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Lorentz Lattice Gases: Basic Theory

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We present several ballistic models of the Lorentz gas in two-dimensional lattices with deterministic and stochastic deflection rules, and their corresponding Liouville equations. Boltzmann-level-equation results are obtained for the diffusion coefficient and velocity autocorrelation function for models with stochastic deflection rules. The long-time behavior of the mean square displacement is briefly discussed and the possibility of abnormal diffusion indicated. Even if the diffusion coefficient exists, its low-density limit may not be given correctly by the Boltzmann equation.

KEY WORDS: Lorentz gas; lattice gases; Liouville equation; Boltzmann equation; diffusion coefficient.

1. INTRODUCTION

The problem of the motion of one particle in an array of randomly placed fixed scatterers was first proposed by Lorentz[(1)] as a model of electronic motion in a solid. Ehrenfest[(2)] introduced a four-velocity version, the wind-tree model. The density dependence of the transport properties and velocity autocorrelation function (VACF) of the Lorentz gas has been extensively studied.[(3,4)] Similar studies have been made for the wind-tree model.[(5,6)] Particularly interesting is the case of overlapping trees, where the mean-square displacement grows more slowly than linearly with time (abnormal diffusion). Several investigators have studied Lorentz models on lattices. Gates and others[(7)] studied the existence of diffusion in lattice wind-tree models. Studies of random walks with excluded sites or bonds, which are

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nonballistic Lorentz models, have answered some questions about particle motion in a statically disordered medium.[8]

Van Beijeren[9] studied extensively one-dimensional Lorentz lattice gases. More recently, Binder[10] proposed lattice models of the Lorentz gas where particles follow ballistic trajectories in the absence of scatterers. These models are of interest because of recent developments of lattice models of hydrodynamics[11] and the large research on the field.[12] Binder[10] gives preliminary results of simulations of the new models. In Section 2 we introduce the models and their corresponding Liouville equation, followed by its formal solution in Section 3. In Section 4 we present the Boltzmann approximation and results for the diffusion coefficient and VACF for the stochastic models. Section 5 contains a discussion of deterministic models and of corrections to the Boltzmann equation.

2. THE MODELS

Consider a d-dimensional, regular, space-filling lattice with N sites, unit lattice distance, and a fraction c of sites—chosen at random—occupied by scatterers. A particle, or a collection of mutually independent particles, moves at times $t = 0, 1, 2,...$ with unit speed from site to site. The trajectories are straight lines until the particle hits a scatterer. The deflection rules, which can be probabilistic or stochastic, define the detailed model.

We will define the models, for simplicity, in a two-dimensional square lattice. The models in different lattices and dimensions can be easily constructed, and we will present some triangular lattice results in Section 4. We define directions $i = 0, 1, 2, 3,...$ (module 4) and associate with them nearest neighbor lattice vectors $\boldsymbol{\rho}_i$, as shown in Fig. 1. The system of many noninteracting particles is described by the probability density in Γ-space, $p_i(n, t; \{c_n\})$, which is the probability of finding a particle moving in direction i at site n in a given configuration of scatterers $\{c_n\}$. We associate with each site n a random variable with value

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

The distribution function of moving particles $f_i(n, t)$ is obtained by averaging $p_i(n, t; \{c_n\})$ over all configurations $\{c_n\}$ of scatterers. We denote this by

$$f_i(n, t) = \langle p_i(n, t) \rangle$$

Collisions between moving particles and scatterers occur only at integer values of time. At such values the velocities are not well-defined. We choose

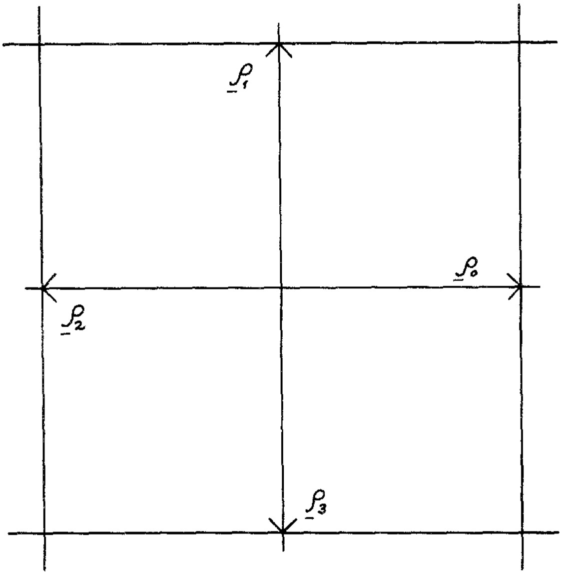

Fig. 1. Direction vectors for the square lattice.

to define $f_i(n, t)$ as the distribution function just *after* time t. We proceed now to describe the models and give their respective Liouville equations, which govern the evolution of p_i.

