \tfrac{1}{4}. \tag{8.6}$$

This expression describes the slope and intercept of $cD(c)$ at $c = 0$ for cases with $\beta = 0$ (see figure 2 for the $\gamma = \frac{1}{2}$ case). It is interesting to observe that $r_1 = 0$ for $\gamma = \frac{1}{2}$, i.e. in Lorentz lattice models where the moving particle, upon collision with a scatterer, is deflected over an angle $\pm\pi/2$. Therefore, in models with $\gamma = \frac{1}{2}$, the diffusion eigenvalue r_1 vanishes at low density up to terms of $\mathcal{O}(c)$ included, and the EMA diffusion coefficient (5.3) is given by the Boltzmann approximation (4.5), $D = (2c)^{-1} - \frac{1}{4}$. Numerical solution of the EMA equations shows, in fact, that $r_1 = 0$ and $r_2 < 0$ *for all densities*, but we could not verify this analytically.

This is an interesting result. Consider the cubic symmetric ring matrix R in (5.9). Its eigenvalue $r_1 = R_{11} - R_{13} = 0$, on account of (A1.4). We recall that $R_{ij} = (G_{00})_{ij}$ is the Laplace transform at $z = 0$ (see (3.5) and (5.1)) of the matrix of conditional probabilities $\langle P_{0i,0j}(t)\rangle$. Hence, $r_1 = 0$ implies that the *probabilities* at long times for the moving particle to be back at the origin *with a velocity parallel or antiparallel to the initial one are equal* in the case of left- or right-turning collisions only ($\gamma = \frac{1}{2}$).

However, as soon as there is a non-vanishing transmission probability α (no backscattering, $\beta = 0$), the probability for antiparallel velocities is larger ($r_1 < 0$). The behaviour of r_2 is as expected. In $\gamma = \frac{1}{2}$ it follows from $r_2 = R_{11} - R_{13} - 2R_{12} = 2(R_{13} - R_{12}) < 0$ that the probability at large times to be back at the origin with a velocity perpendicular to the initial one, is larger than with a parallel one.

In general, the analytic contribution from r_1 in (8.5) (with $0 < \gamma < \frac{1}{2}$ and $\beta = 0$) to the slope of $cD(c)$ in (8.6) at small c is always very small. *Numerically* the contributions from r_1 to $cD(c)$ (with $0 < \gamma < \frac{1}{2}$ and $\beta = 0$) are negligible for all densities and in figure 2 the EMA diffusion coefficient cannot be distinguished from the Boltzmann value. In figure 3(*a*) we have plotted the relative deviations of the EMA results from the Boltzmann results for some cases without reflections.

Also for the models with reflection the EMA result resembles a straight line in the plot of $cD(c)$ against c (figure 2), although this straight line is not described by the Boltzmann expression (4.5). If we linearly interpolate between the EMA value of $cD(c)$

