Transport properties of stochastic Lorentz models

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Diffusion processes are considered for one-dimensional stochastic Lorentz models, consisting of randomly distributed fixed scatterers and one moving light particle. In waiting time Lorentz models the light particle makes instantaneous jumps between scatterers after a stochastically distributed waiting time. In the stochastic Lorentz gas the light particle moves at constant speed and is scattered stochastically at collisions with the scatterers. For the waiting time Lorentz models the Green's function of the diffusion process is calculated exactly. The diffusion coefficient is found to be the same as for a corresponding random walk on a regular lattice, the velocity autocorrelation function exhibits a long-time tail proportional to $t^{-3/2}$ and super Burnett and higher-order transport coefficients are found to diverge. For the stochastic Lorentz gas similar results are found for the diffusion coefficient and the velocity autocorrelation function, but the generalized super Burnett coefficient, as introduced by Alley and Alder, is convergent in this case. For a special case of the waiting time Lorentz models some other aspects are considered, such as periodic boundary conditions, steady-state diffusion and fluctuations of the velocity autocorrelation function about its average value, due to the initial conditions and to the stochastic distribution of scatterers.

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I. DIFFUSION EQUATION AND TIME CORRELATION FUNCTIONS

A. Introduction

The Lorentz gas, introduced by Lorentz (1905) to describe the diffusion of conduction electrons in metals, has gained a great popularity in the past years as one of the simplest nontrivial models on which the ideas developed in kinetic theory could be tested. In this paper I want to discuss certain classes of models that may be regarded as one-dimensional versions of the Lorentz gas, and for which several equilibrium time correlation functions may be calculated—if not completely then at least in the low-frequency limit. This very limit, or equivalently the long-time limit, will be our main concern; we will see how the so-called long-time tails in functions like the velocity autocorrelation function arise for these models. As an introduction I want to present simple phenomenological derivations of the long-time tail in the velocity autocorrelation, both for fluids and for the Lorentz gas, but as preliminaries we need some general connections between quantities characterizing the process of self-diffusion in a physical system and certain equilibrium time correlation functions for the same system.

B. Fick's law

The process of self-diffusion is described by Fick's law as

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t)=D\nabla^2\rho(\mathbf{r},t)\ , \tag{1.1}$$

where $\rho(\mathbf{r},t)$ is the density of diffusing particles at position $\mathbf{r}$ and time t (or, if there is only one diffusing particle, the probability density to find this particle at $\mathbf{r}$ at time t) and D is the coefficient of self-diffusion. The Green's function of this equation, i.e., the solution with initial condition $\rho(\mathbf{r},0)=\delta(\mathbf{r})$ is of the form

$$G^D(\mathbf{r},t)=(4\pi Dt)^{-d/2}e^{-r^2/4Dt}\ , \tag{1.2}$$

where d is the dimensionality of the system. From (1.2) it follows immediately that the mean-square displacement of a diffusing particle in, say, the x direction as a function of time is given by

$$\int d\mathbf{r}\, G^D(\mathbf{r},t)x^2=2Dt\ . \tag{1.3}$$

C. Generalized diffusion equations. Transport coefficients of higher order

In real physical systems the probability density $P(\mathbf{r},t)$ to find a particle tagged 1 and starting off at the origin at $t=0$, at position $\mathbf{r}$ at a time t, is never exactly of the form (1.2); if $P(\mathbf{r},t)$ satisfies the diffusion equation (1.1), it does so only in an asymptotic sense, that is, only on a macroscopic time and length scale. To be more specific, I consider, following McLennan (1973), De Schepper (1975), and De Schepper and Ernst (1979), the Fourier transform of $P(\mathbf{r},t)$ for a system in overall equilibrium,

$$F(\mathbf{k},t)=\int d\mathbf{r}\, e^{-i\mathbf{k}\cdot\mathbf{r}}P(\mathbf{r},t) \equiv\langle e^{-i\mathbf{k}\cdot(\mathbf{r}_1(t)-\mathbf{r}_1(0))}\rangle\ . \tag{1.4}$$

The brackets denote an average over an equilibrium ensemble and $\mathbf{r}_1(t)$ is the position of the tagged particle at time t. The restriction to equilibrium implies that $P(\mathbf{r},t)$ does not depend on the initial time. Without loss of generality $\mathbf{k}$ may be chosen to be parallel to the x direction. Then $F(\mathbf{k},t)$ can be expanded as

$$F(\mathbf{k},t)=\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}k^{2n}\langle[x_1(t)-x_1(0)]^{2n}\rangle \tag{1.5a}$$

$$=\exp\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}k^{2n}\langle[x_1(t)-x_1(0)]^{2n}\rangle_c\ . \tag{1.5b}$$

The odd moments in (1.5) vanish because of the isotropy of $P(\mathbf{r},t)$ in equilibrium and $\langle\ \rangle_c$ denotes cumulant moments (Cramèr, 1951), viz.,

$$\langle[x_1(t)-x_1(0)]^2\rangle_c=\langle[x_1(t)-x_1(0)]^2\rangle-\langle x_1(t)-x_1(0)\rangle^2=\langle[x_1(t)-x_1(0)]^2\rangle\ , \tag{1.6a}$$

$$\langle[x_1(t)-x_1(0)]^4\rangle_c=\langle[x_1(t)-x_1(0)]^4\rangle-3\langle[x_1(t)-x_1(0)]^2\rangle^2\ , \tag{1.6b}$$

etc. One can write a generalized diffusion equation for $F(\mathbf{k},t)$ of the form

$$[\partial/\partial t+k^2D(k,t)]F(\mathbf{k},t)=0\ . \tag{1.6c}$$

This equation merely *defines* $D(k,t)$, which is obtained from (1.5) as

$$D(k,t)=\sum_{n=0}^{\infty}(-1)^n k^{2n}D^{(2n)}(t)\ , \tag{1.7a}$$

$$D^{(2n)}(t)=\frac{1}{(2n+2)!}\frac{d\langle[x_1(t)-x_1(0)]^{2n+2}\rangle_c}{dt}\ . \tag{1.7b}$$

If $P(\mathbf{r},t)$ satisfied Fick's law (1.1), one would simply have $D(k,t)=D$. The requirement one has to impose in order for $P(\mathbf{r},t)$ to satisfy Fick's law asymptotically is that $D=\lim_{t\to\infty}\lim_{k\to 0}D(k,t)$ exists.[1] From (1.7b) an explicit expression for D follows:

$$D=\lim_{t\to\infty}\frac{1}{2}\frac{d}{dt}\langle[x_1(t)-x_1(0)]^2\rangle =\lim_{t\to\infty}\langle[x_1(t)-x_1(0)]v_{1_x}(t)\rangle=\lim_{t\to\infty}\int_0^t d\tau\langle v_{1_x}(\tau)v_{1_x}(t)\rangle \tag{1.8a}$$

$$=\lim_{t\to\infty}\int_0^t d\tau\langle v_{1_x}(0)v_{1_x}(t-\tau)\rangle=\int_0^\infty dt\langle v_{1_x}(0)v_{1_x}(t)\rangle\ , \tag{1.8b}$$

where $v_{1_x}(t)$ is the x component of the velocity $\mathbf{v}_1(t)$ of particle 1 at time t, and one has to require that *the limit exists*. In addition, the fact that in a stationary state the

[1] It is important that the limits are not interchanged (Zwanzig, 1964).

velocity autocorrelation function (abbreviated vaf in the sequel),

$$C(t)=\langle v_{1_x}(t_1)v_{1_x}(t_1+t)\rangle$$
$$=\frac{1}{d}\langle \mathbf{v}_1(t_1)\cdot\mathbf{v}_1(t_1+t)\rangle \quad (1.9)$$

depends only on the time difference t was employed. In (1.8b) one recognizes the well-known Green-Kubo expression (Green, 1952, 1954; Kubo, 1957) for the self-diffusion coefficient. However, from (1.8a) one also sees that this is nothing but the famous Einstein relation (Einstein, 1905)

$$D=\lim_{t\to\infty}\frac{\langle [x_1(t)-x_1(0)]^2\rangle}{2t}\ , \quad (1.10)$$

again, provided the limit exists.[2]

An alternative but equivalent way to characterize the diffusion process makes use of the Laplace transform of $F(\mathbf{k},t)$, that is,

$$G(\mathbf{k},z)=\int_0^\infty dt\, e^{-zt}F(\mathbf{k},t) \quad (1.11a)$$
$$=\frac{1}{z}+\sum_{n=1}^{\infty}\frac{(-1)^n}{(2n)!}k^{2n}\langle x_1^{2n}(z)\rangle\ , \quad (1.11b)$$

where $\langle x_1^{2n}(z)\rangle$ denotes the Laplace transform of $\langle [x_1(t)-x_1(0)]^{2n}\rangle$. Equation (1.11b) follows immediately from (1.5a). For $G(\mathbf{k},z)$ one can again write a formal diffusion equation, of the form

$$[z+k^2U(k,z)]G(\mathbf{k},z)=1\ , \quad (1.12)$$

that *defines* the quantity $U(k,z)$. If $P(\mathbf{r},t)$ satisfied Fick's law, one would have $U(k,z)=D$. Solving for $U(k,z)$ and expanding in powers of k with the aid of (1.11b), one obtains

$$U(k,z)=k^{-2}[G^{-1}(k,z)-z] \quad (1.13a)$$
$$=\sum_{n=0}^{\infty}(-1)^nk^{2n}U^{(2n)}(z)\ , \quad (1.13b)$$

with

$$U^{(0)}(z)=\tfrac{1}{2}z^2\langle x_1^2(z)\rangle\ , \quad (1.14a)$$
$$U^{(2)}(z)=\tfrac{1}{24}[z^2\langle x_1^4(z)\rangle-6z^3\langle x_1^2(z)\rangle^2]\ , \quad (1.14b)$$

etc. Now the condition that Fick's law is asymptotically valid can be formulated as the requirement that $D=\lim_{z\to0}\lim_{k\to0}U(k,z)$ exists.

Phenomenologically there exist different ways to generalize Fick's law by incorporating higher-order derivatives of the density. The simplest of these is of the form (McLennan, 1973)

$$\frac{\partial}{\partial t}P(\mathbf{r},t)=D^{(0)}\nabla^2P(\mathbf{r},t)+D^{(2)}\nabla^2\nabla^2P(\mathbf{r},t)+\cdots \quad (1.15a)$$

or

$$\frac{\partial}{\partial t}F(\mathbf{k},t)=-k^2(D^{(0)}-D^{(2)}k^2+\cdots)F(\mathbf{k},t)\ . \quad (1.15b)$$

These equations are to be understood again as asymptotic equations that are valid for long times. Hence, on comparing with (1.6c)−(1.7), one can make the identifications

$$D^{(2n)}=\lim_{t\to\infty}D^{(2n)}(t)\ , \quad (1.16)$$

provided again these limits exist.

A different generalization of Fick's law takes into account the possibility of memory effects in time by putting (Alley and Alder, 1979),

$$\frac{\partial}{\partial t}F(\mathbf{k},t)=-k^2\sum_{n=0}^{\infty}(-1)^nk^{2n}\int_0^t d\tau\,\phi^{(2n)}(\tau)F(\mathbf{k},t-\tau) \quad (1.17a)$$

or

$$zG(\mathbf{k},z)=-k^2\sum_{n=0}^{\infty}(-1)^nk^{2n}U^{(2n)}(z)G(\mathbf{k},z)+1 \quad (1.17b)$$

The $U^{(2n)}(z)$ are the Laplace transforms of the $\phi^{(2n)}(t)$, and are identical to the quantities defined in (1.14). Phenomenological coefficients can be defined as

$$U^{(2n)}=\lim_{z\to0}U^{(2n)}(z)\ , \quad (1.18)$$

again, provided the limits exist.

D. Long-time behavior of correlation functions

It has been assumed for a long time that the velocity autocorrelation function $C(t)$ would be an exponentially decaying function of time. The intuitive basis of this assumption was the idea that through repeated collisions any particle would rapidly "forget" its initial velocity. This was supported by the explicit solutions of almost all solvable models known by then, such as the linearized Boltzmann equation (Chapman and Cowling, 1970) and the Fokker-Planck equation (Chandrasekhar, 1943). So it came as a great surprise when Alder and Wainwright (1970) discovered in computer simulations that the vaf for a system of moving hard spheres decays only with a negative power of time. Their estimates indicated a long-time behavior proportional to $t^{-d/2}$ in d dimensions. After their discovery theoretical explanations of this phenomenon were rapidly produced, based on kinetic theory (Dorfman and Cohen, 1970, 1972, 1975; Pomeau, 1971; Résibois, 1970; Résibois and Pomeau, 1976; Theo-

[2]If the limit defined in (1.8a) exists, the limit defined in (1.10) also exists and is equal to (1.8a). It is possible, however, that the limit (1.10) does exist and the limit (1.8a) does not. Hence the Einstein relation is slightly more general than the Green-Kubo equation.

dosopulu and Résibois, 1976), mode-coupling theory (Ernst *et al.*, 1970, 1971, 1976; Kawasaki, 1970), fluctuating hydrodynamics (Zwanzig *et al.*, 1972; Bedeaux and Mazur, 1974a, 1974b), Brownian motion theory (Zwanzig and Bixon, 1970; Widom, 1970), and dynamical renormalization group methods (Forster *et al.*, 1976). A review of this subject has been given by Pomeau and Résibois (1975).

1. The velocity autocorrelation function for fluids

Here I want to give a very simple intuitive explanation that, in one form or another, can be recognized easily in most of the above-mentioned more formal derivations.[3]

Suppose a tagged particle in a system in equilibrium is conditioned to be at the origin at $t=0$ with velocity $\mathbf{v}$. This corresponds to an initial nonequilibrium situation with a tagged-particle density and an average overall velocity density given by[4]

$$P(\mathbf{r},0)=\delta(\mathbf{r}) \,, \tag{1.19a}$$

$$\mathbf{u}(\mathbf{r},0)=\mathbf{v}\delta(\mathbf{r}) \,. \tag{1.19b}$$

Since the initial deviation from equilibrium is only a minor one, it seems fair to assume that for not too short times, that is, for times much longer than the mean free time between collisions, the time development of $P(\mathbf{r},t)$ and $\mathbf{u}(\mathbf{r},t)$ is described to a first approximation by the solution of linearized hydrodynamic equations (Foch and Ford, 1970). For $P(\mathbf{r},t)$ this is the diffusion equation (1.1), with the solution (1.2),[5] or for its Fourier transform

$$F(\mathbf{k},t)=e^{-Dk^2t} \,. \tag{1.20}$$

The hydrodynamic equations for the divergence free part $\mathbf{u}_{tr}$ of the velocity density are

$$\frac{\partial \mathbf{u}_{tr}}{\partial t}=-\nu\nabla\times(\nabla\times\mathbf{u}_{tr}) \,, \tag{1.21a}$$

$$\nabla\cdot\mathbf{u}_{tr}=0 \,, \tag{1.21b}$$

where ν is the kinematic viscosity, $\nu=\eta/mn$ with η the shear viscosity, m the mass of the particles, and n the number density. The irrotational part $\mathbf{u}_{long}$ of the velocity density may just as well be obtained by solving the linearized hydrodynamic equations, but, since it does not contribute to the leading long-time tail in the vaf, I will not consider it here. Equations (1.21) are most easily solved for the Fourier transform $\mathbf{u}_{tr}(\mathbf{k},t)$ of $\mathbf{u}_{tr}(\mathbf{r},t)$ with the result

$$\mathbf{u}_{tr}(\mathbf{k},t)=(\mathbf{v}-(\mathbf{v}\cdot\hat{\mathbf{k}})\hat{\mathbf{k}})e^{-\nu k^2t} \tag{1.22}$$

for the initial condition (1.19b). Here $\hat{\mathbf{k}}$ is the unit vector along $\mathbf{k}$. Now assume that, if after a not too short time t, the tagged particle is at a position $\mathbf{r}$, its average velocity is given by $\mathbf{u}(\mathbf{r},t)$. In other words, assume that at time t the tagged particle on the average has the same velocity as the other particles in its neighborhood, and that the average velocity $\mathbf{u}(\mathbf{r},t)$ to first approximation is not influenced by the fact that the tagged particle is located at $\mathbf{r}$ at time t. Then the average velocity of the tagged particle to leading order is found as

$$\begin{aligned}\mathbf{v}(t)&\approx\int d\mathbf{r}\,P(\mathbf{r},t)\mathbf{u}(\mathbf{r},t)\\ &\approx d\mathbf{r}\,P(\mathbf{r},t)\mathbf{u}_{tr}(\mathbf{r},t)\\ &=\frac{1}{(2\pi)^d}\int d\mathbf{k}\,F(\mathbf{k},t)\mathbf{u}_{tr}(-\mathbf{k},t)\\ &=\frac{1}{(2\pi)^d}\int d\mathbf{k}\,[\mathbf{v}-(\mathbf{v}\cdot\hat{\mathbf{k}})\hat{\mathbf{k}}]e^{-(\nu+D)k^2t}\\ &=\frac{d-1}{d}[2\pi(\nu+D)t]^{-d/2}\mathbf{v} \,. \end{aligned}\tag{1.23}$$

The vaf is obtained from this by averaging $\mathbf{v}\cdot\mathbf{v}(t)/d$ over the equilibrium velocity distribution, with the result

$$\begin{aligned}C(t)&=\frac{d-1}{d}[2\pi(\nu+D)t]^{-d/2}\frac{1}{d}\int d\mathbf{v}\,v^2\left[\frac{\beta m}{2\pi}\right]^{d/2}e^{-\beta m v^2/2}\\ &=\frac{d-1}{\beta m d}[2\pi(\nu+D)t]^{-d/2}\end{aligned}\tag{1.24}$$

to leading order in t.

One may conclude that the vaf has a long-time tail, due to the conservation of particle number and momentum. In a time t the particle diffuses over a distance on the order $\sqrt{t}$ from its initial position and there it picks up a fraction of its initial momentum that has been diluted, also by a diffusion process, to a magnitude of order $t^{-d/2}$. The result (1.24) agrees with that of the more sophisticated theories quoted before as well as the results from computer simulations (Alder and Wainwright, 1970; Alder *et al.*, 1970; Wood, 1975)

2. The Lorentz gas

In solids the process of self-diffusion often takes the form of repeated scattering of mobile particles by impurities. One of the simplest models in which this type of process occurs is the Lorentz gas. In this model a number of fixed spherical scatterers are distributed completely at random over a d-dimensional volume (overlapping Lorentz gas), or are distributed randomly under the

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[3] I learned this argument from Knops (1970). Compare also Alder and Wainwright (1970) and Pomeau and Résibois (1975).

[4] In fact, also the overall energy and particle density are disturbed from equilibrium initially. However, the slow relaxation to equilibrium of these quantities does not influence the leading term in the long-time behavior of the velocity autocorrelation function.

[5] I assume here that fixing the initial velocity of the tagged particle does not influence this solution. In fact, this causes a shift of the solution in the direction of the initial velocity over a distance on the order of the mean free path. This shift, however, has no influence on the leading long-time behavior of $C(t)$.

restriction that they may not overlap each other (nonoverlapping Lorentz gas). In addition, there is one light point particle (or a number of mutually noninteracting point particles) that has velocity of constant magnitude (at least in the absence of external forces), and is reflected specularly when hitting a scatterer.