Model I: If a scatterer is present, the particle velocity $\boldsymbol{\rho}_i$ becomes either $\boldsymbol{\rho}_{i+1}$ or $\boldsymbol{\rho}_{i-1}$ (modulo 4), each with probability 1/2.

The Liouville equation can be constructed from Fig. 1:

$$\begin{aligned} p_i(n, t+1) &= (1-c_n)\, p_i(n-\boldsymbol{\rho}_i, t) + \tfrac{1}{2}c_n[p_i(n-\boldsymbol{\rho}_{i+1}, t) + p_i(n-\boldsymbol{\rho}_{i-1}, t)] \\ &= (1+c_n T)\, s^{-1} p_i(n, t) \end{aligned} \tag{2}$$

where s, the free-streaming operator, shifts the argument over one lattice unit in the direction of the velocity $\boldsymbol{\rho}_i$:

$$sA(n) \equiv A(n+\boldsymbol{\rho}_i) \tag{3}$$

The binary collision operator is

$$T = \tfrac{1}{2}(b + b^3 - 2) \tag{4}$$

where $b^m p_i = p_{i+m}$ (modulo 4). In other words, b rotates the index i of p_i by m units, modulo 4.

Model II: A more general stochastic model is one in which reflection occurs with probability $0<r<1$, left or right scattering with probability $0<v<1$, and transmission with probability $1-r-2v\geqslant 0$. In this case the collision operator is

$$T=v(b+b^3-2)+r(b^2-1) \tag{5}$$

A particular example of this is isotropic scattering, with $r=v=\frac{1}{4}$. Model I is also a special case of model II, with $r=0$, $v=\frac{1}{2}$.

Model III: This model, as well as the following two, has deterministic collision rules. The velocity changes according to

$$\rho_i \to \begin{cases} \rho_{i+1}, & t=\text{even} \\ \rho_{i-1}, & t=\text{odd} \end{cases} \tag{6}$$

As usual, the $i\pm 1$ are taken modulo 4. This leads to the Liouville equation

$$\begin{aligned} p_i(n,t+1) &= (1-c_n)\,p_i(n-\boldsymbol{\rho}_i,t)+c_n\,p_{i+\pi(t)}(n-\boldsymbol{\rho}_i,t) \\ &= [1+c_n T(t+1)]\,s^{-1}p_i(n,t) \end{aligned} \tag{7}$$

The binary collision operator is time-dependent:

$$T(t)=b^{\pi(t)}-1, \qquad \pi(t)=(-1)^t \tag{8}$$

Model IV: This model is a modification of model III, in which left-turning and right-turning scatterers occur with equal probability. We define

$$c_n=\begin{cases} 0 & \text{with probability } 1-c \\ 1^+\equiv 1+\varepsilon & \text{with probability } c/2 \\ 1^-\equiv 1-\varepsilon & \text{with probability } c/2 \end{cases}$$

Then, the Liouville equation for this model is Eq. (2) with

$$T=\delta(c_n,1^+)\,b+\delta(c_n,1^-)\,b^3-1 \tag{9}$$

Model V: This is identical to Model V of Gates[7] and has all scatterers as right-turning:

$$T=b^3-1$$

The T operators consist in general of a real part T_r that changes the direction of the moving particle and a virtual part T_v that does not. For instance, in Eq. (5), $T_r=v(b+b^3)+rb^2$ and $T_v=-(r+2v)$.