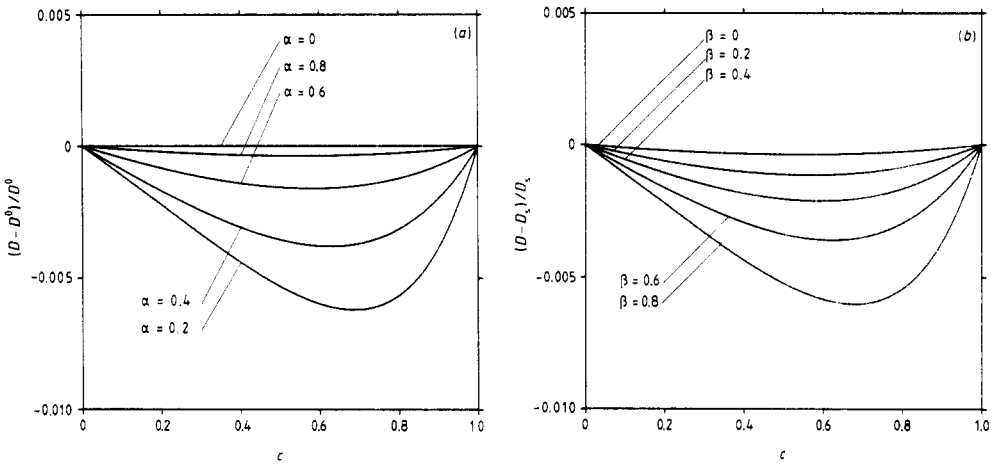

Figure 3. Relative deviations of EMA from linear behaviour for some typical models: (*a*) *without* backscattering ($\beta = 0$), relative to Boltzmann; (*b*) *with* backscattering ($\beta \neq 0$), relative to linear interpolation (D_c) between $c = 0$ and $c = 1$. Here, γ is kept fixed at the value $\gamma = 0.1$.

at $c = 0$ (see end of § 7 and table 1) and the exact value of $cD(c)$ at $c = 1$, then the relative deviation between EMA and linear interpolation is again small, as can be seen in figure 3(*b*) for some cases. For figure 3(*b*) we arbitrarily set the deflection probability to 1/10.

Before closing this section we calculate, also for cases without backscattering, the eigenvalues r_l° for the simple ring matrix R° (see end of § 7) at low densities. It follows from (8.3) by setting $\lambda_l = c\tau_l = 2l\gamma c$ with the result

$$r_1^\circ = r_2^\circ = \left(\frac{1}{4} - \frac{1}{\pi}\right)\gamma c. \tag{8.7}$$

It is interesting to compare the eigenvalues r_l° with the r_l for the self-consistent nested rings in (8.4), where some additional terms appear. One sees that r_1/r_1° decreases from 1 to 0, whereas r_2/r_2° increases from 1 to 2 as γ increases from 0 to its maximum value $\frac{1}{2}$. Thus in models with deflection only ($\gamma = \frac{1}{2}$), the contributions from the simple rings and the nested rings *cancel exactly* in the eigenvalue r_1, relevant for diffusion, *but not* in r_2.

9. Conclusion and discussion

The kinetic description of lattice Lorentz gases is very different for microdynamic collision rules that either forbid or admit backscattering. Only in the first case does the Boltzmann equation give the correct diffusion coefficient (4.5) at low densities of scatterers, as was first derived by Okamura *et al* [9]. In fact, it gives a very good representation of $D(c)$ for all densities in models without backscattering. The contributions from all types of ring collisions are *extremely* small (less than 1%). In models with backscattering ($\beta \neq 0$), the Boltzmann diffusion coefficient (4.5) at low and intermediate densities is quantitatively different from the actual D value. The Boltzmann equation fails not only in two dimensions, but for all values of d, as follows

from the phase space estimates of § 1. The reason is the discrete phase space. In comparison with a *continuous* Lorentz gas, the small set of allowed velocities in the *lattice* version gives an extremely large relative weight to reflected velocities. This introduces into d-dimensional lattice gases certain pathological features of continuous one-dimensional systems, where the Boltzmann equation also fails at low densities [26, 12].

For the square lattice we have performed explicit calculations of the diffusion coefficient by a self-consistent resummation of all ring and repeated ring sequences. This resummation is equivalent to an effective medium theory.

The diffusion coefficient, obtained from analytical and numerical solutions of the effective medium equations (see figure 2), shows excellent agreement with the results from computer simulations, both for models with and without backscattering. In the latter case, $D(c)$ is approximately equal to the Boltzmann value (4.5). Similar results were found in the Lorentz model of [6] with mirrors and no backscattering.

The agreement between EMA and simulations does not only occur at low and high densities, as expected (see §§ 7 and 8), but, surprisingly, also at intermediate densities. These findings are in line with excellent predictions of effective medium theory for diffusion coefficients in hopping models on a square lattice with bond disorder [24, 15]. We also expect that simulations performed on the backscattering models of Gunn and Ortuño [11] will agree with the predictions (7.2)-(7.4) for the diffusion coefficient, at least at low densities.