Lorentz (1905) introduced this model to describe diffusion of electrons in a metal. It is still used as a simplified model to describe the diffusion of electrons controlled by scattering from impurities (Peierls, 1974). Other applications are found in the theories of neutron transport (Case and Zweifel, 1967) and of diffusion in a binary mixture of species with disparate masses (Chapman and Cowling, 1970). The Lorentz gas combines a relative simplicity with the characteristics of a genuine many-particle system. For this reason it has served as a theoretical test case already in several instances [see Hauge (1974) for an excellent review]. Lorentz (1905), elaborating on the work of Drude (1900), derived from it the Wiedemann-Franz law describing the temperature dependence of the ratio between thermal and electrical conductivity of a metal. Much later Van Leeuwen and Weyland [1967; see also Weyland and Van Leeuwen (1968)] showed the occurrence of logarithmic terms in the density expansion of the diffusion coefficient of the Lorentz gas. Sinai and Bunimovich (Sinai, 1970, 1973, 1981; Bunimovich, 1972, 1974, 1979; Bunimovich and Sinai, 1973, 1981, Gallavotti, 1975) performed a deep investigation of the ergodic properties of the Lorentz gas and obtained a number of strong results. Spohn (1978) and Lebowitz (Lebowitz and Spohn, 1978) considered the so-called Boltzmann-Grad limit where the density of scatterers goes to zero. Bruin (1974), Lewis and Tjon (1978), and Alder and Alley (Alder and Alley, 1978; Alley and Alder, 1979; Alley, 1979) performed computer simulations of the Lorentz gas and so did Lagar'kov *et al.* (1975, 1978)—however for the case of a soft potential between the scatterers and the light particle. Recently the model has been devoted new interest because of the possibility of a percolation transition at high-scatterer densities (Shante and Kirkpatrick, 1973; Haan and Zwanzig, 1977) accompanied by the vanishing of the diffusion coefficient (Alder and Alley, 1978; Alley, 1979; Götze *et al.*, 1981).

3. The velocity autocorrelation function for the Lorentz gas

The preceding intuitive argument to explain the occurrence of a long-time tail in the velocity autocorrelation function clearly does not apply to the Lorentz gas, because momentum is not conserved (it can be absorbed by the scatterers). Yet, as Ernst and Weyland (1971) showed with the aid of low-density kinetic theory, a long-time tail arises but is proportional to $t^{-(d/2+1)}$. In this case the long-time tail is entirely caused by the slow decay of density fluctuations; that is, the initial density profile of the light particle decays according to the diffusion equation and the positions of the scatterers are constant in time. In the case of isotropic scattering (after a collision the velocity of the light particle has equal probability to point into any direction) the origins of the long-time tail can be clarified by a simple calculation. Suppose the light particle starts off at $t=0$ with velocity $\mathbf{v}_0$ in the positive x direction and first hits a scatterer at $t=t_0$ at a point O, which I will choose as the origin of the coordinate system describing the model. The position of the center of the scatterer is not specified, however. Because of the isotropy of the scattering mechanism the velocity of the light particle, averaged over the spatial distribution of the scatterers, becomes uncorrelated from the initial velocity after the first collision, and in general subsequent collisions will not change this situation. There is, however, an exception to this: Because the first scattering occurred at the origin, the light particle "knows" that no scatterers are present within the shaded volume $\mathbf{V}_0$, as indicated in Fig. 1. Hence, if the light particle returns within this volume, it maintains its present velocity for a longer time than average. For large t the average density $P(\mathbf{r},t)$ of the light particle may be expected to be described by the solution (1.2) of the diffusion equation, a Gaussian, which for reasons of symmetry has to be centered at the origin. This implies that the particle has a slightly larger probability to return to $\mathbf{V}_0$ from the right than from the left; hence it restores a correlation between the velocity at time t and the initial velocity.[6] This can be quantified in the following way: The average velocity at time t, given the initial velocity $\mathbf{v}_0$ and first-collision time t_0 is approximately given as

$$\langle \mathbf{v}(t) \mid \mathbf{v}_0, t_0 \rangle = \int_{\mathbf{V}_0} d\mathbf{r} \int d\mathbf{v}\, \nu^{-1} \nu f(\mathbf{r},\mathbf{v},t)\mathbf{v} \ . \qquad (1.25)$$

This is to be understood as follows: $\nu f(\mathbf{r},\mathbf{v},t) d\mathbf{r}\, d\mathbf{v}$, with ν equal to the collision frequency, and $f(\mathbf{r},\mathbf{v},t)$, the distribution function for the light particle, is the missing number of collisions per unit time in $d\mathbf{r}$ with velocity $\mathbf{v}$ that would be needed to keep the average velocity equal to zero. The mean free time ν^{-1} is the average time during which the particles that missed a collision in $\mathbf{V}_0$ keep their velocity before being isotropically scattered again. At low scatterer density and for $t >> \nu^{-1}$ the distribution function may be approximated by the normal or Chapman-Enskog solution (Chapman and Cowling, 1970) of the Boltzmann equation. As is shown in Appendix A this solution expanded up to first order in gradients of the density, is of the form

[6] Alley and Alder (1979) want to explain the long-time tail in the vaf on the basis of a larger than average probability for a return to the origin, due to repeated backscattering events. At least for low densities, this explanation is not supported here. The probability for a return to the origin is determined by a diffusion process without memory, and only after such a return is a correlation of the velocity to the initial velocity restored.

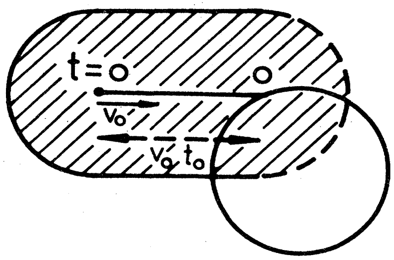

FIG. 1. Initial track of the light particle. Within the shaded area no scattering centers can be present.

$$f(\mathbf{r},\mathbf{v},t)=\left[1-\frac{D_0 d}{v_0^2}(\mathbf{v}\cdot\nabla)\right]\frac{e^{-r^2/4D_0t}}{(4\pi D_0 t)^{d/2}}\phi(\mathbf{v}) \tag{1.26a}$$

$$=\left[1+\frac{\mathbf{v}\cdot\mathbf{r}}{2tv_0^2}\frac{d}{(4\pi D_0 t)^{d/2}}\right]\phi(\mathbf{v}) . \tag{1.26b}$$

Here D_0 is the Boltzmann diffusion coefficient, $D_0=v_0^2(\nu d)^{-1}$ [this value follows also very simply from (1.8b)], and $\phi(\mathbf{v})$ is the equilibrium velocity distribution, i.e., $\phi(\mathbf{v})$ is a constant times a δ function $\delta(|\mathbf{v}|-v_0)$. Substituting (1.26) into (1.25), one finds

$$\langle \mathbf{v}(t)\,|\,\mathbf{v}_0,t_0\rangle=\int_{V_0}d\mathbf{r}\int d\mathbf{v}\frac{\mathbf{v}(\mathbf{v}\cdot\mathbf{r})}{2tv_0^2}\frac{d}{(4\pi D_0t)^{d/2}}\phi(\mathbf{v})$$

$$=\frac{\hat{\mathbf{x}}}{2t(4\pi D_0t)^{d/2}}\int_{V_0}d\mathbf{r}\,x$$

$$\approx\frac{-\hat{\mathbf{x}}v_0^2t_0^2\sigma}{4t(4\pi D_0t)^{d/2}} , \tag{1.27}$$

where σ is the total cross section of a scatterer. In calculating the integral over V_0, this volume was approximated by a cylinder of length v_0t_0, which is correct to lowest order in the density. Next we have to average t_0^2. As the distribution of the first-collision time is purely exponential, this average produces $(t_0^2)_{\rm av}=2\nu^{-2}$. Furthermore, if one uses the expression given above for D_0 and the identity $v_0\nu^{-1}\sigma=n^{-1}$, he finds the following result for the vaf:

$$\frac{1}{d}\langle \mathbf{v}(0)\cdot\mathbf{v}(t)\rangle=\frac{-2\pi D_0^2}{n(4\pi D_0t)^{d/2+1}} \tag{1.28}$$

in agreement with the result of Ernst and Weyland. Basically, my calculation is a special case of theirs, but the formulation given here makes it easier to understand the mechanisms responsible for the long-time tail. It is of some interest to consider the correction resulting from a more precise evaluation of the integral over V_0 occurring in (1.27). The hemisphere to the left of the initial position of the light particle produces a correction factor to (1.28) of magnitude $(1+nV_{\rm sc})$, where $V_{\rm sc}$ is the volume of a single scatterer.

In computer simulations of two-dimensional Lorentz models at fairly low scatterer densities the decay of $C(t)$ as $t^{-(d/2+1)}$ has been confirmed (Alder and Alley, 1978; Lewis and Tjon, 1978; Alley, 1979). However, the coefficient calculated by Ernst and Weyland (1971) remains valid only in a very small density regime (Alley, 1979). Keyes and Mercer (1979) have proposed a generalization of this theory to higher densities, but no comparison of their theory with the most recent computer results has been made.

It is of interest that the $t^{-(d/2+1)}$ long-time tail in the vaf persists, even if the fluctuations of the scatterer density, responsible for the long-time memory effects are not constant in time, but decay diffusively. Notably, this result has been found for one-dimensional systems of particles diffusing independently under the restriction that they may not pass each other (Harris, 1965; Richards, 1977; Fedders, 1978; Kehr *et al.*, 1981). In higher dimensions the vaf for such systems also exhibits the same long-time behavior as for a Lorentz gas. Recently the mean-square displacement for a particle in a sine-Gordon chain at low concentrations of kink sites was found to grow as $t^{1/2}$ with time (Gunther and Imry, 1980; Schneider and Stoll, 1980; Büttiker and Landauer, 1980). This again may be traced back to the same mechanisms that are responsible for the long-time tails in the models discussed above.

4. Consequences of the long-time tails

What are the physical consequences of the existence of the long-time tails? The most dramatic one certainly is that in two-dimensional fluids the occurrence of a $1/t$ tail in time correlation functions such as $C(t)$ leads to divergent integrals in the Green-Kubo formulas, such as (1.8b), hence to nonexistence of the Navier-Stokes transport coefficients. Now there is some inconsistency here, because the derivations of the $t^{-d/2}$ tails assume, explicitly or implicitly, the validity of the Navier-Stokes equations. This problem can be circumvented, however, e.g., by a self-consistent back-coupling of dynamical processes responsible for the long-time tails to the hydrodynamic equations (Wainwright, Alder, and Gass, 1971; Kawasaki, 1971). One then obtains a long-time tail that behaves asymptotically as $(t\sqrt{\log t})^{-1}$, which is still nonintegrable. The problem of divergent transport coefficients can be resolved in certain cases by passing to hydrodynamic equations that cannot be linearized in powers of gradients of the hydrodynamic fields (Onuki, 1975; Ernst *et al.*, 1978). In other cases, such as that of self-diffusion in an equilibrium system, it looks as though the effects of system size and shape come into play unavoidably (Onuki, 1975; Wood, 1975). In three-dimensional fluids the existence of Navier-Stokes transport coefficients is not threatened by the $t^{-3/2}$ tail. There, however, higher-order transport coefficients, like $D^{(2)}$, $D^{(4)}$, etc., as introduced in (1.15), do not exist (Keyes and Oppenheim, 1973; Dufty and Mc Lennan, 1974; De Schepper *et al.*, 1974). Again, this problem can be solved in certain cases by introducing into the hydrodynamic equations some terms that are nonanalytic in the gradients of hydrodynamic fields (Kawasaki and Gunton, 1973; Yamada and Kawasaki, 1975; Onuki, 1975; Ernst *et al.*, 1978).

In Lorentz models the $t^{-(d/2+1)}$ tail occuring in $C(t)$ leads to an existing diffusion coefficient, even in $d=1$ (how to define sensible Lorentz models in one dimension will be the subject of the next section). However, the $D^{(2n)}$ are expected to be divergent for $n \geq d/2$. An interesting conjecture by Alder and Alley [(1979; see also Alley (1979)] is that the $U^{(2n)}$, introduced in (1.18), exist for all n. At low density this conjecture seems to be supported by kinetic theory (Ernst and van Beijeren, 1981). The calculations on one-dimensional models to be reported here show that the conjecture is at least partially fulfilled for one class of models, whereas for another class of models it is not satisfied.

Another important aspect of the long-time tails is that they may contribute appreciably to the transport coefficients, especially at high densities. In fact, this requires a slight generalization of the long-time tail concept for the fluid. Besides the $t^{-d/2}$ contributions to the vaf, which dominate in the asymptotic long-time regime, there exist other contributions with a long-time decay proportional to $t^{-(d/2+1)}$. De Schepper and Cohen (1978) showed that at high densities the most important of these contributions results from the decay of the initial velocity through the product of a diffusive mode and a heat mode, a process that is very similar to the one responsible for the $t^{-(d/2+1)}$ tail in the Lorentz models. From this process a (negative) contribution to the diffusion coefficient may arise, amounting to something in the order of 50% of the total diffusion coefficient (Alder *et al.*, 1970).

Of course the existence of long-time tails in transport kernels like $\phi^{(0)}(t)$, defined in (1.17a), raises the question whether one should not take these into account explicitly in the hydrodynamic equations by introducing frequency dependent transport coefficients, even at low frequencies. Although it seems to me that in principle one should certainly do so, I know of only one real experiment in which the existence of a long-time tail allegedly has been shown directly. This is an experiment by Fedele and Kim (1980) on Brownian motion (where the long-time tail effects should be most pronounced) and even there the interpretation is hard and no complete agreement with theory is found.

E. Rigorous results

From a more formal point of view the long-time tails are definitely of interest. There are, however, hardly any rigorous arguments available for their existence or nonexistence in nontrivial models. This in turn implies that even the existence or nonexistence of transport coefficients cannot be stated with rigor in most cases. Let me list the few exceptions I know of below.

1. Hard spheres in one dimension

For the Jepsen gas, or one-dimensional hard-sphere system with a Maxwellian velocity distribution, the velocity autocorrelation function decays asymptotically as t^{-3} for long times (Jepsen, 1965; Lebowitz and Percus, 1967). Hence the diffusion coefficient exists. This system is somewhat pathological, because it can be considered as an almost ideal gas in which colliding particles merely exchange their identities (at least if the diameters of the spheres are set equal to zero). Therefore self-diffusion is the only type of transport phenomenon that is governed by an equation of hydrodynamic type. The reason why $C(t)$ does not decay in time as $t^{-1/2}$ or anything close to that, is the very absence of momentum diffusion. The initial momentum of the tagged particle just propagates through the system at constant speed.

2. Brownian motion

For a Brownian particle embedded in an ideal gas the existence of the diffusion equation has been proven in the limit where the mass ratio between Brownian particle and bath particles goes to infinity. The velocity autocorrelation function decays exponentially in this limit. The one-dimensional case was treated by Holley (1969), whereas Dürr *et al.* (1981) gave a proof for higher dimensions.

3. Harmonic lattices

For the vaf of a particle in an infinite harmonic lattice Mazur and Montroll (1960) obtained a long-time behavior proportional to $\sin t/t^{-d/2}$ in d dimensions. Hemmer (1959) and Rubin [(1960; see also Morita and Mori (1976)] investigated the motion of a heavy particle in a linear harmonic chain. They found that the diffusion coefficient exists and is nonzero and that, under an appropriate time-scaling, the vaf decays exponentially. For a Brownian particle in a three-dimensional harmonic lattice Rubin (1961) found that the vaf decays exponentially in time, as well, whereas no diffusion occurs; in two dimensions the vaf has a long-time tail proportional to t^{-2}, the diffusion coefficient is zero, and the mean-square displacement grows proportionally to $\log t$.

4. The Boltzmann-Grad limit

In the so-called Boltzmann-Grad limit, where the density goes to zero, while length and time are usually scaled by the mean free path and mean free time, respectively, some rigorous results are available, mainly based on the methods of Lanford (1976a, 1976b). For the d-dimensional Lorentz gas ($d>1$), the vaf approaches the Lorentz-Boltzmann result for all times (Gallavotti, 1969, 1972; Spohn, 1978). The approach is nonuniform as $t \rightarrow \infty$, however; hence the existence of the diffusion coefficient for finite density has not been proven. For steady-state diffusion between two parallel flat reservoirs separated by a distance L, the validity of Fick's law has been proven (Lebowitz and Spohn, 1978) for the case where one first takes the Boltzmann-Grad limit at fixed L and next the limit $L \to \infty$. For fixed finite density, however, the validity of Fick's law in the limit $L \to \infty$ does not follow from this.

For a tagged particle in a system of identical moving hard spheres in two or more dimensions the vaf approaches the Boltzmann value in the Boltzmann-Grad limit for all times (van Beijeren, *et al.*, 1980). Again this does not prove the existence of the diffusion coefficient (actually, as stated before, D is expected to be divergent in two dimensions). For a system of hard spheres in a periodic box a steady state can be set up by coloring all spheres entering from the right white and all spheres entering from the left black (Wood, 1975). In the Boltzmann-Grad limit the distribution functions for spheres of either color approach the Lorentz-Boltzmann value. This again implies the validity of Fick's law if one takes the Boltzmann-Grad limit first and next lets L go to infinity (Spohn, 1981).

5. Spin systems

For one-dimensional XY models several spin-spin equilibrium time correlation functions have been calculated exactly (Niemeyer, 1967, 1968; McCoy *et al.*, 1971; Brandt and Jacoby, 1976, 1977; Perk and Capel; 1977, 1978; Vaidya and Tracy, 1978). For the two-dimensional quadratic nearest neighbor Ising model Allan and Betts (1968, 1969) obtained the time correlation function between transverse spin components.

F. One-dimensional Lorentz models

In view of the considerations given above it seemed fruitful to study certain one-dimensional Lorentz models, some of which are exactly solvable, while others allow for rigorous estimates of the low-frequency behavior of correlation functions such as $G(k,z)$, defined in (1.11).

For these models one can check the existence of the diffusion coefficient, as well as the existence and the precise form of long-time tails in the vaf. Furthermore, one can study in detail the time behavior of the $D^{(2n)}(t)$, defined in (1.7b). It is possible to test the validity of kinetic theory and that of the assumptions made in the semi-intuitive derivation of the long-time tail in the vaf, sketched before. One can calculate for certain models how the correlation functions approach their asymptotic behavior, and how large the contributions from the long-time tail to the diffusion coefficient are. It is clear that the results obtained can serve as a guideline for interpreting computer simulations (Grassberger, 1980). It is possible to check specific conjectures like that of Alder and Alley about the existence of the coefficients $U^{(2n)}$. Perhaps the most useful property of these models is that they make the mechanisms responsible for the occurrence of long-time tails in systems like the Lorentz gas extremely transparent. From a purely mathematical viewpoint it seems of interest to have some treatable examples of stochastic processes of a strongly non-Markovian character. In addition, there are a few other interesting aspects to those models, which I want to sketch briefly below.