3. FORMAL SOLUTION OF THE LIOUVILLE EQUATION

For models I, II, IV, and V with a time-independent collision operator T the formal solution to Eq. (2) is given by

$$p_i(n, t) = [(1 + c_n T)s^{-1}]^t p_i(n, 0) \tag{11a}$$

For model III, with a time-dependent collision operator, this solution is

$$p_i(n, t) = \prod_{\tau=1}^{t} \{[1 + c_n T(\tau)]s^{-1}\} p_i(n, 0) \tag{11b}$$

For convenience, the following discussion will be restricted to models obeying Eq. (11a). The products in this equation can be rearranged in terms containing 0, 1, 2, 3,... T-operators, where each T is followed by at least one s^{-1}-operator:

$$\begin{aligned} p_i(n, t) = \Bigg(& s^{-t} + \sum_{t_1=1}^{t} s^{-t+t_1} c_n T s^{-t_1} \\ & + \sum_{\substack{t_1 t_2 \geqslant 1 \\ t_1 + t_2 < t}} s^{-t+t_1+t_2} c_n T s^{-t_2} c_n T s^{-t_1} \\ & + \sum_{\substack{t_1 t_2 t_3 \geqslant 1 \\ t_1 + t_2 + t_3 < t}} s^{-t+t_1+t_2+t_3} c_n T s^{-t_3} c_n T s^{-t_2} c_n T s^{-t_1} + \cdots \Bigg) p_i(n, 0) \end{aligned} \tag{12}$$

This representation of the formal solution of the Liouville equation is completely analogous to the binary collision expansion in the theory of hard-sphere gases.[13]

The first term in Eq. (12) represents free streaming without any collisions, i.e., $s^{-t}A(n) = A(n - t\mathbf{p}_i)$. The remaining terms represent time convolutions involving free streaming over a time interval $t_1 \geqslant 1$, a collision, free streaming over a time $t_2 \geqslant 1$, etc.,..., and finally free streaming over a time $t - t_1 - t_2 - \cdots \geqslant 0$.

In view of the convolution products in Eq. (12), it is natural to change to a generating function ("Laplace transform" of the t variable, $\xi = e^{-z}$) using

$$\hat{p}_i(n, \xi) = \sum_{t=0}^{\infty} \xi^t p_i(n, t) \tag{13}$$

Then, Eq. (12) becomes

$$\begin{aligned}\hat{p}_i(n, \xi) &= (1 - \xi s^{-1})^{-1} + (1 - \xi s^{-1})^{-1} c_n T \xi s^{-1}(1 - \xi s^{-1})^{-1} + \cdots \\ &= [(1 + c_n T)\, \xi s^{-1}]^{-1} \end{aligned} \tag{14}$$

The distribution function $\hat{f}_i(n, \xi)$ is obtained by averaging over all configurations $\{c_n\}$ of scatterers: $\hat{f}_i(n, \xi) = \langle \hat{p}_i(n, \xi) \rangle$.

4. THE BOLTZMANN APPROXIMATION; RESULTS

The successive terms in the time evolution of Eqs. (12) and (14) represent trajectories with 0, 1, 2,... particle–scatterer collisions, respectively. Collisions after the first one may occur with new scatterers or with one of the previously visited ones. For most of the models, the dominant contribution at low densities of scatterers comes from collisions with new scatterers. We will discuss possible exceptions in the next section. When collisions occur with new scatterers only, the term (12) contains sequences $c_{n_1} c_{n_2} c_{n_3},...$, where all the sites $n_1 n_2 n_3,...$ are different and the random variables $c_{n_1}, c_{n_2},...$ are independent. Their average is the product of the average $c = \langle c_n \rangle$,

$$\langle c_{n_1} c_{n_2} \cdots c_{n_m} \rangle = c^m$$

The initial distribution $p_i(n, 0)$ relevant for describing diffusion coefficients does not depend on the random variable c_n, as we shall see below.

We now take the ensemble average of Eq. (12), accounting only for uncorrelated collisions, and replace all c_n by $\langle c_n \rangle = c$. The resulting kinetic equation is the Boltzmann equation,

$$f_i(n, t) = \langle p_i(n, t) \rangle = [(1 + cT)\, s^{-1}]^t\, p_i(n, 0)$$

or, as a kinetic equation,

$$\begin{aligned} f_i(n, t+1) &= (1 + cT)\, s^{-1} f_i(n, t) \\ &= (1 + cT)\, f_i(n - \boldsymbol{\rho}_i, t) \\ &= (1 - c)\, f_i(n - \boldsymbol{\rho}_i, t) + \tfrac{1}{2} c[f_{i-1}(n - \boldsymbol{\rho}_{i-1}, t) + f_{i+1}(n - \rho_{i+1}, t] \end{aligned} \tag{15}$$