Notwithstanding the excellent agreement between diffusion coefficients from computer simulations and our effective medium theory, the values at small densities are by no means exact. Consider first Lorentz gases *with* backscattering. The EMA diffusion coefficient $cD = (1 + r_1\tau_1)/(2\tau_1)$ with r_1 from (7.3), (7.4) may *not* represent the *exact* value of $cD(c)$ as $c \to 0$. In fact, all tree-like collision trajectories (as nested and repeated rings in figure 1), in which the branches are retraced an arbitrary number of times, are proportional to $(ct)^k \sim \mathcal{O}(1)$ for $t \to \infty$ and $c \to 0$, similar to those in figure 1. For the one-dimensional continuous Lorentz gas with stochastic collision rules these collision trajectories can be resummed using a transfer matrix method [27]. However, it is not clear how this analysis can be extended to the two-dimensional case and how the exact value of $cD(c)$ at $c = 0+$ for models with reflections can be determined.

Next consider Lorentz gases *without* backscattering. Here the Boltzmann diffusion coefficient does indeed represent the dominant low-density behaviour. However, the expression for $D(c)$ in (8.6) does not include *all* contributions of relative $\mathcal{O}(c)$. The orbiting collision events of figure 1 are non-ring-type events, missing in effective medium theory. A separate calculation is required, but we have not yet carried this out. Their contributions are expected to be very small in our stochastic Lorentz model, because the probability of retracing the same closed orbit decreases exponentially with time (as opposed to periodic orbits in a deterministic Lorentz gas [5, 6]).

Finally we point out that the EMA equation (5.8) is rather similar, but not equivalent to a self-consistent resummation of nested rings or of (nested) repeated rings, where T^c in (5.8) is replaced respectively by T^N or T^{RR}, defined as

$$T^N = T + TRT$$
$$T^{RR} = T + TRT^{RR}. \tag{9.1}$$

For models *without* backscattering, these methods (standardly used in kinetic theory) are equivalent to EMA at low and high densities of scatterers. For models *with* backscattering, this is only the case for high densities (the region of random walks with

impurities). At low densities, only the second method (repeated rings) yields dominant behaviour which agrees with EMA. The expression for the ring integral, given in [1], should be replaced (for low densities *with* backscattering) by

$$R(z) = \int_q \{(1+z)e^{iqV} - 1 - cT[1 - R(z)T]^{-1}\}^{-1}.$$

The details given in [1] nevertheless remain valid, as they are in fact obtained using this representation.

In a forthcoming paper we will analyse the relations between ring, repeated ring and effective medium approximation in more detail.

The implications of backscattering on transport properties in CA fluids have been discussed in [1], where also further simulations have been suggested.

Acknowledgments

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Appendix 1

In this appendix we present the definitions and some properties of cubic symmetric matrices and their eigenvectors. Important simplifications come from the fact that all matrices have cubic symmetry. Consider the set of $2d$-vectors:

$$\begin{aligned}
&|1\rangle = (1, 1, 1, \ldots, 1, 1)\\
&|V_x\rangle = V_x|1\rangle = (1, 0, \ldots, 0, -1, 0, \ldots, 0)\\
&|V_y\rangle = V_y|1\rangle = (0, 1, 0, \ldots, 0, 0, -1, 0, \ldots, 0)\\
&\quad\vdots\\
&|V_d\rangle = V_d|1\rangle = (0, \ldots, 1, 0, \ldots, 0, -1)\\
&|V_x^2\rangle = V_x^2|1\rangle = (1, 0, \ldots, 0, 1, 0, \ldots, 0)\\
&\quad\vdots\\
&|V_d^2\rangle = V_d^2|1\rangle = (0, \ldots, 0, 1, 0, 0, \ldots, 1).
\end{aligned} \tag{A1.1}$$