1. Periodic boundary conditions

All the results concerning long-time tails in functions such as the velocity autocorrelation function are strictly taken true in the thermodynamic limit only, that is for infinite systems. In systems with periodic boundary conditions, as studied mostly in computer simulations, the asymptotic long-time behavior of these functions changes to an exponential decay (Wood, 1975). This is not hard to understand: The solutions of diffusion equations that govern the time evolution of the densities of conserved quantities can be expanded in eigensolutions which for periodic systems are typically of the form $e^{-Dk^2t}e^{i\mathbf{k}\cdot\mathbf{r}}$, with $k_i = 2\pi n_i/L_i$; n_i is an integer, and L_i is the period in the i direction. This means that the slowest decaying contribution to $\mathbf{u}(r,t)P(\mathbf{r},t)$, as considered in (1.23), decays in time as $\exp(-4\pi^2(\nu+D)t/L^2)$. For times that are short compared to the decay time $L^2/4\pi^2(\nu+D)$, but long enough that for the infinite system the long-time tails appear,[7] the latter will show up also in the periodic system. For Lorentz models similar arguments are valid, because the probability for return of the light particle to the neighborhood of its starting position is also governed by the solution of the diffusion equation. For the exactly solvable models the influence of periodic boundary conditions can be studied in a simple way again.

If one replaces the periodic boundary conditions by more general ones, the situation becomes somewhat less transparent. However, one still expects an exponential decay, because the eigenvalue spectrum for the diffusion equation in a finite system is discrete under all boundary conditions.

2. Fluctuating hydrodynamics

As mentioned before, the long-time tails can also be explained with the aid of fluctuating hydrodynamics. In the fluid case the most important fluctuating quantity is the velocity density. In the case of the Lorentz gas this does not enter the hydrodynamic equation. There the

[7]For fluids finite system effects appear already at times on the order of the sound-mode traversal time L/c, where c is the speed of sound, due to couplings between the tagged particle density and the irrotational part of the velocity (Wood, 1975) (although these do not contribute to the asymptotic long-time tail).

fluctuating quantity is the diffusion coefficient, which is driven by spatial fluctuations in the density of scatterers (Dorfman *et al.*, 1981). It is interesting to check also this interpretation of the long-time tails against the exactly solvable models.

3. Steady-state diffusion

A common way to define the diffusion coefficient is as the ratio between density current and density gradient in a steady state. Such a steady state can be set up, for instance, by placing the system between an emitting plate at $x=0$ and an absorbing plate at $x=L$. Strictly taken, one has to go to the limits $L\to\infty$ and $d\rho/dx\to 0$, where ρ is the density of diffusing particles. In Lorentz models, which are strictly linear in ρ, the second limit need not be taken. Now one can ask the question how the density fluctuations, responsible for the long-time tails, influence this ratio for finite L, as well as in the limit $L\to\infty$.

The next sections of the paper are organized as follows. In Sec. II I introduce waiting time Lorentz models and the stochastic Lorentz gas and discuss some of their properties. Section III contains a calculation of several properties for a specific simple example. Different interpretations of the long-time tail effects, the influence of periodic boundary conditions and finite system effects, steady-state diffusion, and Sinai's fluctuations (introduced in Sec. II) are discussed in detail. In Sec. IV I calculate the Green's function $G(k,z)$ for a quite general class of waiting time models, I consider the low-frequency and high-frequency limits of this function and that of the generalized transport coefficients $U(k,z)$, $U^{(2n)}(z)$, and $D^{(2n)}(t)$, and, in addition, I consider several special cases that may be of interest. In Sec. V the Green's function for the stochastic Lorentz gas, which resembles the usual Lorentz gas more closely than the waiting time Lorentz models, is calculated in the form of an expansion in powers of k and z. The first few terms in this expansion are given explicitly and the results are compared to the results for the waiting time Lorentz models and those from kinetic theory. The last section finally contains a summary and evaluation of the results and a review of possible extensions of the theory developed here.

II. STOCHASTIC LORENTZ MODELS

A. Introduction

The distinction between stochastic and deterministic Lorentz models lies in the nature of the scattering mechanism. In deterministic Lorentz models the velocity of the light particle after a collision with a scatterer is uniquely defined; in stochastic Lorentz models this velocity follows some stochastic distribution, depending on the precollisional velocity and the relative position of the light particle with respect to the scatterer at the collision. Certain two-dimensional stochastic Lorentz models have been studied by Alder and Alley [(1978); see also Alley and Alder (1979)]. They found qualitative agreement between the long-time behavior of time correlation functions in stochastic and deterministic Lorentz models. This is not surprising, as the explanation for the long-time tail in the vaf of the Lorentz model does not depend on the details of the scattering mechanism [Ernst and Weyland (1971); see also Sec. I].

B. Lattice models

In certain cases one is forced to consider stochastic, rather than deterministic, Lorentz models. One such case consists of Lorentz models on d-dimensional lattices. In these models a given fraction of the lattice sites is occupied by scatterers and the light particle moves along the lattice bonds. In those versions of the model that are most analogous to the continuum Lorentz gas the light particle moves at constant speed without changing direction until it hits a scatterer. Then it suffers a change of direction, according to some predescribed probability distribution (for example, on a simple two-dimensional lattice it may have probability $\frac{1}{8}$ to be reflected, $\frac{3}{8}$ to continue its course, and $\frac{1}{4}$ to make a 90° angle in either possible direction). One reason to study such lattice models is that one might hope these to be mathematically simpler than the continuum models. Another good reason is that some of these models may give a fairly good picture of certain diffusion processes in crystals. In that case one must identify the lattice points of the Lorentz model with the interstitial positions of the crystal. Instead of letting the light particle run along the lattice bonds at constant speed, one must let it hop from lattice site to lattice site with a stochastically distributed waiting time between subsequent hoppings and possibly a probability distribution for the different hopping directions, which may depend, for instance, on the direction of the preceding jump. If all lattice points are equivalent, this is nothing but some type of random walk process. To introduce the character of a Lorentz model one has to introduce randomly distributed inhomogeneities, which are the equivalent of the scatterers in the continuum model. There are several ways to do this. For instance, one can occupy a certain fraction of the lattice sites with impurities that make these sites inadmissable to the light particle. Or one may block a certain fraction of the lattice bonds to the light particle by an impenetrable barrier. One could merge a certain fraction of neighboring sites to mimic vacancies in the lattice. One may consider a random A-B alloy where sites are inequivalent, depending on the configuration of surrounding atoms, and where barriers between neighboring sites are also inequivalent. The hopping probabilities may then be chosen to depend on the types of neighboring sites and/or barriers. Another variant is the model introduced by Scher and Montroll [(1975); see also Pfister and Scher (1978); Montroll and West (1979)]. They consider a light particle hopping between traps that are distributed randomly over a lattice. The hopping rate for a jump between two given traps depends strongly on the distance between them. They treat this model approximately by dividing the lattice into equal cells each containing many traps and assuming an effective waiting time distribution for jumps between neighboring cells. A one-dimensional version of this hopping model has been treated with exact methods by Bernasconi *et al.* [Alexander *et al.* (1981) and references quoted there]; and for a similar one-dimensional model Anshelevich and Vologodskii (1981) proved the validity of the diffusion equation in a certain scaling limit.

C. Related models

The common feature of all these models is that *they contain randomly distributed spatial inhomogeneities on a microscopic scale.* Systems and models with this property have been studied in a much wider context over the past years. Perhaps the simplest example is a diffusion process with a spatially fluctuating diffusion coefficient. For such a process Papanicolao and Varadhan (1980) rigorously prove the approach to a normal diffusion process in a certain scaling limit, and Dorfman *et al.* (1981) treat the low-frequency behavior of the diffusion coefficient. In a review paper Elliott *et al.* (1974) treat the mathematically very similar problems of elastic and optical properties of disordered crystals. A vast body of work has been done on the electrical conductivity of disordered crystals and the closely related problem of quantum-mechanical motion in a random potential, where the problems of localization and the existence of mobility edges play an important role. Recent reviews have been given by Mott and Davis (1979), Landauer (1978), and Thouless (1978). Another class of problems that are closely related to hopping processes with random barriers is the problem of conduction in random resistor networks [Kirkpatrick (1973); see also Shklovskii and Efros (1975)].

D. One-dimensional Lorentz models

For one-dimensional systems drastic simplifications arise and therefore I will concentrate my attention on these from now on.

1. A pseudo-one-dimensional deterministic Lorentz model

The deterministic Lorentz model in a strictly one-dimensional system leads to a light particle that just keeps running back and forth between two neighboring scatterers and is not of great physical interest. One way to improve on this would be to consider a pseudo—one-dimensional system consisting of an infinitely long cylinder of cross-section 1 containing randomly distributed infinitely thin scatterers of cross-section p, oriented perpendicular to the cylinder axis (see Fig. 2).

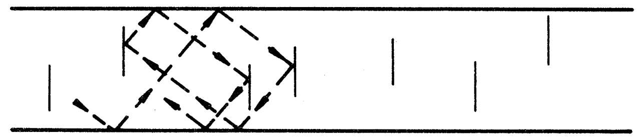

FIG. 2. A pseudo-one-dimensional deterministic Lorentz model

The light particle makes specular collisions both with the cylinder wall and the scatterers. Let n be the number density of scatterers. If one passes to the limit $p \rightarrow 0$, keeping np constant [this is the so-called Boltzmann-Grad limit (Lanford, 1976; Spohn, 1980)], the probability of hitting the same scatterer twice within a given time t will go to zero. Hence all collisions of the light particle with a scatterer are independent of each other. This implies that the time evolution of the distribution function of the light particle is described exactly by the Lorentz-Boltzmann equation (Spohn, 1978).

2. Strictly one-dimensional models

On the other hand, one may also consider a strictly one-dimensional stochastic Lorentz model in which the light particle moves with constant speed among randomly distributed point scatterers on the real axis. At a collision the probability for a reversal of the velocity of the light particle is p, and the probability that it continues its course is $(1-p)$. It is obvious that in the Boltzmann-Grad limit this stochastic Lorentz model becomes equivalent to the deterministic model sketched above. Therefore the parameter p may be considered to play a role equivalent to that of the density in higher dimensions, as has been noted by Spohn (1980) and Grassberger (1980).

Unlike in higher dimensions the scatterers need not be confined to lying on the sites of a periodic lattice, although they may be. Additionally, the scatterers need not be distributed independently over the real axis or over the lattice sites. Generally the models I will consider can be described in the following way, as shown in Fig. 3: Fixed scatterers labeled $(\ldots,-n, -n+1,\ldots -1,0,1,\ldots n,\ldots)$ are located in this sequence on the real axis. the intervals x_i, with $x_i>0$, between scatterers i and $i+1$ are independently distributed random variables with the same probability distribution μ such that

$$\int_0^\infty dx\, \mu(x)=1 \;, \tag{2.1}$$

$$\int_0^\infty dx\, x\mu(x)=l \;, \tag{2.2}$$

$$\int_0^\infty dx (x-l)^2\mu(x)=\Delta^2 \;. \tag{2.3}$$

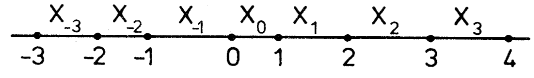

FIG. 3. A configuration of scatterers on the real axis.

Hence the average and the variance of the interval length must exist.

3. The stochastic Lorentz gas

I will now call *the stochastic Lorentz gas* the model in which the light particle runs with constant speed v and makes instantaneous collisions with the scatterers. The probability for a reflection will be p, that for transmission $(1-p)$. In the simplest case p is the same for all scatterers. For the initial distribution of the position x and velocity V of the light particle the simplest choice is a uniform distribution over the interval x_0 with equal probabilities for positive and negative velocity, viz.,[8]

$$f(x,V,t=0)=(2l)^{-1}[\delta(V-v)+\delta(V+v)] \quad \text{if } x\in x_0 , \tag{2.4}$$
$$=0 \quad \text{if } x\notin x_0 .$$

When one calculates quantities that are averages over the distribution of all intervals, this initial condition is equivalent to distributing the light particle uniformly over the real axis and subsequently relabeling the interval where it happens to be as x_0 (and relabeling the other intervals accordingly). Of course for a fixed configuration of scatterers (2.4) is not equivalent to a uniform distribution of the light particle. In addition $(2l)^{-1}$ must be replaced by $(2x_0)^{-1}$ in this case to warrant a correct normalization.

Further I will consider *waiting time Lorentz models*. In these models the light particle sits on one of the scatterers and jumps instantaneously to a neighboring scatterer after a stochastically distributed waiting time. The most general case I will consider is that where the waiting time distribution for a jump in the direction opposite the previous one is given as $\tilde{p}(t)$ and the waiting time distribution for a jump in the same direction as $\tilde{q}(t)$.[9] These distributions must be the same for all sites, the time integral of $\tilde{p}(t)+\tilde{q}(t)$ must be normalized to unity (no emission or absportion of light particles occurs) and the average waiting time τ must be finite, or

$$\int_0^\infty dt[\tilde{p}(t)+\tilde{q}(t)]=1 , \tag{2.5}$$

$$\int_0^\infty dt\, t(\tilde{p}(t)+\tilde{q}(t))=\tau . \tag{2.6}$$

As initial condition I will usually consider the situation where the light particle sits on scatterer 0, with equal probability that it came there from the left or from the right.

4. Waiting time Lorentz models

Compared to the stochastic Lorentz gas the waiting time Lorentz models show an enormous simplification: The probabilaity to get from scatterer 0 to scatterer n in a given time t is independent of the lengths of the intervals x_i and therefore can be simply calculated, just as for a random walk on a regular one-dimensional lattice, or for the generalized random walk with different probabilities $\tilde{p}(t)$ and $\tilde{q}(t)$, for backward and forward jumps, respectively. The difference with the (generalized) regular random walk is that the position of the nth scatterer is a stochastic variable, and it is precisely the fluctuations of this quantity about its average that are responsible for long-time tails. On the other hand, although the waiting time Lorentz models are much simpler to treat mathematically than the stochastic Lorentz gas, the physical behavior is not very different. This becomes plausible immediately if one considers the intuitive explanations for the occurrence of long-time tails. The basic ingredients, like the existence of a diffusion equation and a memory of the positions of scatterers, apply to both classes of models equally well. Explicit calculations will show that, although there are differences, those do not show up in the form of the leading contribution to the long-time tail in the velocity autocorrelation function.

5. Special interval and waiting time distributions

Although it is possible to treat general distributions $\mu(x)$ for the interval lengths and $\tilde{p}(t)$, $\tilde{q}(t)$ for the waiting times, certain cases are of special interest. For the interval distribution this is the exponential distribution, corresponding to a Poisson distribution of scatterers,

$$\mu(x)=l^{-1}e^{-x/l} , \tag{2.7}$$

or its discrete counterpart,

$$\mu(x)=\rho\sum_{n=1}^{\infty}(1-\rho)^{n-1}\delta(x-n\rho l) , \quad 0<\rho\le 1 . \tag{2.8}$$

In the limit $\rho\to 0$ (2.8) approaches (2.7). For the waiting time distributions the most interesting special cases are those where $\tilde{p}(t)=\tilde{q}(t)$ and especially where both are exponential

$$\tilde{p}(t)=\tilde{q}(t)=(2\tau)^{-1}e^{-t/\tau} , \tag{2.9}$$

which corresponds to a Poisson distribution for the times at which the light particle makes a jump.

E. Generalizations

In principle several generalizations of the models discussed above are possible. One could allow for correlations between the interval lengths, such as would arise from a long-range potential between the scatterers. One could make the waiting time distribution dependent on the configuration of neighboring scatterers, but that would go at the cost of the simplifications discussed above. Another possibility still would be to consider a mixture of different kinds of scatterers. For instance, if

[8]This distribution is normalized only in conjunction with the distribution $\mu(x_0)$ for the interval x_0.

[9]In the case of a regular random walk (all intervals have the same length) such models have been considered by Haus and Kehr (1979) and by Zwerger and Kehr (1980).

one would add to a system of scatterers with a small or intermediate reflection coefficient a small fraction of scatterers with high reflection coefficient, one might be able to mimic the so-called cage effect occuring in higher dimensions at high scatterer denisties (Alder and Alley, 1978). However, none of these generalizations will be discussed here.

F. Sinai's fluctuations

A final remark to be made here is the following: Owing to the stochastic nature of the dynamics of the light particle one may distinguish two types of averaging that can be applied to a dynamical quantity. The first one is an average over all paths of the light particle for a given configuration of scatterers and given initial conditions on position and velocity of the light particle (for example, fixed initial position and equal probability for both velocity directions or fixed position and velocity). This average, if needed explicitly, will be denoted by $\{\ \}$. The second average is over the distribution of the interval lengths x_i plus possibly a further average over the initial conditions on the light particle. This average will be denoted as $\langle\ \rangle$, but in many cases the same symbol will be used instead of $\langle\{\ \}\rangle$. It was noted by Sinai that averages of the first type may still be considered stochastic quantities with respect to the second average (Sinai, 1980). Hence one may consider fluctuations of the type $\langle\{\ \}^2\rangle-\langle\{\ \}\rangle^2$. We will be especially interested in fluctuations of the velocity autocorrelation function and the mean-square displacement,

$$\delta C(t)=\langle\{V(0)V(t)\}^2\rangle-\langle\{V(0)V(t)\}\rangle^2\ , \tag{2.10a}$$

$$\delta x^2(t)=\langle\{[x(t)-x(0)]^2\}^2\rangle-\langle\{[x(t)-x(0)]^2\}\rangle^2\ . \tag{2.10b}$$

These quantities are of interest for computer simulations where one computes, say, $\langle\{V(0)V(t)\}\rangle$ by calculating $\{V(0)V(t)\}$ for several configurations and initial conditions and averaging subsequently. The magnitude of $\delta C(t)$ gives an indication of the amount of averaging that will be needed for a given time t, and, in addition, one may manage to reduce the amount of averaging needed by a judicious choice of the initial conditions on $\{\ \}$.

III. VELOCITY AUTOCORRELATION FUNCTION AND MEAN-SQUARE DISPLACEMENT FOR THE SYMMETRIC EXPONENTIAL WAITING TIME LORENTZ MODEL

A. The Green's function

In this section I want to consider the waiting time Lorentz model with isotropic scattering [i.e., $\widetilde{p}(t)=\widetilde{q}(t)$] and an exponential distribution for the waiting times as given by (2.9). Assume that initially the light particle is located at scatterer 0 and that this position is chosen as the origin on the real axis. The first quantity of interest is the Green's function or probability density $P(x,t)$, already introduced in Sec. I, to find the light particle at position x at time t. First calculate the probability $p(m,t)$ of finding the particle at scatterer m at time t (Feller, 1971, Sec. II, 7). This quantity, which is obviously an even function in m, is obtained for non-negative m as

$$p(m,t)=\sum_{k=0}^{\infty}\frac{(m+2k)!}{(m+k)!k!}2^{-(m+2k)}\frac{e^{-t/\tau}}{(m+2k)!}\left[\frac{t}{\tau}\right]^{m+2k}\ .\qquad m\geq 0 \tag{3.1}$$

The factor $[(m+2k)!/(m+k)!k!](2^{-(m+2k)})$ is the probability that the light particle arrives at scatterer m after $m+2k$ jumps, and $e^{-t/\tau}(t/\tau)^{m+2k}/(m+2k)!$ is the probability, according to the Poisson distribution, that the light particle makes $m+2k$ jumps during a time t. In (3.1) one recognizes the series expansion of a Bessel function of imaginary argument (Gradshteyn and Ryzhik, 1965); hence

$$p(m,t)=e^{-t/\tau}I_m(t/\tau)\ , \tag{3.2}$$

which holds for positive and negative m equally. From this $P(x,t)$ can be obtained as

$$P(x,t)=p(0,t)\delta(x)+\sum_{m=1}^{\infty}p(m,t)\left\langle\delta\left[x-\sum_{i=0}^{m-1}x_i\right]\right\rangle,\qquad x\geq 0 \tag{3.3}$$

and the evenness of $P(x,t)$ in x can be used to define this function for negative x.