For the Lorentz gas the diffusion coefficient is given by the Green–Kubo formula

$$\begin{aligned} D &= \int_0^t d\tau\, \varphi(\tau) \\ \varphi(\tau) &= \langle v_x(\tau)\, v_x(0) \rangle \\ &= \int dr\, dv\, dR^M\, v_x(\tau)\, v_x(0)\, D_0(r, v, R^M) \end{aligned} \tag{16}$$

Here R^M denotes the configurations of M scatterers and (v, r) the phase of the moving particle, and $D_0(r, v, R^M)$ is the distribution function of the canonical ensemble. In the stochastic Lorentz models there is a unique equilibrium distribution, which is $D_0 = 1/(4N)$ for the square lattice. For the deterministic model, phase space decomposes into closed orbits, and the equilibrium state depends on the initial distribution of particles over these orbits. Therefore, there is an infinity of stationary states. For this reason, we limit the following discussion to stochastic models.

In lattice models, the VACF is defined through

$$\varphi(t) = \sum_{i,n} \langle \rho_{ix}(t)\, \rho_{ix}(0) \rangle = \sum_{i,n} \rho_{ix} \langle p_i(n, t) \rangle \tag{17}$$

with initial value $p_i(n, 0) = \rho_{ix}/(4N)$, independent of the random variables $\{c_n\}$. The diffusion coefficient is given by

$$D = \sum_{t=0}^{\infty} \varphi(t) = \sum_{t=0}^{\infty} \rho_{ix} \langle p_i(n, t) \rangle$$

where $p_i(n, t)$ obeys the Liouville equation with formal solution (11a):

$$p_i(n, t) = (1/4N)[(1 + c_n T)\, s^{-1}]^t \rho_{ix}$$

Then, the diffusion coefficient is

$$D = (1/4N) \sum_{t=0}^{\infty} \sum_{i,n} \rho_{ix} \langle [(1 + c_n T)\, s^{-1}]^t \rangle\, \rho_{ix} \tag{18}$$

The Laplace transform of the VACF is

$$\Phi(\xi) = \sum_{t=0}^{\infty} \xi^t \varphi(t) = \frac{1}{4} \sum_{i,n} \rho_{ix} \left\langle \frac{1}{1 - \xi(1 + c_n T)\, s^{-1}} \right\rangle \rho_{ix} \tag{19}$$

with $D = \Phi(\xi = 1)$.

In the Boltzmann approximation, one replaces all c_n in (19) by $\langle c_n \rangle = c$, according to the discussion at the beginning of this section. Consequently, all space dependence in (19) has disappeared, and the translation operator s^{-1} may be replaced by unity. This yields

$$\Phi_{\mathrm{B}}(\xi) = \frac{1}{4} \sum_{i} \rho_{ix} \frac{1}{1 - \xi(1 + cT)} \rho_{ix} \tag{20}$$

We observe that $\boldsymbol{\rho}_i$ is an eigenvector of the 4×4 matrix T with eigenvalue

$-\lambda$. This eigenvalue for models I and II is $\lambda = 1$ and $\lambda = 2(r+v)$, respectively. Thus, we have

$$\Phi_{\mathrm{B}}(\xi) = \frac{1}{1-\xi(1-\lambda c)} \frac{1}{4} \sum_{i=0}^{3} \rho_{ix}^2 = \frac{1}{2} \frac{1}{1-\xi(1-\lambda c)} \tag{21}$$

Since $\Phi_{\mathrm{B}}(\xi) = \sum_{t=0}^{\infty} \xi^t \varphi_{\mathrm{B}}(t)$, one finds

$$\varphi_{\mathrm{B}}(t) = \tfrac{1}{2}(1-\lambda c)^t \tag{22}$$

and for the diffusion coefficient

$$D = \Phi_{\mathrm{B}}(1) = 1/(2\lambda c)$$

This yields, for model I,

$$\varphi_{\mathrm{B}}(t) = \tfrac{1}{2}(1-c)^t, \qquad D_{\mathrm{B}} = (2c)^{-1} \tag{23}$$

and for model II,

$$\varphi_{\mathrm{B}}(t) = \frac{1}{2}(1-2cr-2cv)^t, \qquad D_{\mathrm{B}} = \frac{1}{4c(r+v)} \tag{24}$$

There are two special cases of interest in this model. One is isotropic scattering, in which the particle scatters in any of the four directions with probability one-quarter. For this case, corresponding to $r = v = \frac{1}{4}$, we have

$$\varphi_{\mathrm{B}} = \tfrac{1}{2}(1-c)^t, \qquad D_{\mathrm{B}} = (2c)^{-1} \tag{25}$$