Then, a biorthonormal basis $|\psi_{li}\rangle$, $|\tilde{\psi}_{li}\rangle$ $(l = 0, 1, 2)$ is defined through

$$\begin{aligned}
&|\psi_0\rangle = |\tilde{\psi}_0\rangle = |1\rangle\\
&|\psi_{1\alpha}\rangle = |\tilde{\psi}_{1\alpha}\rangle = \sqrt{d}\,|V_\alpha\rangle \qquad \alpha = x, y, \ldots, d\\
&|\psi_{2\alpha}\rangle = |dV_\alpha^2 - 1\rangle\\
&|\tilde{\psi}_{2\alpha}\rangle = |V_\alpha^2 - V_d^2\rangle \qquad \alpha = x, y, \ldots, d-1
\end{aligned} \tag{A1.2}$$

satisfying $\langle\tilde{\psi}_{l'\alpha'}|\psi_{l\alpha}\rangle = \delta_{ll'}\delta_{\alpha\alpha'}$, where an inner product is defined in (2.10). The completeness of the $2d$ basis can be expressed in terms of projectors $P_0 + P_1 + P_2 = 1$, where

$$\begin{aligned} P_0 &= |1\rangle\langle 1| \\ P_1 &= \sum_{\alpha=x}^{d} |\psi_{1\alpha}\rangle\langle\tilde{\psi}_{1\alpha}| \\ P_2 &= \sum_{\alpha=x}^{d-1} |\psi_{2\alpha}\rangle\langle\tilde{\psi}_{2\alpha}|. \end{aligned} \tag{A1.3}$$

We further observe that any $2d \times 2d$ matrix K possessing cubic symmetry and having constant coefficients (no dependence on (reciprocal) lattice vectors n or q) has necessarily the same form as W in (2.3) with α, β and γ replaced by arbitrary numbers a, b and c without the constraint (2.2). One easily verifies that any cubic symmetric matrix K has only *three* different eigenvalues k_l ($l = 0, 1, 2$) and $2d$-eigenvectors:

$$\begin{aligned} K|\psi_{l\alpha}\rangle &= k_l|\psi_{l\alpha}\rangle \\ k_0 &= a + b + 2(d-1)c \\ k_1 &= a - b \\ k_2 &= a + b - 2c \end{aligned} \tag{A1.4}$$

where $l = 0$ refers to the scalar $|1\rangle$, $l = 1$ to the vector $|V_\alpha\rangle$ (d-fold degenerate) and $l = 2$ to the tensor $|dV_\alpha^2 - 1\rangle$ ($(d-1)$-fold degenerate). Its spectral representation is

$$K = k_0P_0 + k_1P_1 + k_2P_2. \tag{A1.5}$$

Appendix 2

Here we give a detailed calculation of the eigenvalues of the ring matrix that occur in the effective medium equation (5.8). We write

$$r_l = \langle\tilde{\psi}_{lx}|R|\psi_{lx}\rangle = \langle\tilde{\psi}_{ly}|R|\psi_{ly}\rangle = \int_q \langle\tilde{\psi}_{lx}|A_l\rangle \tag{A2.1}$$

where $|A_l\rangle$ satisfies (6.5). Using the spectral representation (A1.5) of $-cT^e$ with $\lambda_0 = 0$ (see below (6.2a)), this equation can be written as

$$\{e^{iqV} - 1 + \lambda_1P_1 + \lambda_2P_2\}|A_l\rangle = |\psi_{lx}\rangle. \tag{A2.2}$$