B. Velocity autocorrelation function and mean-square displacement

To introduce the velocity autocorrelation function one first has to say what is meant by the velocity. As the light particle moves by making instantaneous jumps, it does not have a velocity in the proper sense of this word. However, it is possible to attribute to a jump from, say, scatterer j to scatterer $j+1$ at a time t_0, a generalized velocity

$$V(t)=x_j\delta(t-t_0)\ . \tag{3.4}$$

With this definition in mind we can attribute to a particle that sits on scatterer 0 at $t=0^+$ an "average initial velocity" $(x_{-1}-x_0)/2\tau$. One easily convinces himself that integration of this quantity from $t=-\epsilon$ to $t=0^+$ correctly yields the average displacement of the light particle during this small time interval.[10] Likewise, if the light particle is at scatterer m at time t, its "average velocity" is $(x_m-x_{m-1})/2\tau$. The vaf now is obtained as

[10]Only those processes contribute to the velocity autocorrelation function where the light particle jumps just at $t=0$. I have chosen here the convention of labeling the particle on which the jump ends as 0. I could also have chosen to label 0 the particle from which this initial jump starts. But then the effective initial distribution for the light particle that contributes to the vaf has a probability of $\frac{1}{2}$ of sitting on scatterer 1, with effective initial velocity x_0/τ, and a probability of $\frac{1}{2}$ of sitting on scatterer -1, with effective velocity $-x_{-1}/\tau$.

$$C(t)=\sum_{m=-\infty}^{\infty} p(m,t)\langle (x_{-1}-x_0)(x_m-x_{m-1})\rangle/(4\tau^2) + [\langle x_{-1}^2+x_0^2\rangle/(2\tau^2)]\delta(t/\tau) \tag{3.5a}$$

$$=e^{-t/\tau}[I_1(t/\tau)-I_0(t/\tau)]\frac{\Delta^2}{2\tau^2}+\delta(t/\tau)\frac{l^2+\Delta^2}{\tau^2} . \tag{3.5b}$$

Here I used the property $\langle x_i x_j\rangle = l^2$ for $i\neq j$, as a result of which the only remaining contributions come from $m=0, \pm 1$. The initial δ function accounts for the correlation of a jump at $t=0$ to itself.[11] From the known asymptotic expansion of I_m for large argument (Gradshteyn and Ryzhik, 1965),

$$e^{-x}I_m(x)=(2\pi x)^{-1/2}\left[1-\frac{\left[\frac{2m+1}{2}\right]\left[\frac{2m-1}{2}\right]}{2x}+\frac{\left[\frac{2m+3}{2}\right]\left[\frac{2m+1}{2}\right]\left[\frac{2m-1}{2}\right]\left[\frac{2m-3}{2}\right]}{2!(2x)^2}-\cdots\right] \tag{3.6a}$$

$$=(2\pi x)^{-1/2}e^{-m^2/2x}\left[1+\frac{1}{x}\left[\frac{1}{8}-\frac{m^2}{4x}+\frac{m^4}{24x^2}\right]+\cdots\right], \tag{3.6b}$$

one readily obtains the long-time behavior of the vaf as

$$C(t)\approx\frac{-\Delta^2}{4\tau^2\sqrt{2\pi}}(t/\tau)^{-3/2} . \tag{3.7}$$

The diffusion coefficient is found as

$$D=\int_0^\infty dt\; C(t)=l^2/2\tau , \tag{3.8}$$

and the mean-square displacement as a function of time is obtained by integrating (3.5b) twice with respect to time, with the result, setting $x(0)=0$,

$$\langle x^2(t)\rangle = l^2 t/\tau+\Delta^2\int_0^{t/\tau} dx\; e^{-x}I_0(x) \tag{3.9a}$$

$$\approx l^2 t/\tau+\Delta^2(2t/\pi\tau)^{1/2} \quad \text{for } t/\tau >> 1 . \tag{3.9b}$$

The remainder of this section is devoted to a discussion of certain aspects of the above results plus a consideration of steady-state diffusion.

C. Contribution of the long-time tail of the velocity autocorrelation function to the diffusion coefficient

First, the diffusion coefficient exists, and it is the same as for a random walk on a lattice with a fixed distance between neighboring scatterers. This is certainly no surprise; the probability $p(m,t)$ is the same for the lattices with fixed and with random intervals, the average distance to the origin of the mth scatterer in the random case is just ml, and the relative fluctuations of this distance are small for large m. Notice, however, that correlations between the initial jump and jumps at later times are of paramount importance in establishing this result! If all jumps were uncorrelated, the diffusion coefficient would be given by $(l^2+\Delta^2)/2\tau$. For instance, in the case of a Poisson distribution of scatterers, where $\Delta=l$, this would make a difference of a factor 2. Now it would be unrealistic to attribute this difference entirely to the long-time tail in the vaf because there are also memory effects occurring on the time scale of a few mean jump times. Figure 4 shows the vaf as a function of t/τ together with the asymptotic approximation (3.7). One sees that the asymptotic behavior sets in already surprisingly early, say, around $t/\tau=4$. If $\Delta=l$, the contribution to the diffusion coefficient from the area of $C(t)$ for t/τ between 4 and ∞ amounts to almost 30% (with negative sign!) of the diffusion coefficient.

D. Connection between density fluctuations and the long-time tails

It is interesting to calculate the long-time behavior of the mean-square displacement also from (3.3) and (3.2) with the aid of the asymptotic expansion (3.6b). This yields

$$\langle x^2(t)\rangle = \sum_{m=-\infty}^{\infty} p(m,t)\left\langle\left[\sum_{i=0}^{|m|-1} x_i\right]^2\right\rangle \tag{3.10a}$$

$$\approx \sum_{m=-\infty}^{\infty}\frac{1}{\sqrt{2\pi t/\tau}}e^{-m^2\tau/2t}(m^2l^2+|m|\Delta^2) \tag{3.10b}$$

$$\approx l^2t/\tau+\Delta^2(2t/\pi\tau)^{1/2} . \tag{3.10c}$$

One sees again that the main contribution comes from the average distance to the origin ml, of the mth scatterer, whereas the $\sqrt{t}$ term responsible for the long-time tail in the vaf is due to the fluctuations in this distance (or, equivalently, to fluctuations in the density of scatter-

[11]To understand this contribution one may consider a model in which the jumps are not instantaneous but instead require a fixed time $t_0 << \tau$. In this case the self-correlation of a jump starting between $t=-t_0$ and $t=0$ on the average contributes $(l^2+\Delta^2)\,|\,t_0-t\,|\,\tau^{-1}t_0^{-2}\;\mathrm{H}(t_0-|\,t\,|)$ to $C(t)$. In the limit $t_0\to 0$ this approaches the δ-function contribution in (3.5).

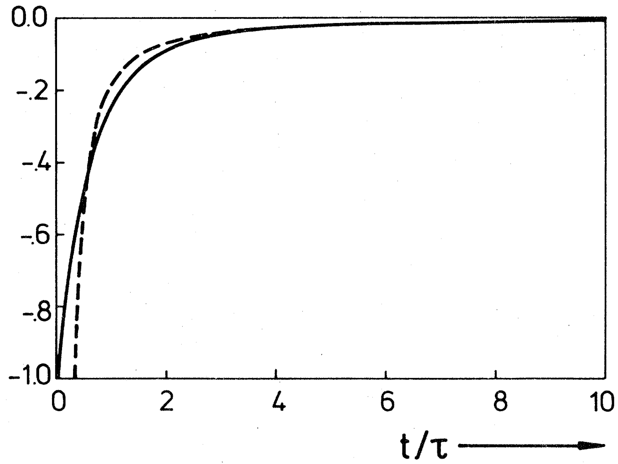

FIG. 4. The normalized velocity autocorrelation function $2C(t)\tau^2/\Delta^2$ (solid line) for the symmetric, exponential waiting time model, and the asymptote $-(1/2\sqrt{2\pi})(t/\tau)^{-3/2}$ (dashed line) as a function of t/τ.

ers). The latter are typically of a magnitude $\sqrt{m}$. An equivalent interpretation is to attribute the $\sqrt{t}$ term to spatial fluctuations of the diffusion coefficient. Spatial fluctuations in the average length of the intervals directly lead to spatial fluctuations in the diffusion coefficient, as can be seen from (3.8). From these the correct long-time behavior of $\langle x^2(t)\rangle$ can also be obtained (Dorfman *et al.*, 1981).

E. Comparison with the theory of Ernst and Weyland

From the calculation of the vaf given above one may conclude that the picture for the origin of the long-time tail, as sketched in Sec. I, applies also in the case of the waiting time Lorentz models. The long-time tail is entirely due to recurrences of the light particle to the interval of its first jump, the probability of such a recurrence is described to leading order by the solution of the diffusion equation, and the slight difference between the probabilities of returning from the right or from the left, depending on the direction of the initial jump, introduces a factor $1/t$.

In the case of a Poisson distribution of scatterers, where $l=\Delta$, (3.7) agrees entirely with the result of Ernst and Weyland (1.28) if one uses instead of D_0 the complete diffusion coefficient, given by (3.8).

F. Periodic boundary conditions

Periodic boundary conditions can be imposed in different ways. The most straightforward is to put a fixed number N of scatterers into a periodic box of length L and to impose the distribution $\mu(x)$ on each of the interval lengths, under the constraint that the total length equals L. This leads to a joint distribution for the N intervals of the form

$$\mu(x_0,\ldots,x_{N-1})=\prod_{i=0}^{N-1}\mu(x_i)\delta\left[\sum_{j=0}^{N-1}x_j-L\right]Z^{-1}, \tag{3.11}$$

where Z is a normalization constant.

The average length of an interval now is L/N, due to the constraint, and the variance,

$$\Delta_{LN}^2=\langle (x_0-L/N)^2\rangle , \tag{3.12}$$

in general differs from Δ^2. As a consequence of the constraint the lengths of different intervals are not uncorrelated any more. One has

$$\begin{aligned}&\left\langle (x_0-\langle x_0\rangle)\sum_{i=0}^{N-1}(x_i-\langle x_i\rangle)\right\rangle=0 ,\\ &\Delta_{LN}^2+(N-1)\langle (x_0-\langle x_0\rangle)(x_1-\langle x_1\rangle)\rangle=0 ,\\ &\langle (x_0-\langle x_0\rangle)(x_1-\langle x_1\rangle)\rangle=-\Delta_{LN}^2/(N-1) ,\end{aligned} \tag{3.13}$$

provided $N>1$. In the limit $N\to\infty$ this correlation disappears, and, if $L/N=l$, the quantity Δ_{LN} approaches Δ.

The infinite periodic lattice can be related to the periodic box in the usual way by imposing the conditions

$$x_{m+kN}=x_m \quad (0\le m<N;\ k=\pm1,\pm2,\ldots) . \tag{3.14}$$

The vaf still can be obtained from (3.5a), with Δ replaced by Δ_{LN} and l by L/N, but, as a result of the periodicity conditions (3.14), Eq. (3.5b) is to be replaced by

$$C(t)=\frac{1}{2\tau^2}e^{-t/\tau}\sum_{k=-\infty}^{\infty}[I_{Nk+1}(t/\tau)-I_{Nk}(t/\tau)]\Delta_{NL}^2\frac{N}{N-1}+\frac{1}{\tau^2}[(L/N)^2+\Delta_{NL}^2]\delta(t/\tau) . \tag{3.15}$$

For the periodic box the function $p(m,t)$, with $0\le m<N$, can be expanded in plane waves by means of a discrete Fourier decomposition. The result reads

$$p(m,t)=e^{-t/\tau}\sum_{k=-\infty}^{\infty}I_{Nk+m}(t/\tau)=\frac{1}{N}\sum_{q=0}^{N-1}\exp\left\{\frac{2\pi imq}{N}-\left[1-\cos\left[\frac{2\pi q}{N}\right]\right]\frac{t}{\tau}\right\} . \tag{3.16}$$

For large N and t/τ (3.16) can be approximated as

$$p(m,t)\approx\frac{1}{N}+\frac{2}{N}\sum_{q=1}^{\infty}\cos\left[\frac{2\pi qx}{L}\right]\exp\left[-Dt\left[\frac{2\pi q}{L}\right]^2\right] , \tag{3.17}$$

where we put $mL/N=x$. In (3.17) one recognizes the decay of an initial δ function through the eigenfunctions of the diffusion equation for a periodic system. The exact eigenfunctions for the time evolution of the random walk process under consideration are of course given in (3.16). Substitution of (3.16) into (3.15) leads to

$$C(t)=-\frac{\Delta_{NL}^2}{2\tau^2(N-1)}\sum_{q=1}^{N-1}\left[1-\cos\left[\frac{2\pi q}{N}\right]\right]\exp\left\{-\left[1-\cos\left[\frac{2\pi q}{N}\right]\right]\frac{t}{\tau}\right\}+\frac{1}{\tau^2}\left[(L/N)^2+\Delta_{NL}^2\right]\delta(t/\tau)\,.$$

From (3.15) and (3.18) one can infer the behavior of the vaf in different time regimes. For $t/\tau<<N^2$, that is, for times in which the light particle has a very small probability to reach the boundary of the box, only the $k=0$ term in (3.15) contributes. Hence in this time regime the infinite-system result (3.5b) is reproduced, except for a change in the coefficients! For example, in the case that the N scatterers are distributed independently over the box L one finds

$$\Delta_{NL}^2=\frac{L^2(N-1)}{N^2(N+1)}\,, \tag{3.19}$$

so, if one chooses $L/N=l$ the coefficient of the apparent long-time tail is reduced by a factor $N/N+1$. This is typical for a finite size correction (Wood, 1975).

For $t/\tau>>N^2$ the terms with $q=1$ and $q=N-1$ in (3.18) become dominant. In this time regime the vaf decays exponentially, due to the exponential decay of the nonconstant eigenmodes of the diffusion equation. This type of crossover from a power-law decay to an asymptotic exponential time decay is well known in computer simulations (Wood, 1975).

The diffusion coefficient is readily obtained from (3.18), with the aid of (1.8b), as

$$D=\frac{1}{2\tau}\left[\frac{L}{N}\right]^2. \tag{3.20}$$

This is the same again as the diffusion coefficient for a random walk with constant lattice spacing L/N, as one would expect.

It is interesting to consider also a different way of introducing periodic boundary conditions, namely by distributing the intervals $x_0\cdots x_{N-1}$ independently of each other according to $\mu(x)$ plus imposing the periodicity condition (3.14). In this case the periodicity length L is a fluctuating quantity. The coefficient of the apparent long-time tail for $t/\tau<<N^2$ now becomes the same as in the nonperiodic infinite system, but the diffusion coefficient becomes a fluctuating quantity dependent on L, as the average interval length is L/N. If one averages over the distribution of the intervals, he obtains an average diffusion constant

$$D_{\rm av}=(l^2/2\tau)(1+\Delta^2/Nl^2)\,. \tag{3.21}$$

Finally, it is illuminating also to consider the mean-square displacement. Owing to the periodicity condition the fluctuation in the distance of the mth scatterer to the origin does not grow as $\sqrt{m}$, but is bounded to be at most of the order $\sqrt{N}$. Therefore the contributions to the mean-square displacement from these fluctuations saturate at a value proportional to N as soon as t/τ becomes much larger than N^2.

G. Sinai's fluctuations

As discussed already in Sec. II, quantities such as the vaf can be considered as resulting from a twofold averaging procedure, namely, an average over random walks at fixed scatterer configuration, indicated by $\{\ \}$, followed by an average over scatterer configurations, indicated by $\langle\ \rangle$. The quantities resulting after the first averaging are still stochastic variables with respect to the second averaging. A typical measure for the degree of stochasticity of a variable is its variance. In the case of the vaf for the waiting time Lorentz models I consider the quantity $\langle\{V(0)V(t_1)\}\ \{V(0)V(t_2)\}\rangle$ from which the variance of the vaf is readily obtained by putting $t_1=t_2$ and subtracting the square of the average vaf. A straightforward calculation, based on (3.5), yields

$$\begin{aligned}\langle\{V(0)V(t_1)\}\{V(0)V(t_2)\}\rangle=&\frac{1}{16\tau^4}\sum_{m=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}e^{-(t_1+t_2)/\tau}I_m(t_1/\tau)\\&\times I_q(t_2/\tau)\langle(x_{-1}-x_0)^2(x_m-x_{m-1})(x_q-x_{q-1})\rangle\\&+\frac{1}{8\tau^4}\left[\sum_{m=-\infty}^{\infty}e^{-t_1/\tau}I_m(t_1/\tau)\delta(t_2/\tau)\langle(x_{-1}^2+x_0^2)(x_{-1}-x_0)(x_m-x_{m-1})\rangle\right.\\&\left.+\sum_{q=-\infty}^{\infty}e^{-t_2/\tau}I_q(t_2/\tau)\delta(t_1/\tau)\langle(x_{-1}^2+x_0^2)(x_{-1}-x_0)(x_q-x_{q-1})\rangle\right]\\&+\frac{1}{4\tau^4}\delta(t_1/\tau)\delta(t_2/\tau)\langle(x_{-1}^2+x_0^2)^2\rangle\end{aligned} \tag{3.22a}$$

$$\begin{aligned}=&\sum_{m=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\frac{1}{16\tau^4}e^{-(t_1+t_2)/\tau}I_m(t_1/\tau)I_q(t_2/\tau)\\&\times\langle(x_{-1}-x_0)^2\rangle\langle(x_m-x_{m-1})(x_q-x_{q-1})\rangle+\mathscr{T}_{\rm corr}\,,\end{aligned} \tag{3.22b}$$

the correction terms $\mathscr{T}_{corr}$ resulting solely from m or $q=0, \pm 1$. The only nonvanishing contributions to the leading term come from $q=m, m\pm 1$; hence (3.22b) can be reduced to

$$\begin{aligned}\langle\{V(0)V(t_1)\}\{V(0)V(t_2)\}&=\frac{\Delta^4}{8\tau^4}e^{-(t_1+t_2)/\tau}\sum_{m=-\infty}^{\infty}I_m(t_1/\tau)[2I_m(t_2/\tau)-(I_{m+1}(t_2/\tau)+I_{m-1}(t_2/\tau))]+\mathscr{T}_{corr}\\&=\frac{\Delta^4}{4\tau^4}\left[-\frac{d}{d(t_2/\tau)}\right]\sum_{m=-\infty}^{\infty}e^{-(t_1+t_2)/\tau}I_m(t_1/\tau)I_m(t_2/\tau)+\mathscr{T}_{corr}\\&=\frac{\Delta^4}{4\tau^4}\left[-\frac{d}{d(t_2/\tau)}\right]e^{-(t_1+t_2)/\tau}I_0((t_1+t_2)/\tau)+\mathscr{T}_{corr}\\&=\frac{\Delta^4}{4\tau^4}e^{-(t_1+t_2)/\tau}[I_0((t_1+t_2)/\tau)-I_1((t_1+t_2)/\tau)]+\mathscr{T}_{corr}\,.\end{aligned}$$

The similarity of this result to Eq. (3.5b) for the vaf itself immediately strikes the eye; and, as a matter of fact, this similarity is not incidental. Some reflection reveals that the two independent random walks, both starting at $t=0$, can be linked together to one random walk, starting at $t=-t_1$ passing through scatterer 0 at $t=0$ and ending at $t=t_2$. Indeed, if on the right-hand side of (3.22b) one takes out a factor $-\langle(x_{-1}-x_0)^2\rangle/4\tau^2$, the remaining expression is just the vaf for such a random walk. It is clear that the condition that the random walk must pass through scatterer 0 at $t=0$ does not affect the value of the vaf, as all scatterers are equivalent under the average $\langle\ \rangle$.