For the case of one-dimensional diffusion, we have $v = 0$, $r > 0$:

$$\varphi_{\mathrm{B}}(t) = \tfrac{1}{2}(1-2cr)^t, \qquad D_{\mathrm{B}} = (4cr)^{-1} \tag{26}$$

We also present results for models in a triangular lattice. The directions, as shown in Fig. 2, are

$$\boldsymbol{\rho}_0 = -\boldsymbol{\rho}_3 = (1, 0), \qquad \boldsymbol{\rho}_1 = -\boldsymbol{\rho}_4 = \tfrac{1}{2}(1, \sqrt{3}), \qquad \boldsymbol{\rho}_2 = -\boldsymbol{\rho}_5 = \tfrac{1}{2}(-1, \sqrt{3})$$

(a) Left–right scattering ($\pi/3$ rad) with equal probability:

$$T = \tfrac{1}{2}(b + b^5 - 2); \qquad \lambda = \tfrac{1}{2}$$

$$\varphi_{\mathrm{B}}(t) = \tfrac{1}{2}(1 - \tfrac{1}{2}c)^t; \qquad D = 1/c \tag{27}$$

Here b^n denotes a rotation by $n\pi/3$ deg.

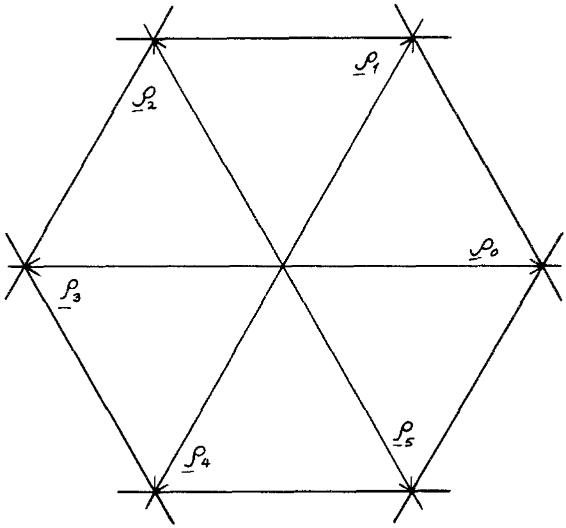

Fig. 2. Direction vectors for the triangular lattice.

(b) Uniform, isotropic scattering:

$$T = \frac{1}{6} \sum_{i=0}^{5} b^i - 1; \qquad \lambda = 1$$

$$D = (2c)^{-1}; \qquad \varphi_B(t) = \tfrac{1}{2}(1-c)^t \tag{28}$$

5. DISCUSSION AND CONCLUSIONS

We have proposed several lattice models for the Lorentz gas. We develop the Liouville equation for these models and present its formal solution. We solve the Liouville equation in the Boltzmann approximation and obtain results for the diffusion coefficient and the velocity autocorrelation function even in the case where no diffusion exists. This may happen in deterministic models. Here a return to a previously visited node with the same velocity (which happens with probability 1 in the equivalent random walk) implies that the particle gets locked in a cycle. Thus, for very long times, we expect that the mean square displacement will grow more slowly than linearly (abnormal diffusion). It has been suggested[14] that the mean square displacement may grow as some power of log t. For intermediate times shorter than the length of most orbits, one expects the mean-square displacement to grow linearly with time. The diffusion coefficient may be calculated from ordinary kinetic theory for these intermediate times. We intend to do this in subsequent publications.

Even if diffusion exists, the Boltzmann approximation does not always yield the correct low-density value of the transport coefficient. This is the case, for instance, in the stochastic models that allow reflection (like our model II). In such models the ring collisions resulting from two collinear scatterers yield such strong divergences that the Boltzmann result is modified. More specifically, the coefficient of c^k, the kth-order density correction to the diffusion coefficient, diverges as t^k for large t. Resummation of the leading divergences effectively replaces t by the mean free time $t_0 \sim 1/c$, yielding at low densities a relative correction of $O(ct_0) \sim O(1)$ to the Boltzmann result. The same situation occurs in the self-diffusion of a one-dimensional hard-rod gas.[15] After locating the mechanism that modifies the lowest order Boltzmann transport, it will be straightforward to construct deterministic Lorentz lattice gases where the diffusion coefficient on the intermediate time scale has the same properties.

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