As already mentioned, we restrict ourselves to the two-dimensional case; the eigenvectors are $|\psi_{1\alpha}\rangle = |\tilde{\psi}_{1\alpha}\rangle = \sqrt{2}|V_\alpha\rangle$ ($\alpha = x, y$) and $|\psi_2\rangle = |\tilde{\psi}_2\rangle = |V_x^2 - V_y^2\rangle$ and P_l ($l = 1, 2$) is a projection operator on the eigenspace spanned by $|\psi_l\rangle$ ($l = 1, 2$). The required functions $\langle\tilde{\psi}_{lx}|A_{lx}\rangle$ are contained in the components of $P_{l'}|A_{lx}\rangle$ ($l' = 1, 2$) for which a closed set of linear equations can be obtained. Multiplying (A2.2) by $((1+z)\,e^{iqV} - 1)^{-1}$ and applying P_1 and P_2, respectively, yields the closed set of equations. With the definition

$$B_{l'\alpha',l\alpha} = \langle\tilde{\psi}_{l'\alpha'}|((1+z)\,e^{iqV} - 1)^{-1}|\psi_{l\alpha}\rangle$$

one arrives at three coupled equations:

$$\begin{pmatrix} \delta_{\alpha\beta} + \lambda_1 B_{1\alpha,1\beta} & \lambda_2 B_{1\alpha,2} \\ \lambda_1 B_{2,1\beta} & 1 + \lambda_2 B_{22} \end{pmatrix} \begin{pmatrix} \langle\tilde{\psi}_{1\beta}|A_l\rangle \\ \langle\tilde{\psi}_2|A_l\rangle \end{pmatrix} = \begin{pmatrix} B_{1\alpha,lx} \\ B_{2,lx} \end{pmatrix}$$

where α, β are equal to x or y. The matrix elements can be evaluated from (2.2) and (2.3), yielding

$$\begin{aligned} &B_{1\alpha,1\beta} = -\tfrac{1}{2}\delta_{\alpha\beta} \qquad B_{22} = -\tfrac{1}{2} \\ &B_{2,1\alpha} = B_{1\alpha,2} = (1/2\sqrt{2})\{\mathrm{i}s_\alpha/(1-c_\alpha)\}(1-2\delta_{\alpha x}) \equiv \mathrm{i}f_\alpha(1-2\delta_{\alpha x}) \end{aligned} \tag{A2.3}$$

where $s_\alpha = \sin q_\alpha$ and $c_\alpha = \cos q_\alpha$. We thus obtain for the eigenvalues:

$$r_l = \int_q [A_l + 8B_l(f_x^2+f_y^2)][E+8F(f_x^2+f_y^2)]^{-1} \tag{A2.4}$$

where the integrand has been symmetrised with respect to q_x and q_y, and A_l, B_l, E and F are given by (6.7). Observing that $8f_x^2 = (1+c_x)/(1-c_x)$, the q_x-integration is carried out. We use that $\pi^{-1}\int_0^\pi \mathrm{d}x(a+bc_x)^{-1} = (a^2-b^2)^{-1/2}$ for $a^2 > b^2$; this, and other integrals needed in the following, are found in [28]. For $E > F$ we then have

$$r_l(\lambda_1,\lambda_2) = \frac{A-2B}{E-2F} + \frac{(BE-AF)}{(E-2F)F}\,\delta(1+I_+(\delta)) \tag{A2.5}$$

where $A = A_l$, $B = B_l$ and $\delta^2 = F/(E-F)$. The remaining integral has the form

$$I_+(\delta) = \int_0^\pi \frac{\mathrm{d}x}{\pi} \frac{(1-c_x)^{3/2}}{[(1+\delta^2)(1-\delta^2)^{-1}-c_x][1+2\delta^2-c_x]^{1/2}} \tag{A2.6}$$

and reduces to an elementary integral through the subsequent substitutions $1-c_x = 2\sin^2\varphi$, $\cos\varphi = z$, $(1+\delta^2)^{1/2}z = t$ and $t = \sin\psi$. This yields

$$I_+(\delta) = \frac{2}{\pi}\int_0^{\psi_0} \mathrm{d}\psi - \frac{2}{\pi}\delta^2K^2\int_0^{\psi_0} \frac{\mathrm{d}\psi}{K^2-\sin^2\psi} \tag{A2.7}$$

with $\tan\psi_0 = \delta^{-1}$ and $K^2 = (1-\delta^4)^{-1}$. With the help of [28] the result can be shown to be

$$I_+(\delta) = \frac{2}{\pi}\tan^{-1}\tfrac{1}{2}[\delta^{-1}-\delta]. \tag{A2.8}$$