The correction terms resulting from $m, q=0, \pm 1$ are easily expressed in terms of moments of the interval distribution function $\mu(x)$. We have to require the existence of the third and fourth moments, denoted as $\langle x^3\rangle$ and $\langle x^4\rangle$, respectively. The final form for the fluctuation formula becomes

$$\begin{aligned}\langle\{V(0)V(t_1)\}\{V(0)V(t_2)\}\rangle&=\frac{\Delta^4}{4\tau^4}e^{-(t_1+t_2)/\tau}[I_0((t_1+t_2)/\tau)-I_1((t_1+t_2)/\tau)]\\&\quad+\frac{1}{8\tau^4}e^{-(t_1+t_2)/\tau}[I_0(t_1/\tau)-I_1(t_1/\tau)][I_0(t_2/\tau)-I_1(t_2/\tau)]\\&\quad\times(\langle x^4\rangle-4\langle x^3\rangle l+\langle x^2\rangle^2+4\langle x^2\rangle l^2-2l^4)\ +\frac{1}{2\tau^4}\delta(t_1/\tau)\delta(t_2/\tau)(\langle x^4\rangle+\langle x^2\rangle^2)\\&\quad+\frac{1}{4\tau^4}(\delta(t_1/\tau)e^{-t_2/\tau}[I_0(t_2/\tau)-I_1(t_2/\tau)]+\delta(t_2/\tau)e^{-t_1/\tau}[I_0(t_1/\tau)-I_1(t_1/\tau)])\\&\quad\times(-\langle x^4\rangle+2\langle x^3\rangle l-\langle x^2\rangle^2)\,.\end{aligned}\tag{3.24}$$

From this result one may immediately extract the long-time behavior of the fluctuations. The variance $\langle\{V(0)V(t)\}^2\rangle-\langle\{V(0)V(t)\}\rangle^2$ decays asymptotically as $t^{-3/2}$, just as the vaf itself does. This implies that the stochastic variable $\{V(0)V(t)\}$ is typically of magnitude $t^{-3/4}$.[12]

Hence, if one would like to extract the long-time behavior of the vaf from a stochastic average applied on $\{V(0)V(t)\}$ (e.g., by a Monte Carlo simulation on a computer), one would have to average over extremely many configurations of scatterers. One way to improve on this situation is by considering each configuration of scatterers together with the configuration that obtains by the interchange of the intervals x_{-1} and x_0. One may then define an average $\{\ \}'$ consisting of both an average over random walks and an average over the two selected configurations of scatterers. In either configuration the light particle starts off at scatterer 0 at $t=0^+$. The average value $\{x_{-1}-x_0\}'$ now is equal to zero. Hence in (3.24) only the correction terms survive (they are not changed!), and the stochastic vaf $\{V(0)V(t)\}'$ is of order $t^{-3/2}$ for long times. This, in fact, can be seen directly from (3.5a): $\{(x_{-1}-x_0)(x_m-x_{m-1})\}'$ vanishes for $|m|>1$, and one has

$$\begin{aligned}&\sum_{m=-\infty}^{\infty}p(m,t)\frac{1}{4\tau^2}\{(x_{-1}-x_0)(x_m-x_{m-1})\}'+\frac{1}{2\tau^2}\{x_{-1}^2+x_0^2\}'\delta(t/\tau)\\&\quad=\frac{1}{4\tau^2}[e^{-t/\tau}[I_1(t/\tau)-I_0(t/\tau)](x_{-1}-x_0)^2+2(x_{-1}^2+x_0^2)\delta(t/\tau)]\,.\end{aligned}\tag{3.25}$$

[12]Sinai (1980) has obtained stronger results concerning the distribution of $\{V(0)V(t)\}$ with respect to $\mu(x_i)$ in the case of the stochastic Lorentz gas.

Of course there is no reason to compute the vaf for the waiting time Lorentz model by stochastic methods. In more complicated systems, however, for which the vaf cannot be calculated exactly, one may want to use computer simulations for a calculation of the vaf. Then it will be very useful if the spread in the computed values can be reduced substantially by a judicious choice of the averaging procedure.

It is also of interest to calculate the variance of the mean-square displacement $\{x^2(t)\}$. With the aid of (3.10) one readily finds

$$\langle \{x^2(t_1)\}\{x^2(t_2)\}\rangle - \langle \{x^2(t_1)\}\rangle\langle \{x^2(t_2)\}\rangle$$
$$=2\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} e^{-(t_1+t_2)/\tau} I_m(t_1/\tau)I_n(t_2/\tau)$$
$$\times[\min(m,n)(\langle x^4\rangle-\langle x^2\rangle^2)+2\min(m,n)(m+n-2)(\langle x^3\rangle l-\langle x^2\rangle l^2)$$
$$+2\min(m,n)[\min(m,n)-1](\langle x^2\rangle^2-l^4)+4\min(m,n)(m-1)(n-2)\Delta^2 l^2]\ . \tag{3.26}$$

For t_1 and t_2 large the last term between square brackets dominates. With the aid of (3.1), (3.2), and (3.6) the asymptotic behavior of this term is found as

$$\langle \{x^2(t_1)\}\{x^2(t_2)\}\rangle - \langle \{x^2(t_1)\}\rangle\langle \{x^2(t_2)\}\rangle \approx \frac{8D^2 t_1 t_2}{\{\pi D(t_1+t_2)\}^{1/2}}\frac{\Delta^2}{l}\ . \tag{3.27}$$

This implies that $\{x^2(t)\}-\langle\{x^2(t)\}\rangle$ for long times is of order $t^{3/4}$, whereas the long-time tail contribution to $\langle\{x^2(t)\}\rangle$ was found in (3.9b) to be of order $t^{1/2}$. This may be an indication of why in computer simulations the long-time tail in the vaf is usually observed with much greater accuracy in the mean-square displacement than in the vaf directly (Wood and Lado, 1971) (although the averages performed for a fixed configuration of scatterers are usually different from the average considered here). For long times also the spread in the mean-square displacement becomes large compared to the long-time tail contribution, but the ratio of the two increases much more slowly with time than in the case of the vaf. On the other hand, it does not seem possible to reduce the variance of the mean-square displacement by a simple change in the averaging procedure { }, as could be done for the vaf.

H. Steady-state diffusion

As discussed already in Sec. I, a common way of defining the diffusion constant is as the ratio between the average values of current and density gradient of diffusing particles in a steady state. In our one-dimensional models we can set up such a steady state by placing a source at the origin which emits particles to the right at a constant rate $\alpha/2\tau$ and which, in addition, absorbs all particles hitting it, by placing N scatterers at positions $\xi_1, \xi_2, \ldots, \xi_N$, such that $0<\xi_1<\xi_2\cdots<\xi_N$, and by putting a sink that absorbs all particles hitting it at $L>\xi_N$. If $\rho_i(t)$ is the number of light particles located at scatterer i at time t,[13] the steady state is characterized by occupation numbers $\{\rho_i\}$ averaged over the random walk process that satisfy

$$\{\rho_i\}=\frac{\alpha(N+1-i)}{N+1}\ . \tag{3.28}$$

One simple way of seeing this is by noting that the $\{\rho_i(t)\}$ satisfy a master equation

$$\frac{d}{dt}\{\rho_i(t)\}=\tau^{-1}(\tfrac{1}{2}\{\rho_{i+1}(t)\}+\tfrac{1}{2}\{\rho_{i-1}(t)\}-\{\rho_i(t)\})\ ,\quad (1<i<N) \tag{3.29}$$
$$\frac{d}{dt}\{\rho_1(t)\}=\tau^{-1}(\tfrac{1}{2}\alpha+\tfrac{1}{2}\{\rho_2(t)\}-\{\rho_1(t)\})\ ,$$
$$\frac{d}{dt}\{\rho_N(t)\}=\tau^{-1}(\tfrac{1}{2}\{\rho_{N-1}(t)\}-\{\rho_N(t)\})\ .$$

Equation (3.28) is just the steady solution to these equations. Notice that the density profile is linear in the label i. The precise location of the scatterers is completely immaterial, as was to be expected. The average current is given as

$$j=\frac{\alpha}{2\tau(N+1)}\ . \tag{3.30}$$

The average gradient of the density of light particles is $-\alpha(N+1)/L^2$; hence the diffusion coefficient as a function of N and L follows as

$$D(N,L)=\frac{L^2}{2\tau(N+1)^2}=\frac{1}{2\tau n^2}\left[\frac{N}{N+1}\right]^2\ , \tag{3.31}$$

where n is the average density of scatterers.

It is worth noticing that the results obtained here remain essentially unchanged for the steady states of the

[13]Although in this picture it is natural to consider systems containing a large number of light particles, I maintain the requirement that these do not interact with each other.

stochastic Lorentz gas with isotropic scattering. There the densities of light particles moving away in either direction from each scatterer take the role of the $\{n_i\}$, but except for this trivial modification everything discussed here remains the same.

One must now ask the question how the stochastic distribution of the scatterers influences the average value of the diffusion coefficient. The answer to this question depends on the way in which the sources are added to the system and on the constraints one wants to impose on the distribution of scatterers. I want to consider three different possibilities.

1. A given number of scatterers is distributed over an interval of fixed length L. Then the result (3.31) is valid for each configuration of scatterers and the stochastic nature of the distribution of scatterers does not appear.

2. The number of scatterers is fixed, but the length L of the total interval may fluctuate. The simplest possibility for these fluctuations is the assumption that all nearest-neighbor distances, including those between the sources and the scatterers 1 and N, are distributed according to $\mu(x)$. Then the average of (3.31) over these distribution yields

$$D=\frac{l^2}{2\tau}\left[1+\frac{\Delta^2}{(N+1)l^2}\right]. \tag{3.32}$$

The correction to the infinite volume value of D is of order $1/N$, that is, of the same order of magnitude as boundary effects [compare also (3.21)].

3. The length of the interval L is kept fixed, but the number of scatterers is allowed to fluctuate. The diffusion coefficient for given L is then determined by the distribution of the number of scatterers on this interval. The simplest choice is to neglect the influence of the sources on this distribution and to consider the probability of finding N scatterers on an arbitrary interval of length L if the nearest-neighbor distances are distributed according to $\mu(x)$. A fairly long but straightforward calculation, which is given in Appendix B, yields the following result for the distribution of N at given L:

$$\begin{aligned}
P_L(N)=\frac{l}{\Delta}\frac{e^{-(N-n_0)^2l^2/2\Delta^2 n_0}}{\sqrt{2\pi n_0}}\Bigg\{&1+\frac{1}{n_0}\left[\frac{\langle x^3\rangle_c}{6l\Delta^2}-\frac{\Delta^2}{4l^2}-\frac{l^2}{12\Delta^2}+\frac{\langle x^4\rangle_c}{8\Delta^4}-\frac{5}{24}\frac{\langle x^3\rangle_c^2}{\Delta^6}\right.\\
&\left.+O\left[\frac{1}{n_0^2}\right]+\frac{N-n_0}{n_0}\left[-\frac{3}{2}+\frac{l\langle x^3\rangle_c}{2\Delta^4}+O\left[\frac{1}{n_0}\right]\right]\right]\\
&+\frac{(N-n_0)^2}{n_0^2}\left[\frac{17}{8}-\frac{17l\langle x^3\rangle_c}{12\Delta^4}+\frac{l^4}{12\Delta^4}-\frac{l^2\langle x^4\rangle_c}{4\Delta^6}+\frac{5l^2\langle x^3\rangle_c^2}{8\Delta^8}+O\left[\frac{1}{n_0}\right]\right]\\
&+\frac{(N-n_0)^3}{n_0^2}\left[\frac{l^2}{2\Delta^2}-\frac{l^3\langle x^3\rangle_c}{6\Delta^6}+O\left[\frac{1}{n_0}\right]\right]\\
&+\frac{(N-n_0)^4}{n_0^3}\left[\frac{-5l^2}{4\Delta^2}+\frac{5l^3\langle x^3\rangle_c}{6\Delta^6}+\frac{\langle x^4\rangle_c l^4}{24\Delta^8}-\frac{5l^4\langle x^3\rangle_c^2}{24\Delta^{10}}+O\left[\frac{1}{n_0}\right]\right]\\
&+\frac{(N-n_0)^6}{n_0^4}\left[\frac{\langle x^3\rangle_c^2}{72}+\frac{l^4}{8\Delta^4}-\frac{l^5\langle x^3\rangle_c}{12\Delta^8}+O\left[\frac{1}{n_0}\right]\right]\\
&+O\left[\frac{(N-n_0)^7}{n_0^5}\right]+\cdots\Bigg\},
\end{aligned} \tag{3.33}$$

where $n_0=L/l$ and $\langle x^m\rangle_c$ are the cumulant moments of x with respect to the distribution $\mu(x)$ (provided these exist).

With the aid of this result and (3.31) one obtains for the diffusion coefficient

$$D=\frac{l^2}{2\tau}\sum_N P_L(N)\frac{N^2}{(N+1)^2}$$
$$\approx\frac{l^2}{2\tau}\int_{-\infty}^{\infty}dx\, P_L(x)\frac{n_0^2}{(n_0+1)^2}\times\left[1-\frac{2(x-n_0)}{n_0+1}+\frac{3(x-n_0)^2}{(n_0+1)^2}+\cdots\right]$$
$$=\frac{l^2}{2\tau}\left[+\frac{1}{n_0}\left[3\frac{\Delta^2}{l^2}-2\right]+O\left[\frac{1}{n_0^2}\right]\right]. \tag{3.34}$$

Again, the corrections to the infinite-system diffusion coefficient are of order $1/N$, and the leading correction can be separated into a term due to the length fluctuations of the intervals [the term $(1/n_0)3\Delta^2/l^2$] and a term due to boundary effects (the term $-2/n_0$). For the case of a Poisson distribution of the scatterers the calculation simplifies enormously, and from (3.31) one obtains immediately

$$D=\frac{l^2}{2\tau}\sum_{N=0}^{\infty}\frac{(L/l)^{N+2}e^{-L/l}}{N!(N+1)^2}$$
$$=\frac{l^2}{2\tau}\sum_{N=0}^{\infty}\frac{(L/l)^{N+2}}{(N+2)!}\left[1+\frac{1}{N+1}\right]e^{-L/l} \tag{3.35}$$
$$\approx\frac{l^2}{2\tau}\left[1+\frac{l}{L}\right]=\frac{l^2}{2\tau}\left[1+\frac{1}{n_0}\right]$$

in agreement with (3.34).

Further quantities of interest are the Green's functions $F(k,t)$ and $G(k,z)$ defined in (1.4) and (1.11), respectively, and the higher-order diffusion coefficients $D^{(2n)}(t)$ and $U^{(2n)}(z)$, defined in (1.7) and (1.13). Instead of discussing these quantities for the special case treated above, I will consider them for the general waiting time Lorentz model, which will be the subject of the next section.

IV. THE GENERAL WAITING TIME LORENTZ MODEL

A. Calculation of the Green's function

As mentioned already in Sec. II, the most general waiting time Lorentz model that can be solved by the simple methods discussed here, is the one in which the waiting time distribution $\tilde{p}(t)$ for a backward jump is different from the distribution $\tilde{q}(t)$ for a forward jump, but $\tilde{p}(t)$ and $\tilde{q}(t)$ are the same for all scatterers. For the usual random walk, with equal distances between the scatterers, such models have been discussed by Haus and Kehr (1979) and by Zwerger and Kehr (1980).

From the Green's function $G(k,z)$, as defined in (1.11), all other quantities of interest may be obtained easily. The calculation of this function is straightforward and can be done by combining the following steps.

(i) Start from the situation where the light particle is initially at the origin, at scatterer 0, with equal probability to have arrived from either side. Then the probability density for a first jump to the right, respectively to the left, is given as (Feller, 1968 Sec. XIII, 5)

$$\tilde{r}^{+}(t)=\tilde{r}^{-}(t)=\tau^{-1}\int_t^{\infty}dt'\tfrac{1}{2}[\tilde{p}(t')+\tilde{q}(t')] , \tag{4.1a}$$

or after a Laplace transform, defined by $f(z)=\int_0^{\infty}dt\, e^{-zt}\tilde{f}(t)$,

$$r^{+}=r^{-}=\frac{1}{2z\tau}(1-p-q) , \tag{4.1b}$$

where the z dependence of p, q, and $r^{\pm}$ is omitted. Equation (4.1a) is easily understood by noting that the unconditional probability density for arrival of the light particle at scatterer 0 at time $t-t'$ is just τ^{-1}, and that the probability density for a first jump to the right at time t, after arrival at time $t-t'$, is $\frac{1}{2}[\tilde{p}(t')+\tilde{q}(t')]$ if the previous jump had no preferred direction.

(ii) Similarly, after arrival of the light particle at a given scatterer at time t_0, the probability to find it at the same scatterer, without having jumped, at time t_0+t is given by

$$\tilde{s}(t)=\int_t^{\infty}dt'[\tilde{p}(t')+\tilde{q}(t')] , \tag{4.2a}$$

or, after a Laplace transform

$$s=(1-p-q)/z . \tag{4.2b}$$

(iii) The probability of finding the light particle, sitting originally at scatterer 0, still at scatterer 0, without having jumped, at time t, is given as

$$\tilde{s}_0(t)=\tau^{-1}\int_t^{\infty}dt'\int_{t'}^{\infty}dt''[\tilde{p}(t'')+\tilde{q}(t'')] , \tag{4.3a}$$

or

$$s_0=\frac{z-\tau^{-1}(1-p-q)}{z^2} . \tag{4.3b}$$

(iv) The (Laplace-transformed) probability density X for a first return to the origin (scatterer 0), *just after* the light particle has jumped to the right (or to the left) from the origin is obtained from the equation

$$X=p+\sum_{n=1}^{\infty}q^2p^{n-1}X^n=p+\frac{q^2X}{1-pX} . \tag{4.4}$$

The first term on the right-hand side of (4.4) gives the probability that the particle jumps right back to the origin. The terms in the series describe the probability that the particle jumps back to the origin after n returns from the right to scatterer 1. The solution of (4.4) reads

$$X=\frac{1+p^2-q^2-\sqrt{(1-p-q)(1+p+q)(1-p+q)(1+p-q)}}{2p} . \tag{4.5}$$

(v) The probability density for an unconditioned return to the origin just after the first jump, is given as

$$R=\sum_{n=1}^{\infty} X^n(p+q)^{n-1}=\frac{X}{1-(p+q)X} . \tag{4.6}$$

(vi) Combination of $i-v$ yields for the total probability of ending up at the origin

$$P(0)=\frac{z-\tau^{-1}(1-p-q)}{z^2}+\frac{1-p-q}{z\tau}\frac{X}{1-(p+q)X}\frac{1-p-q}{z} . \tag{4.7}$$

(vii) Suppose the light particle arrives from the left at scatterer m. Then the probability density for 0,1,2,. . .subsequent returns to m from the right, followed by a jump to $m+1$ is given as

$$\Delta=q\sum_{n=0}^{\infty}(Xp)^n=\frac{q}{1-pX} . \tag{4.8}$$

(viii) The probability density for 1,2,. . .subsequent returns from the right to a given scatterer, just after arrival from the left is given as

$$R^+=\sum_{n=1}^{\infty} qX(pX)^{n-1}=\frac{qX}{1-pX} . \tag{4.9}$$

(ix) The probability $P(m)$ of ending up at scatterer m, with $|m|>0$, is obtained by combining (i), (v), (vii), (viii), and (ii) into

$$P(m)=\frac{1}{z\tau}(1-p-q)\left[\frac{1}{2}+R\left[\frac{p+q}{2}\right]\right]\Delta^{|m|-1}(1+R^+)\frac{1-p-q}{z} \tag{4.10a}$$

$$=\frac{1-p-q}{2z\tau}\frac{1}{1-(p+q)X}\left[\frac{q}{1-pX}\right]^{|m|-1}\frac{1+(q-p)X}{1-pX}\frac{1-p-q}{z} . \tag{4.10b}$$

Finally the Green's function is obtained as

$$G(k,z)=P(0)+\sum_{m=1}^{\infty}\left[P(m)\prod_{i=0}^{m-1}\int_0^{\infty}dx_i e^{-ikx_i}\mu(x_i)+P(-m)\prod_{i=1}^{m}\int_0^{\infty}dx_i e^{ikx_i}\mu(x_i)\right]$$

$$=P(0)+\sum_{m=1}^{\infty}P(m)[M^m(k)+M^m(-k)] \tag{4.11a}$$

$$=\frac{z-\tau^{-1}(1-p-q)}{z^2}+\frac{1-p-q}{z}\frac{1-p-q}{2z\tau[1-(p+q)X]}$$

$$\times\left[2X+\sum_{m=1}^{\infty}\left[\frac{q}{1-pX}\right]^m(M^m(k)+M^m(-k))\frac{1+(q-p)X}{q}\right] \tag{4.11b}$$

$$=\frac{1}{z}-\frac{1-p-q}{\tau z^2}\left[1-\frac{(1-pX)[X+M(k)](1-p-q)}{2[1-(p+q)X][1-pX-qM(k)]}-\frac{(1-pX)[X+M(-k)](1-p-q)}{2[1-(p+q)X][1-pX-qM(-k)]}\right] \tag{4.11c}$$

where I introduced the Fourier transform of the interval distribution function,

$$M(k)=\int_0^{\infty}dx\, e^{-ikx}\mu(x) . \tag{4.12}$$

As consequence of (2.1) one has

$$\lim_{k\to 0}M(k)=1 . \tag{4.13}$$

Substituting this result and (4.5) into (4.11) one easily checks the relation,

$$\lim_{k\to 0}G(k,z)=\frac{1}{z} , \tag{4.14}$$

which is an obvious consequence of the conservation of the light particle. It is useful to introduce the quantities

$$A(k)=M(k)+M(-k)-M(k)M(-k)-1 , \tag{4.15a}$$

$$B(k)=M(k)M(-k)-1 . \tag{4.15b}$$

In the limit $k\to 0$ one finds for these

$$\lim_{k\to 0}A(k)/k^2=-l^2 \tag{4.16a}$$

$$\lim_{k\to 0}B(k)/k^2=-\Delta^2 . \tag{4.16b}$$

One may express $G(k,z)$ in terms of these quantities by means of some algebraic rearrangements on (4.11c), in which Eq. (4.5) for X has to be used. The result reads

$$G(k,z)=\frac{1}{z}\left[1+\frac{1}{2\tau z}\frac{\frac{1-p+q}{1+p-q}A(k)+\left[\frac{(1-p-q)(1-p+q)}{(1+p+q)(1+p-q)}\right]^{1/2}B(k)}{1-\frac{q}{(1+p-q)(1-p-q)}A(k)+\frac{1}{2}\left[1-\left[\frac{(1+p+q)(1-p+q)}{(1-p-q)(1+p-q)}\right]^{1/2}\right]B(k)}\right]. \tag{4.17}$$

For the generalized diffusion coefficient $U(k,z)$ defined in (1.13a) this yields

$$\begin{aligned}U(k,z)=&-\frac{1}{2\tau k^2}\left[\frac{1-p+q}{1+p-q}A(k)+\left[\frac{(1-p-q)(1-p+q)}{(1+p+q)(1+p-q)}\right]^{1/2}B(k)\right]\\&\times\left\{1+\frac{1-p+q}{2\tau z(1+p-q)}\left[1-\frac{2q\tau z}{(1-p+q)(1-p-q)}\right]A(k)\right.\\&\left.+\frac{1}{2}\left[1-\left[1-\frac{1-p-q}{\tau z(1+p+q)}\right]\left[\frac{(1+p+q)(1-p+q)}{(1-p-q)(1+p-q)}\right]^{1/2}\right]B(k)\right\}^{-1}.\end{aligned} \tag{4.18}$$

It is interesting to consider the simplifications occurring in these expressions for certain special cases, but before doing so I first want to consider certain general properties.

B. The coefficient of self-diffusion

The diffusion coefficient is obtained from (1.13) and (4.18). Let us assume the jump frequencies p and q can be expanded as

$$p(z)=p_0-p_1z+O(z^2)\ , \tag{4.19a}$$

$$q(z)=1-p_0-q_1z+O(z^2)\ , \tag{4.19b}$$

where (2.5) was used, and as a consequence of (2.6) one has

$$p_1+q_1=\tau\ . \tag{4.20}$$

In addition, it is assumed in (4.19) that the second moments of p and q exist. The diffusion coefficient is then found as

$$D=\lim_{z\to 0}\lim_{k\to 0}U(k,z)=\frac{1-p_0}{2p_0\tau}l^2\ . \tag{4.21}$$

This is the same again as the diffusion coefficient for the corresponding random walk on a lattice with fixed lattice-spacing l (Haus and Kehr, 1979).

The frequency-dependent (or z-dependent) diffusion coefficient now follows from (1.13) and (4.18) as

$$U^{(0)}(z)=\frac{1}{2\tau}\left[\frac{1-p+q}{1+p-q}l^2+\left[\frac{(1-p-q)(1-p+q)}{(1+p+q)(1+p-q)}\right]^{1/2}\Delta^2\right]. \tag{4.22}$$

The first term on the right-hand side again is the result for the random walk with constant lattice spacing; obviously, the second term represents the effect of fluctuations in the interval lengths.

C. Low-frequency and high-frequency behavior. Higher-order diffusion coefficients

Let us next consider the limiting behaviors for small and large frequencies. For $\tau z<<1$ one finds for $G(k,z)$ and $U(k,z)$, respectively,

$$G(k,z)=\frac{1+O(1)A(k)-\left[\frac{1}{2}\left[\frac{1-p_0}{2\tau zp_0}\right]^{1/2}+O(1)\right]B(k)}{z\left[1-\left[\frac{1-p_0}{2\tau zp_0}+O(1)\right]A(k)-\left[\left[\frac{1-p_0}{2\tau zp_0}\right]^{1/2}+O(1)\right]B(k)\right]} \tag{4.23a}$$

$$U(k,z)=\frac{-\left\{\left[\frac{1-p_0}{p_0}+O(z)\right]A(k)+\left[\left[\frac{\tau z(1-p_0)}{2p_0}\right]^{1/2}+O(z)\right]B(k)\right\}}{2\tau k^2\left\{1+O(1)A(k)-\left[\frac{1}{2}\left[\frac{1-p_0}{2\tau zp_0}\right]^{1/2}+O(1)\right]B(k)\right\}}\ . \tag{4.23b}$$

Let us assume that all moments of $\mu(x)$ exist. Then $A(k)$ and $B(k)$ can be expanded in powers of k^2, the first terms in these expansions being given by (4.16). Expansion of $G(k,z)$ and $U(k,z)$ in powers of k^2 yields

$$G(k,z)=\frac{1}{z}\left[1+\sum_{n=1}^{\infty}\left[\frac{-(1-p_0)l^2k^2}{2\tau z p_0}\right]^n\left\{1+(n-\tfrac{1}{2})\frac{\Delta^2}{l^2}\left[\frac{2\tau z p_0}{1-p_0}\right]^{1/2}+O(z)\right\}\right] \tag{4.24a}$$

$$=\frac{1}{z}\left[1+\sum_{n=1}^{\infty}\left[\frac{-Dk^2}{z}\right]^n\left\{1+(n-\tfrac{1}{2})\Delta^2\left[\frac{z}{Dl^2}\right]^{1/2}+O(z)\right\}\right]. \tag{4.24b}$$

$$U(k,z)=\frac{\dfrac{l^2(1-p_0)}{2\tau p_0}+\dfrac{\Delta^2}{2}\left[\dfrac{(1-p_0)z}{2\tau p_0}\right]^{1/2}+O(z)}{1+\left[1/2\left[\dfrac{1-p_0}{2\tau z p_0}\right]^{1/2}\Delta^2+O(1)\right]k^2} \tag{4.25a}$$

$$U^{(0)}(z)=D+\frac{\Delta^2}{2l}\sqrt{zD}+O(z) \tag{4.25b}$$

$$U^{(2n)}(z)=D\left[\frac{\Delta^2}{2l}\left[\frac{D}{z}\right]^{1/2}\right]^n(1+O\sqrt{z})\quad(n=1,2\cdots). \tag{4.25c}$$

Here definition (1.13b) of the $U^{(2n)}(z)$ was used.

Clearly the asymptotic small-frequency or long-time behavior of all these quantities is entirely determined by the diffusion coefficient and the variance of the interval length. The finer details of the waiting time distributions and the interval distribution do not show up. From (4.25) it is obvious that all higher-order transport coefficients $U^{(2n)}(z)$ with $n\geq 1$ diverge as $z^{-n/2}$ when z tends to zero. Hence the conjecture of Alley and Alder (1979) that these coefficients would have a finite limit as $z\to 0$ is not satisfied for the one-dimensional waiting time Lorentz models considered here. Let us next consider the time-dependent transport coefficients $D^{(2n)}(t)$, defined in (1.7a). For the asymptotic long-time behavior of the moments of displacement Eqs. (1.11) and (4.24b) yield

$$\langle x^{2n}(t)\rangle\sim(Dt)^n(2n)!\left[\frac{1}{n!}+\frac{\Delta^2}{(Dl^2t)^{1/2}\Gamma(n-\frac{1}{2})}\right], \tag{4.26}$$

where $\Gamma(x)$ is the gamma function. The cumulants of these moments are found from (1.5) as follows:

$$\log F(k,t)\approx\log\left[1+\sum_{n=1}^{\infty}(-Dtk^2)^n\left[\frac{1}{n!}+\frac{\Delta^2}{(Dl^2t)^{1/2}\Gamma(n-\frac{1}{2})}\right]\right] \tag{4.27a}$$

$$=-Dtk^2+\log\left[1+\sum_{n=1}^{\infty}e^{Dtk^2}(-Dtk^2)^n\frac{\Delta^2}{(Dl^2t)^{1/2}\Gamma(n-\frac{1}{2})}\right] \tag{4.27b}$$

$$\approx-Dtk^2+\frac{\Delta^2}{(Dl^2t)^{1/2}}\sum_{n=1}^{\infty}(-Dtk^2)^n\sum_{m=0}^{n-1}\frac{(-1)^m}{m!\Gamma(n-m-\frac{1}{2})}. \tag{4.27c}$$

Hence

$$\langle x^{2n}(t)\rangle_c\approx\frac{\Delta^2}{l}(Dt)^{n-1/2}\sum_{m=0}^{n-1}\frac{(-1)^m(2n)!}{m!\Gamma(n-m-\frac{1}{2})}+2Dt\delta_{n1}, \tag{4.28}$$

and (1.7b) yields for the time-dependent transport coefficients

$$D^{(2n)}(t)\approx D\delta_{0n}+\frac{\Delta^2 D}{l}(Dt)^{n-1/2}(n+\tfrac{1}{2})\times\sum_{m=0}^{n}\frac{(-1)^m}{m!\Gamma(n-m+\frac{1}{2})}. \tag{4.29}$$

This implies that for $n \geq 1$ the coefficients $D^{(2n)}(t)$ diverge as $t^{n-1/2}$ for $t \to \infty$, although the coefficient of this power decreases rapidly with increasing n. This corresponds to a divergence $z^{1/2-n}$ as $z \to 0$ for the Laplace transform $z\int_0^\infty dt\; e^{-zt}D^{(2n)}(t)$. This at least seems to lend some support to the statement (Alley and Alder, 1979) that the coefficients $U^{(2n)}(z)$ are more suited for a description of the generalized diffusion process than the coefficients $D^{(2n)}(t)$. Notice also that within the theory presented here the quantity $U(k,z)$ is obtained much more straightforwardly than $D(k,t)$.

Consider next the high-frequency limit. Let us assume that both $p(z)$ and $q(z)$ tend to zero in the limit $z \to \infty$. Then the limiting behavior of $G(k,z)$ and $U(k,z)$ is given by

$$G(k,z) \approx \frac{1}{z}\left[1+\frac{A(k)+B(k)}{2z\tau}\right], \tag{4.30a}$$

$$U(k,z) \approx -\frac{A(k)+B(k)}{2\tau k^2}, \tag{4.30b}$$

as follows from (4.17) and (4.18). For the limiting behavior of the coefficient $U^{(0)}$ this leads to

$$\lim_{z\to\infty} U^{(0)}(z) = (l^2+\Delta^2)/2\tau = \frac{p_0}{1-p_0}(1+\Delta^2/l^2)D\ . \tag{4.31}$$

In a sense these results are an artifact of the model: The existence of a nonzero limit as $z \to \infty$ for (4.30b) and (4.31) is a consequence of the assumption of instantaneous jumps [Compare Eqs. (3.5b) and (3.8)]. However, under the condition that the average duration of a jump τ_{jump} is very much shorter than the average waiting time (this condition must be satisfied anyhow for the waiting time Lorentz model to be a good approximation), one can find a frequency range such that the conditions $z\tau >> 1$ and $z\tau_{\text{jump}} << 1$ are simultaneously satisfied. In this frequency range (4.30) holds to a very good approximation and the ratio $(p_0/1-p_0)(1+\Delta^2/l^2)$ between $U^{(0)}(z)$ and D is virtually exact. It is noteworthy that in the high-frequency limit the fluctuations in the interval lengths lead to a noticeable increase in the diffusion coefficient in comparison to the case of constant lattice spacing.

D. Special choices for waiting time and interval distributions

In a number of special cases for the waiting time distribution and/or the distribution of the interval lengths the expressions for $G(k,z)$ and $U(k,z)$ simplify considerably. We consider the following examples.

1. Fixed intervals

If the interval lengths have the fixed value l, one has $B(k)=0$ and $A(k)=2[\cos(kl)-1]$. For $G(k,z)$ and $U(k,z)$ one obtains the known results (Haus and Kehr, 1979; Zwerger and Kehr, 1980)

$$G(k,z) = \frac{1}{z}\left[1+\frac{\dfrac{1-p+q}{1+p-q}\left[\cos(kl)-1\right]}{\tau z\left[1-\dfrac{2q}{(1+p-q)(1-p-q)}\right][\cos(kl)-1]}\right] \tag{4.32a}$$

$$U(k,z) = \frac{-\dfrac{1-p+q}{1+p-q}[\cos(kl)-1]/k^2}{\tau\left[1+\dfrac{1-p+q}{\tau z(1+p-q)}\left[1-\dfrac{2q\tau z}{(1-p+q)(1-p-q)}\right][\cos(kl)-1]\right]}\ . \tag{4.32b}$$

2. The symmetric waiting time distribution

In this case $p=q$ and we may put

$$p(z)=q(z)=\nu(z)/2\ . \tag{4.33}$$

The resulting expressions for $G(k,z)$ and $U(k,z)$ are

$$G(k,z)=\left\{1+\frac{1-\nu(z)(1+\tau z)}{2\tau z[1-\nu(z)]}A(k)+\frac{1}{2}\left[1+\frac{1-\tau z-\nu(z)(1+\tau z)}{\tau z[1+\nu(z)]}\left[\frac{1+\nu(z)}{1-\nu(z)}\right]^{1/2}\right]B(k)\right\}$$
$$\times\left[z\left\{1-\frac{\nu(z)}{2[1-\nu(z)]}A(k)+\frac{1}{2}\left[1-\left[\frac{1+\nu(z)}{1-\nu(z)}\right]^{1/2}\right]B(k)\right\}\right]^{-1} \tag{4.34a}$$

$$U(k,z)=-\left[A(k)+\left[\frac{1-\nu(z)}{1+\nu(z)}\right]^{1/2}B(k)\right]\Big/k^2$$
$$\times\left[2\tau\left\{1+\frac{1-\nu(z)(1+\tau z)}{2\tau z[1-\nu(z)]}A(k)+\frac{1}{2}\left[1+\frac{1-\tau z-\nu(z)(1+\tau z)}{\tau z[1+\nu(z)]}\left[\frac{1+\nu(z)}{1-\nu(z)}\right]^{1/2}\right]B(k)\right\}\right]^{-1} \tag{4.34b}$$

For the frequency-dependent diffusion coefficient $U^{(0)}(z)$ one obtains

$$U^{(0)}(z)=\left[l^2+\left[\frac{1-\nu(z)}{1+\nu(z)}\right]^{1/2}\Delta^2\right]\Big/2\tau\,. \tag{4.35}$$

One sees immediately that for a fixed interval length $U^{(0)}(z)$ becomes frequency independent, as was noted by Tunaley (1974). In general, there is an additional frequency-dependent part that is proportional to the variance of the interval length and otherwise is determined entirely by the waiting time distribution. If one knows $U^{(0)}(z)$ as a function of z, the constants l, Δ, τ and the function $\nu(z)$ can be calculated right away. The value of $U^{(0)}(\infty)/U^{(0)}(0)$ fixes Δ/l, and from $U^{(0)}(0)$ and the coefficient of the square-root cusp in $U^{(0)}(z)$ as z tends to zero one then finds the values of τ, l, and Δ. The function $\nu(z)$ follows as

$$\nu(z)=\frac{\Delta^4-[2\tau U^{(0)}(z)-l^2]^2}{\Delta^4+[2\tau U^{(0)}(z)-l^2]^2}\,. \tag{4.36}$$

Also of interest is the quasisymmetric waiting time distribution, by which I mean the case where the light particle after arriving at a scatterer, has probability c to jump immediately to the next scatterer and probability density $(1-c)\nu(t)/2$ to jump in either direction after a waiting time t.[14] This corresponds to the following values for p and q:

$$p(z)=(1-c)\nu(z)/2\,, \tag{4.37a}$$

$$q(z)=c+(1-c)\nu(z)/2\,. \tag{4.37b}$$

For $G(k,z)$ and $U(k,z)$ one obtains in this case

$$G(k,z)=\frac{1}{z}\left[1+\frac{\dfrac{1+c}{1-c}A(k)+\left[\dfrac{(1+c)[1-\nu(z)]}{1+c+(1-c)\nu(z)}\right]^{1/2}B(k)}{2\tau z\left\{1-\dfrac{c+\dfrac{1-c}{2}\nu(z)}{(1-c)^2[1-\nu(z)]}A(k)+\dfrac{1}{2}\left[1-\left[\dfrac{(1+c)[1+c+(1-c)\nu(z)]}{(1-c)^2[1-\nu(z)]}\right]^{1/2}\right]B(k)\right\}}\right], \tag{4.38a}$$

$$U(k,z)=-\frac{1}{2\tau k^2}\left[\frac{1+c}{1-c}A(k)+\left[\frac{(1+c)[1-\nu(z)]}{[1+c+(1-c)\nu(z)]}\right]^{1/2}B(k)\right]$$
$$\times\left[1+\frac{1+c}{2\tau z(1-c)}\left[1-\frac{[2c+(1-c)\nu(z)]\tau z}{(1-c^2)[1-\nu(z)]}\right]A(k)\right.$$
$$\left.+\frac{1}{2}\left[1-\left[1-\frac{(1-c)[1-\nu(z)]}{\tau z[1+c+(1-c)\nu(z)]}\right]\left[\frac{(1+c)[1+c+(1-c)\nu(z)]}{(1-c)^2[1-\nu(z)]}\right]^{1/2}\right]B(k)\right]^{-1} \tag{4.38b}$$

The function $U^{(0)}(z)$ has a similar structure as for the completely symmetric case.