For $E < F$ one has to be more careful. Define for this case $\eta^2 = F/(F-E)$ $(= -\delta^2)$. From a z-dependent analysis analogous to (A2.1)-(A2.4), yielding nine coefficients instead of the six coefficients A_l, B_l, E and F in (6.7), we can show that $\mathrm{Im}\,\eta > 0$ for $z = +\mathrm{i}\varepsilon$. The equivalent of (A2.5) is then

$$r_l(\lambda_1,\lambda_2) = \frac{A-2B}{E-2F} + \frac{(BE-AF)}{(E-2F)F}\,\eta(\mathrm{i}+I_-(\eta)) \tag{A2.9}$$

with

$$I_-(\eta) = \int_0^\pi \frac{\mathrm{d}x}{\pi} \frac{(1-c_x)^{3/2}}{[(1-\eta^2)(1+\eta^2)^{-1}-c_x][c_x-1+2\eta^2]^{1/2}}. \tag{A2.10}$$

Using substitutions $1-c_x = 2\sin^2\varphi$, $\cos\varphi = z$, $z = (\eta^2-1)^{1/2}y$ and $y = \sinh t$:

$$I_-(\eta) = \frac{2}{\pi}\int_0^{y_0} \frac{\mathrm{d}y}{(1+y^2)^{1/2}} + \frac{2}{\pi}\eta^2K^2\int_0^{t_0} \frac{\mathrm{d}t}{K^2-\sinh^2 t} \tag{A2.11}$$

with $y_0=(\eta^2-1)^{-1/2}$, $\tanh t_0=\eta^{-1}$ and $K^2=(\eta^4-1)^{-1}$. The first integral yields $\pi^{-1}\ln(\eta+1)/(\eta-1)$; the second can be written in the form $\int dx(a-\cosh x)^{-1}$ with $x=2t$, and then gives $\pi^{-1}\ln(\eta+1)/(1-\eta)$. As $\mathrm{Im}\,\eta>0$, the result for $I_-(\eta)$ is

$$I_-(\eta)=\frac{2}{\pi}\eta\ln\frac{\eta+1}{\eta-1}-\mathrm{i}. \tag{A2.12}$$

The imaginary term cancels the other imaginary term in (A2.9). Note that these terms would also cancel if $\mathrm{Im}\,\eta<0$. So, finally, the general result can be written as

$$r_l(\lambda_1,\lambda_2)=\frac{A-2B}{E-2F}+\frac{(BE-AF)}{(E-2F)F}J \tag{A2.13}$$

with

$$J=\begin{cases}\delta\left(1+\dfrac{2}{\pi}\tan^{-1}\tfrac{1}{2}(\delta^{-1}-\delta)\right) & \text{for} \quad \delta^2>0\\[2ex] \dfrac{2}{\pi}\eta\ln\dfrac{\eta+1}{\eta-1} & \text{for} \quad \delta^2=-\eta^2<0.\end{cases} \tag{A2.14}$$

In fact, the first line of this equation leads to the second line if we consider its analytical continuation for $\delta=-\mathrm{i}\eta$, and vice versa. In two special cases the eigenvalues become particularly simple: for $E=2F$ one has

$$r_l=\left(1-\frac{2}{\pi}\right)\frac{A}{E}+\frac{4}{\pi}\frac{B}{E} \tag{A2.15}$$

and for $E\to F$ one has $J=4/\pi$ and

$$r_l=\left(\frac{4}{\pi}-1\right)\frac{A}{E}+\left(2-\frac{4}{\pi}\right)\frac{B}{E}. \tag{A2.16}$$

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