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[14]This may also be interpreted as a situation in which the probability for a jump to bring the light particle from the initial scatterer—say, n_0—to scatterer n_0+m is equal to $\frac{1}{2}c^{|m|-1}(1-c)$ and the jump frequency as a function of time is $\nu(t)$, independent of the length and direction of the jump.

3. The exponential waiting time distribution

If $\tilde{p}(t)$ and $\tilde{q}(t)$ are exponential with the same decay time τ, their Laplace transforms are of the form

$$p(z)=\frac{p_0}{1+\tau z}\,, \tag{4.39a}$$

$$q(z)=\frac{1-p_0}{1+\tau z}\,. \tag{4.39b}$$

Putting $1+\tau z=\zeta$ and $2p_0-1=\alpha$, one obtains

$$G(k,z)=\frac{1+\dfrac{\alpha}{2(\zeta+\alpha)}A(k)+\dfrac{1}{2}\left[1-\dfrac{\zeta}{1+\zeta}\left[\dfrac{(\zeta+1)(\zeta-\alpha)}{(\zeta-1)(\zeta+\alpha)}\right]^{1/2}\right]B(k)}{\left\{1-\dfrac{(1-\alpha)\zeta}{2(\zeta-1)(\zeta+\alpha)}A(k)+\dfrac{1}{2}\left[1-\left[\dfrac{(\zeta+1)(\zeta-\alpha)}{(\zeta-1)(\zeta+\alpha)}\right]^{1/2}\right]B(k)\right\}z}\,, \tag{4.40a}$$

$$U(k,z)=\frac{-\left[\dfrac{\zeta-\alpha}{\zeta+\alpha}A(k)+\left[\dfrac{(\zeta-1)(\zeta-\alpha)}{(\zeta+1)(\zeta+\alpha)}\right]B(k)\right]\Big/2\tau k^2}{1+\dfrac{\alpha}{2(\zeta+\alpha)}A(k)+\dfrac{1}{2}\left[1-\dfrac{\zeta}{1+\zeta}\left[\dfrac{(\zeta+1)(\zeta-\alpha)}{(\zeta-1)(\zeta+\alpha)}\right]^{1/2}\right]B(k)}\,. \tag{4.40b}$$

In the quasisymmetric case, with $\nu(z)=\dfrac{1-c}{1-c+\tau z}$, the functions $G(k,z)$ and $U(k,z)$ assume the forms

$$G(k,z)=\frac{1-\dfrac{c}{(1-c)^2}A(k)+\dfrac{1}{2}\left[1-\dfrac{1-c+(1+c)\tau z}{1-c}\left[\dfrac{1+c}{\tau z[2(1-c)+\tau z(1+c)]}\right]^{1/2}\right]B(k)}{\left\{1-\dfrac{1-c^2+2c\tau z}{2(1-c)^2\tau z}A(k)+\dfrac{1}{2}\left[1-\left[\dfrac{(1+c)[2(1-c)+(1+c)\tau z)]}{(1-c)^2\tau z}\right]^{1/2}\right]B(k)\right\}z}\,, \tag{4.41a}$$

$$U(k,z)=\frac{-\left[\dfrac{1+c}{1-c}A(k)+\left[\dfrac{(1+c)\tau z}{2(1-c)+(1+c)\tau z}\right]^{1/2}B(k)\right]\Big/2\tau k^2}{1-\dfrac{c}{(1-c)^2}A(k)+\dfrac{1}{2}\left[1-\dfrac{1-c+(1+c)\tau z}{1-c}\left[\dfrac{1+c}{\tau z[2(1-c)+\tau z(1+c)]}\right]^{1/2}\right]B(k)}\,. \tag{4.41b}$$

The completely symmetric case, which was discussed to some extent in Sec. III, is recovered by putting $\alpha=0$ in (4.40) or $c=0$ in (4.41).

4. The Poisson distribution of scatterers

If the scatterers are distributed independently over the real axis with density $1/l$, the interval lengths are distributed according to (2.7). For $M(k)$, $A(k)$, and $B(k)$ this results into

$$M(k)=\frac{1}{1+i\kappa}\,, \tag{4.42a}$$

$$A(k)=B(k)=\frac{-\kappa^2}{1+\kappa^2}\,, \tag{4.42b}$$

with $\kappa=kl$. Substitution of this into (4.17) and (4.18) yields

$$G(k,z)=\frac{1+\frac{1}{2}\kappa^2\left[1-\frac{1-p+q}{\tau z(1+p-q)}\left[1-\frac{2q\tau z}{(1-p+q)(1-p-q)}\right]+\left[1-\frac{1-p-q}{\tau z(1+p+q)}\right]\left[\frac{(1+p+q)(1-p+q)}{(1-p-q)(1+p-q)}\right]^{1/2}\right]}{1+\frac{1}{2}\kappa^2\left[1+\frac{2q}{(1+p-q)(1-p-q)}+\left[\frac{(1+p+q)(1-p+q)}{(1-p-q)(1+p-q)}\right]^{1/2}\right]} \tag{4.43a}$$

$$U(k,z)=\frac{\frac{1}{2\tau}l^2\left[\frac{1-p+q}{1+p-q}+\left[\frac{(1-p-q)(1-p+q)}{(1+p+q)(1+p-q)}\right]^{1/2}\right]}{1+\frac{1}{2}\kappa^2\left[1-\frac{1-p+q}{\tau z(1+p-q)}\left[1-\frac{2q\tau z}{(1-p+q)(1-p-q)}\right]+\left[1-\frac{1-p-q}{\tau z(1+p+q)}\right]\left[\frac{(1+p+q)(1-p+q)}{(1-p-q)(1+p-q)}\right]^{1/2}\right]} \tag{4.43b}$$

In this case the $U^{(2n)}(z)$, defined in (1.13b), can be written immediately for all n, but I will not bother to do so. Similarly, one may consider the symmetric case, the exponential waiting time distribution, etc., in conjunction with a Poisson distribution and write $G(k,z)$ and $U(k,z)$ for those cases.

If the scatterers are constrained to occupy discrete lattice sites with a lattice constant l_0, and the lattice sites have independent occupation probabilities ρ, $\mu(z)$ is described by (2.8), and one obtains for $M(k)$, $A(k)$, and $B(k)$ the following expressions:

$$M(k)=\rho e^{-ik\rho l}[1-(1-\rho)e^{-ik\rho l}]^{-1}, \tag{4.44a}$$

$$\begin{aligned}A(k)&=-2[1-\cos(k\rho l)]\\&\quad\times\{\rho^2+2(1-\rho)[1-\cos(k\rho l)]\}^{-1},\\&\equiv\alpha(k)\end{aligned} \tag{4.44b}$$

$$B(k)=(1-\rho)\alpha(k), \tag{4.44c}$$

where I used that for this model $l=l_0/\rho$. With the aid of these expressions one may consider again $G(k,z)$ and $U(k,z)$ for several cases. As an example I consider $U(k,z)$ for the symmetric case with exponential waiting time distribution. This is found as

$$U(k,z)=\frac{-\frac{\alpha(k)}{2\tau k^2}\left[1+(1-\rho)\left[\frac{\tau z}{2+\tau z}\right]^{1/2}\right]}{1+\frac{1-\rho}{2}\alpha(k)\left[1-(1+\tau z)\left[\frac{1}{\tau z(2+\tau z)}\right]^{1/2}\right]}. \tag{4.45}$$

From this result one sees that for this waiting time Lorentz model the relative importance of the $\sqrt{z}$ term in $U^{(0)}(z)$ increases with decreasing ρ, or with increasing density of vacancies on the lattice. If one passes to the limit $\rho\to 0$, he recovers the results for the continuous Poisson distribution.

In summary, one may conclude that for all waiting time distributions satisfying (4.19), combined with interval distributions satisfying (2.1)–(2.3) the same qualitative results apply. The diffusion coefficient is the same as for a random walk on a lattice with constant lattice spacing. If all moments of the interval distribution exist, the higher-order diffusion coefficients $U^{(2n)}(z)$ diverge as $z^{n/2}$ as $z\to 0$, with a coefficient proportional to the variance Δ^2 of the interval length. The infinite-frequency limit of the diffusion coefficient has the value $(p_0/1-p_0)(1+\Delta^2/l^2)D$ [provided $\widetilde{p}(t)$ and $\widetilde{q}(t)$ contain no contribution proportional to $\delta(t)$]. For several specific choices of the waiting time distributions and/or the interval distribution the expressions for $G(k,z)$ and $U(k,z)$ simplify considerably.

V. THE STOCHASTIC LORENTZ GAS

A. Counting the walks

In this section I want to consider the stochastic Lorentz gas, as introduced in Sec. II. As a reminder: This is the model in which the light particle always runs at velocity v or $-v$, and when it collides with a scatterer it is reflected with probability p, or transmitted with probability $1-p$. For this model the probability density for a light particle starting off at scatterer 0 at $t=0$, of reaching scatterer m at time t, cannot be calculated as simply as for the waiting time Lorentz model. The reason is that for a fixed configuration of scatterers this probability density depends on the interval lengths x_i.

Yet for small values of k and z the Green's function can be obtained in the form of an asymptotic expansion in these parameters by means of a calculation that I will sketch below. A more detailed and rigorous account will be given by Van Beijeren and Spohn (1981).

The first ingredient of the calculation of the Green's function $G(k,z)$ consists of finding the probability for a light particle starting off with velocity V_0 (restricted to be $\pm v$) within the interval x_0 to end up with velocity V_f within the interval x_f (I assume $f\geq 0$, the results for negative f follow by symmetry) after traversing each of the intervals x_i a given number of times n_i as specified below:

$n_i=2m_i,\ \ m_i=0,1,\ldots,\ \text{for } i<0 \text{ or } i>f\ ,$

$n_i=2m_i+1,\ \ m_i=0,1,\ldots,\ \text{for } 0<i<f\ ,$

$n_0=2m_0+1,\ \ m_0=0,1,\ldots,\ \text{if } V_0=v \text{ and } f>0\ ,$

$n_0=2m_0+2,\ \ m_0=0,1,\ldots,\ \text{if } V_0=-v \text{ and } f>0\ ,$

$n_f=2m_f+1,\ \ m_f=0,1,\ldots,\ \text{if } V_f=v \text{ and } f>0\ ,$

$n_f=2m_f+2,\ \ m_f=0,1,\ldots,\ \text{if } V_f=-v \text{ and } f>0\ ,$

$n_0=2m_0+2,\ \ m_0=0,1,\ldots,\ \text{if } f=0 \text{ and } V_0=-V_f\ ,$

$n_0=2m_0+1,\ \ m_0=1,2,\ldots,\ \text{if } f=0 \text{ and } V_0=V_f\ .$

The numbers n_0 and n_f include the incomplete initial—respectively, final—passage of the interval x_0—respectively, x_f. This problem requires a combinatorial analysis, enumerating all different paths traversing the intervals x_i just n_i times and attributing to each path factors p for each reflection and factors $(1-p)$ for each transmission of the light particle at a collision with a scatterer. This analysis is given in Appendix C. The results read

$$P(x_0,x_f\mid V_0,V_f,m_i)=t_{q_0m_{-1}}\prod_{i=-1}^{-\infty}t_{m_im_{i-1}}\prod_{j=0}^{f-1}s_{m_jm_{j+1}}t_{q_fm_{f+1}}\prod_{l=f+1}^{\infty}t_{m_lm_{l+1}}\ ,\qquad (f\geq 1)\quad (5.1a)$$

$$P(x_0,x_0\mid V_0,V_f,m_i)=t_{r_0m_{-1}}\prod_{i=-1}^{-\infty}t_{m_im_{i-1}}t_{s_0m_1}\prod_{j=1}^{\infty}t_{m_jm_{j+1}}\ ,\qquad (5.1b)$$

with $q_0=m_0$ if $V_0=v$ and $q_0=m_0+1$ if $V_0=-v$; $q_f=m_f$ if $V_f=v$ and $q_f=m_f+1$ if $V_f=-v$; $r_0=m_0+1$ if $V_0=-v$ and $V_f=v$; $r_0=m_0$ otherwise; $s_0=m_0+1$ if $V_0=v$ and $V_f=-v$; $s_0=m_0$ otherwise. For the quantities s_{mn} and t_{mn} the following expressions are obtained:

$$t_{mn}=\sum_{l=0}^{\min(m,n)}\frac{m!}{(m-l)!l!}\frac{(n-1)!}{(n-l)!(l-1)!}p^{n+m-2l}(1-p)^{2l}\ ,\qquad (5.2)$$

$$s_{mn}=\sum_{l=0}^{\min(m,n)}\frac{m!}{(m-l)!l!}\frac{n!}{(n-l)!l!}p^{n+m-2l}(1-p)^{2l+1}\ ,\qquad (5.3)$$

with the convention $p!/(-1!)=\delta_{p-1}$. Hence one has

$$t_{0n}=\delta_{0n}\ .\qquad (5.4)$$

Also in Appendix C the following properties are derived:

$$\sum_{n=0}^{\infty}t_{mn}x^n=\left\{\frac{p+(1-2p)x}{1-px}\right\}^m\ ,\qquad (5.5)$$

$$\sum_{n=0}^{\infty}s_{mn}x^n=\frac{1-p}{1-px}\left\{\frac{p+(1-2p)x}{1-px}\right\}^m\ .\qquad (5.6)$$

One may interpret s_{mn} and t_{mn} as matrix elements of transfer matrices describing the probability that an interval with $2m+1$—respectively, $2m$—passages of the light particle is followed by an interval with $2n+1$—respectively, $2n$—passages. In the case of s_{mn} the neighboring intervals must both lie on the line piece between the scatterers 0 and $f+1$; in the case of t_{mn} at least the second interval (the one that is crossed $2n$ times) must lie outside this line piece, and if both intervals lie outside this line piece, the second interval must be farther away from it than the first one.

B. The Green's function

The contribution to $G(k,z)$ of a random walk starting at ξ_0, ending between ξ_f and $\xi_f+d\xi$ and lasting between t and $t+dt$ is $e^{-zt}e^{-ik(\xi_f-\xi_0)}dt\,d\xi$, times the probability of this walk to occur. For the sets of walks considered above, the quantity $e^{-zt}e^{-ik(\xi_f-\xi_0)}$ can be factorized into a product of contributions from separate intervals. For a given set of interval lengths x_i, the intervals with $i<0$ or $i>f$ contribute a factor $e^{-2m_izx_i/v}$; the intervals with $0<i<f$ contribute a factor $\exp\{[-(2m_i+1)z/v-ik]x_i\}$; and the intervals x_0 and x_f yield slightly different contributions depending on the initial and final position and velocity of the light particle. Next these factors must be averaged over the interval distributions $\mu(x_i)$ and over the initial distribution (2.4) of the light particle over x_0, and summations over f and m_i must be performed. Introducing the mean free time between collisions,

$$\tau=l/v\ ,\qquad (5.7)$$

and the generating function,

$$\phi(z)=M(-iz/v)=\int_0^\infty dx\,\mu(x)e^{-zx/v}\qquad (5.8a)$$

$$=e^{-z\tau}\exp\sum_{n=2}^{\infty}(-z/v)^n\langle x^n\rangle_c/n!\qquad (5.8b)$$

with $M(k)$ defined in (4.12), one may write down the following expression for the Green's function (Van Beijeren and Spohn, 1981):

$$G(k,z)=\frac{1}{2\tau}\Bigg[\prod_{l=-1}^{-\infty}\sum_{m_l=0}^{\infty}T_{m_lm_{l-1}}\sum_{m_0=0}^{\infty}\Bigg\{\frac{Q_{m_0m_{-1}}}{\phi((2m_0+1)z+ikv)}\sum_{f=1}^{\infty}\prod_{j=1}^{f}\sum_{m_j=0}^{\infty}S_{m_{j-1}m_j}\sum_{m_{f+1}=0}^{\infty}Q_{m_fm_{f+1}}$$

$$+\frac{Q^*_{m_0m-1}}{\phi((2m_0+1)z-ikv)}\sum_{f=1}^{\infty}\prod_{j=1}^{f}\sum_{m_j=0}^{\infty}S^*_{m_{j-1}m_j}\sum_{m_{f+1}=0}^{\infty}Q^*_{m_fm_{f+1}}\Bigg\}$$

$$\times\prod_{l=f+2}^{\infty}\sum_{m_l=0}^{\infty}T_{m_{l-1}m_l}+\prod_{j=-1}^{-\infty}\sum_{m_j=0}^{\infty}T_{m_jm_{j-1}}\prod_{l=1}^{\infty}\sum_{m_l=0}^{\infty}T_{m_lm_{l+1}}$$

$$\times\Bigg\{\sum_{m_0=1}^{\infty}t_{m_0m_{-1}}t_{m_0m_1}(\phi^{++}(m_0)+\phi^{--}(m_0))+\sum_{m_0=0}^{\infty}(t_{m_0m_{-1}}t_{m_0+1m_1}+t_{m_0+1m_{-1}}t_{m_0m_1})\phi^{+-}(m_0)\Bigg\}\Bigg]+G^{00}(k,z)\,. \tag{5.9}$$

Here I introduced the following symbols:

$$S_{mn}=s_{mn}\phi((2m+1)z+ikv)\,, \tag{5.10a}$$

$$T_{mn}=t_{mn}\phi(2mz)\,, \tag{5.10b}$$

$$Q_{mn}=t_{mn}\frac{\phi(2mz)-\phi((2m+1)z+ikv)}{z+ikv}+t_{m+1n}\frac{\phi((2m+1)z+ikv)-\phi((2m+2)z)}{z-ikv}\,, \tag{5.10c}$$

$$\phi^{++}(m)=\left\langle e^{-(2m-1)zx/v}\left[\frac{1-e^{-(z+ikv)x/v}}{z+ikv}\right]^2\right\rangle, \tag{5.11a}$$

$$\phi^{--}(m)=[\phi^{++}(m)]^*\,, \tag{5.11b}$$

$$\phi^{+-}(m)=\left\langle e^{-2mzx/v}\frac{(1-e^{-(z+ikv)x/v})(1-e^{-(z-ikv)x/v})}{(z+ikv)(z-ikv)}\right\rangle, \tag{5.11c}$$

$$G^{00}(k,z)=\frac{z}{z^2+(kv)^2}-\frac{[z^2-(kv)^2](1-\langle e^{-zx/v}\cos(kx)\rangle)}{\tau(z^2+(kv)^2)^2}\,. \tag{5.12}$$

These results require some explanation. The first term between square brackets contains the contributions from all random walks starting and ending in different intervals. Furthermore, this term was split up into the contributions with $f>0$ (the first term between curly brackets) and $f<0$ [the second term between curly brackets; for convenience f has been replaced by $-f$ in (5.9)]. These two terms obviously are each other's complex conjugate. The second term between square brackets contains the contributions for which x_0 and x_f coincide, and at least one collision occurs. The terms with ϕ^{++} and ϕ^{--} correspond to the cases that initial and final velocity are both positive—respectively, negative; the terms with ϕ^{+-} correspond to the cases where these velocities have opposite sign. The contribution $G^{00}(k,z)$ finally comes from those processes where the light particle encounters no scatterers at all between the initial and final times.

The quantities S_{mn} and T_{mn} can be interpreted as matrix elements of transfer matrices **S** and **T** again. S_{mn} and T_{mn} are the Fourier and Laplace transforms of the conditional probability density for a given interval having length x and being traversed $2m+1$—respectively, $2m$—times during time t, conditioned on a neighboring interval being traversed $2n+1$—respectively, $2n$—times. The matrix **Q** with matrix elements Q_{mn} may be interpreted similarly as a transfer matrix.

C. Further reductions and asymptotic expansions

The matrix **T** has one invariant vector, or eigenvector, with (maximal) eigenvalue 1, Ψ^T. For small z (that is $z\tau<<1$) and for $m\lesssim(z\tau)^{-1/2}$ one can explicitly derive an asymptotic expansion in powers of $z\tau$ for the components Ψ^T_m (with $m=0,1,2,\ldots$) of this invariant vector. The leading terms in this expansion can be arranged in the form

$$\Psi^T_m=Y^m\left[1+\frac{\Delta^2}{4l^2}z\tau m+\frac{\Delta^2}{2l^2}\left[\frac{1-p}{2p}\right]^{1/2}(z\tau)^{3/2}m^2+O((z\tau)^{3/2}m)+O((z\tau)^2m^2)+\cdots\right], \tag{5.13}$$

with

$$Y=\frac{1-e^{-2z\tau}(1-2p)-[1-2e^{-2z\tau}(1-2p+2p^2)+e^{-4z\tau}(1-2p)^2]^{1/2}}{2p} \tag{5.14a}$$

$$=1-\left[2z\tau\frac{(1-p)}{p}\right]^{1/2}+\frac{(1-2p)}{p}z\tau+O(z\tau)^{3/2}\ . \tag{5.14b}$$

Notice that, but for a multiplicative factor $e^{-z\tau}$, the quantity Y is identical to X, defined in (4.5), for the case of a fixed waiting time, i.e., $p(z)=pe^{-z\tau}$ and $q(z)=(1-p)e^{-z\tau}$. It can be interpreted as the first-return probability for a particle starting off at the origin on a lattice with constant lattice spacing. Indeed, if we set $\phi(2mz)=e^{-2mz\tau}$, as one would find for such a lattice, it is seen from (5.10b) and (5.4) that the invariant vector of $\mathbf{T}$ is just given by $\Psi_m^T=Y^m$. The corrections to this are found by treating the deviation of $\phi(2mz)$ from $e^{-2mz\tau}$ as a perturbation. In this perturbation expansion each power of m is effectively of order $(z\tau)^{-1/2}$. To understand this, notice that from (5.14b) one readily obtains the property

$$\sum_{m=0}^{\infty} m^k Y^{2m}\Big/\sum_{m=0}^{\infty} Y^{2m}\sim(z\tau)^{-k/2}\quad(z\tau\to 0)\ . \tag{5.15}$$

Next introduce the inner product

$$(\boldsymbol{\phi},\boldsymbol{\Psi})=\sum_{m=0}^{\infty}\phi_m\Psi_m\ . \tag{5.16}$$

It then follows from (5.13) that the leading contribution to $(\boldsymbol{\Psi}^T,\boldsymbol{\Psi}^T)$ results from the terms Y^m in Ψ_m^T. Indeed, when additional contributions to this inner product are calculated, each factor m results in a factor $(z\tau)^{-1/2}$. With this convention for estimating the order of factors m it follows that (5.13) contains all contributions to Ψ_m^T up to corrections of order $z\tau$ relative to the leading term.

The situation where, with probability 1, a given interval is never traversed by the light particle (e.g., because it is too far away from the origin to be reached with a given time interval) may be characterized by a vector $\boldsymbol{\Psi}^{(0)}$ with the components

$$\Psi_m^{(0)}=\delta_{0m} \tag{5.17}$$

describing the probability for $2m$ traversals of the interval. It can be proven (Van Beijeren and Spohn, 1981) that the invariant vector $\boldsymbol{\Psi}^T$ of $\mathbf{T}$ may be obtained as

$$\boldsymbol{\Psi}^T=\lim_{N\to\infty}\mathbf{T}^N\boldsymbol{\Psi}^{(0)}\ . \tag{5.18}$$

With the aid of this relation an alternative useful representation of Ψ^T can be obtained in the form

$$\Psi_m^T=\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\sum_{m_3=0}^{\infty}\cdots T_{mm_1}\prod_{l=1}^{\infty}T_{m_lm_{l+1}}\ . \tag{5.19}$$

From (5.18) one may infer that the components Ψ_m^T can be interpreted as the average z-dependent probabilities for the mth return to the origin of a light particle starting off at the origin on a half-infinite lattice with a reflecting boundary at the origin. In the case of fixed lattice spacing this probability is just Y^m. Clearly, the corrections due to the fluctuations of the interval lengths are of relative order $(z\tau)^{1/2}$ for small z. Similarly, the components $[(\mathbf{S})^f\mathbf{Q}\boldsymbol{\Psi}^T]_m$ can be interpreted as the average probabilities for the $(m+1)$th arrival at the origin of a similar half-infinite lattice of a light particle starting off within the interval x_f with an initial distribution of the form (2.4) (where x_0 must be replaced by x_f).

For $z>0$ the eigenvalues of $\mathbf{S}$, denoted as s^α, all have a norm $|s^\alpha|$ that is <1. There is one eigenvector $\boldsymbol{\Psi}^S$ with an eigenvalue s^0 of maximal norm. The leading terms in the expansion of the components Ψ_m^S and of s^0 are given as

$$\Psi_m^S=Y^m\left[1+\frac{\Delta^2}{2l^2}z\tau m+\frac{\Delta^2}{2l^2}\left[\frac{1-p}{2p}\right]^{1/2}(z\tau)^{3/2}m^2+\frac{\Delta^2}{l^2}\left[\frac{1-p}{2p}\right]^{1/2}(z\tau)^{1/2}mikl+O(z\tau)+O(kl(z\tau)^{1/2})+O(kl)^2\right], \tag{5.20}$$

$$s^0=1-\left[\frac{2p}{1-p}\right]^{1/2}(z\tau)^{1/2}+\frac{p}{1-p}\left[1+\frac{\Delta^2}{2l^2}\right]z\tau-ikl-\tfrac{1}{2}(kl)^2\left[1+\frac{\Delta^2}{l^2}\right]+ikl\left[\frac{2p}{1-p}\right]^{1/2}(z\tau)^{1/2}\left[1+\frac{\Delta^2}{2l^2}\right]+O(z\tau)^{3/2}+O(kl)^3+O((kl)^2(z\tau)^{1/2})+O(klz\tau)\ . \tag{5.21}$$

In estimating the neglected terms in (5.21) I used again the convention that $m\sim(z\tau)^{-1/2}$. The structure of s^0 can be understood as follows: The terms not containing Δ result from an expansion of $e^{-ikl-z\tau}(1-p)/(1-pY)$, which is the value of s^0 for a lattice of constant lattice spacing l, as follows from (5.10a), (5.6), and (5.8b). The other terms are correction terms resulting again from a perturbation expansion about the result for the regular lattice. Notice further that $\boldsymbol{\Psi}^T$ and $\boldsymbol{\Psi}^S$ differ only by terms of relative orders $\sqrt{z\tau}$ and k. In the case of the regular lattice they are identical.

One may also construct the left eigenvector corresponding to $\boldsymbol{\Psi}^S$. For a general vector $\boldsymbol{\Psi}$ I define a related vector $\overline{\boldsymbol{\Psi}}$ with components given as

$$\overline{\Psi}_m=\phi^{-1}((2m+1)z+ikv)\Psi_m\ . \tag{5.22}$$

Then the left eigenvector corresponding to $\boldsymbol{\Psi}^S$ is just $\overline{\boldsymbol{\Psi}}^S$ and, in general, if $\boldsymbol{\Psi}^\alpha$ is a right eigenvector of $\mathbf{S}$, then $\overline{\boldsymbol{\Psi}}^\alpha$

is the corresponding left eigenvector.[15]

Now (5.9), (5.18), and (5.22) may be combined to reexpress the Green's function $G(k,z)$ as

$$G(k,z)=\frac{1}{2\tau}\{[(\overline{\mathbf{Q}\Psi^T}),\mathbf{S}(1-\mathbf{S})^{-1}\mathbf{Q}\Psi^T] +[(\overline{\mathbf{Q}\Psi^T}),\mathbf{S}(1-\mathbf{S})^{-1}\mathbf{Q}\Psi^T]^* +[\Psi^T,(\Phi^{++}+\Phi^{--}+\Phi^{+-}+\Phi^{-+})\Psi^T]\} +G^{00}(k,z)\,, \tag{5.23}$$

where I introduced the matrices Φ^{++}, Φ^{--}, Φ^{+-}, and Φ^{-+}, which are defined below through their components:

$$\Phi^{++}_{mn}=\frac{\phi^{++}(m)}{\phi^2(2mz)}\delta_{mn}(1-\delta_{m0})\,, \tag{5.24a}$$

$$\Phi^{--}_{mn}=\frac{\phi^{--}(m)}{\phi^2(2mz)}\delta_{mn}(1-\delta_{m0})\,, \tag{5.24b}$$

$$\Phi^{+-}_{mn}=\frac{\phi^{+-}(m)}{\phi(2mz)\phi(2(m+1)z)}\delta_{m+1n}\,, \tag{5.24c}$$

$$\Phi^{-+}_{mn}=\frac{\phi^{+-}(m)}{\phi(2mz)\phi(2(m-1)z)}\delta_{mn+1}\,. \tag{5.24d}$$

For a further evaluation of (5.23) the explicit form of $\mathbf{Q}\Psi^T$ is needed. Combining Eqs. (5.10c), (5.8b), (5.10b), (5.13), and (5.14b), one obtains for this

$$(\mathbf{Q}\Psi^T)m\approx\tau\sum_n\left\{T_{mn}\left[1-\frac{2m\Delta^2}{l^2}z\tau-\frac{1}{2}(z\tau+ikl)\left[1+\frac{\Delta^2}{l^2}\right]\right]+T_{m+1n}\left[1-\frac{2(m+1)\Delta^2}{l^2}z\tau-\frac{1}{2}(z\tau+ikl)\right]\left[1+\frac{\Delta^2}{l^2}\right]\right\}\Psi^T_n \tag{5.25a}$$

$$=2\tau Y^m\left[1-\left[\frac{1-p}{2p}\right]^{1/2}(z\tau)^{1/2}-\frac{7}{4}\frac{\Delta^2}{l^2}z\tau m +\frac{\Delta^2}{2l^2}\left[\frac{1-p}{2p}\right]^{1/2}(z\tau)^{3/2}m^2-\frac{1}{2}\left[1+\frac{\Delta^2}{l^2}\right]ikl+O(z\tau)+O(kl(z\tau)^{1/2})+O(kl)^2\right]. \tag{5.25b}$$

Obviously, $(\mathbf{Q}\Psi^T)$ also differs from Ψ^S only by terms of relative orders $(z\tau)^{1/2}$ and k. In general, the projection of a vector Ψ upon Ψ^S can be defined as

$$\mathbf{p}_s\Psi=\Psi^S(\overline{\Psi}^S,\Psi)/(\overline{\Psi}^S,\Psi^S)\,, \tag{5.26}$$

and from (5.16), (5.21), and (5.14b) one obtains

$$(\overline{\Psi}^S,\Psi^S)=\frac{1}{2}\left[\frac{p}{2(1-p)}\right]^{1/2}(z\tau)^{-1/2}\left[1+\left[\frac{2(1-p)}{p}\right]^{1/2}(z\tau)^{1/2} +\frac{3}{4}\left[\frac{p}{2(1-p)}\right]^{1/2}(z\tau)^{1/2}\frac{\Delta^2}{l^2}+ikl\left[1+\frac{\Delta^2}{2l^2}\right]+O(z\tau)+O(kl(z\tau)^{1/2})+O(kl)^2\right]. \tag{5.27}$$

From (5.25)–(5.27) it follows that $\mathbf{Q}\Psi^T$ can be expressed as

$$\mathbf{Q}\Psi^T=2\tau\left[1-\left[\frac{1-p}{2p}\right]^{1/2}\left[1+\frac{9}{8}\frac{p}{1-p}\frac{\Delta^2}{l^2}\right](z\tau)^{1/2}-\left[\frac{1}{2}+\frac{3}{4}\frac{\Delta^2}{l^2}\right]ikl\right]\Psi^S+\Delta\Psi\,, \tag{5.28}$$

---

[15]The inequality of left and right eigenvectors is due to the asymmetric definition of **S**. If one replaces **S** and **T** by **S'** and **T'**, with

$$S'_{mn}=\phi^{1/2}[(2m+1)z+ikv]s_{mn}\phi^{1/2}[(2n+1)z+ikv]$$

and

$$T'_{mn}=\phi^{1/2}(2mz)t_{mn}\phi^{1/2}(2nz)\,,$$

respectively, right and left eigenvectors of **S'** become identical, e.g.,

$$\Psi^{s'}_m=\phi^{-1/2}[(2m+1)z+ikv]\Psi^S_m\,.$$

However, the physical interpretation of transfer matrices and vectors becomes less transparent this way.

where $\Delta\Psi$ is orthogonal to Ψ^S and consists of contributions that are of $O(z\tau)^{1/2}$ or $O(k)$ relative to Ψ^S, in the sense of the norm (5.16).

The third term in (5.23) is readily estimated as

$$(\Psi^T,(\Phi^{++}+\Phi^{--}+\Phi^{+-}+\Phi^{-+})\Psi^T)=\left[\frac{2p}{1-p}\right]^{1/2}(z\tau)^{-1/2}\left[1+\frac{\Delta^2}{l^2}+O(z\tau)^{1/2}+O(k^2)\right], \tag{5.29}$$

and the contribution $G^{00}(k,z)$ may be ignored to leading orders in k and z.

D. Low-frequency results

Now $G(k,z)$ may be calculated, putting together (5.23), (5.28), (5.27), (5.22), and (5.29), with the result

$$G(k,z)=\frac{1+(kl)^2O(1)+O((kl)^4(z\tau)^{-1/2})}{z\left\{1+k^2\left[\frac{1-p}{2pz\tau}l^2+\frac{1}{2}\left[\frac{1-p}{2pz\tau}\right]^{1/2}\Delta^2+O(1)\right]+O((kl)^4(z\tau)^{-1})\right\}}. \tag{5.30}$$

For the generalized diffusion coefficient $U(k,z)$ this leads to

$$U(k,z)=\frac{\frac{1-p}{2p}l^2+\frac{1}{2}\left[\frac{1-p}{2p}\right]^{1/2}(z\tau)^{1/2}\Delta^2+O(z\tau)+O(kl)^2}{\tau[1+(kl)^2O(1)+O((kl)^4(z\tau)^{-1/2})]}. \tag{5.31}$$

Let us consider these results in some detail. First, the diffusion coefficient takes the value $\tau^{-1}l^2(1-p)/2p$ again, just as for the corresponding regular random walk, or for the corresponding waiting time Lorentz models with waiting time distributions of the form (4.19). Also the small-z behavior of $U^{(0)}(z)$ is the same as for the corresponding waiting time Lorentz models [compare Eq. (4.25b)]. The higher-order diffusion coefficients are surprisingly different, however. From (5.31) it follows that the coefficient $U^{(2)}(z)$ has a finite limit as z tends to zero. This implies that the conjecture of Alley and Alder (1979) is satisfied for the stochastic Lorentz model, at least for the coefficient $U^{(2)}$. Whether the conjecture is also satisfied for the coefficients $U^{(2n)}$ with $n>1$ cannot be concluded from the present calculation. However, an extension of this calculation so as to uncover the asymptotic small-z behavior of the higher-order transport coefficients seems straightforward and is currently under way.

For a Poisson distribution of scatterers, and in the limit $p\to 0$, kinetic theory, based on Lorentz-Boltzmann plus ring terms, also predicts convergence of $U^{(2)}$ in the limit $z\to 0$ (Ernst and Van Beijeren, 1981). Perhaps the methods developed by Grassberger (1980) will allow extension of this result to all values of p, maintaining the Poisson distribution of scatterers. This is certainly no simple task, however: It requires an estimate of the small-k and z behavior of all contributing diagrams, and, although Grassberger managed to find such estimates for $U^{(0)}(z)$, it remains to be seen if these can be generalized so as to find estimates of $U(k,z)$ for general k. A treatment of general distributions $\mu(x)$ for the interval lengths seems to be somewhat outside the scope of kinetic theory.

E. Comparison with waiting time Lorentz models

It is interesting to apply the method used in this section also to the waiting time Lorentz models and to make a comparison to the stochastic Lorentz gas. This can be done very straightforwardly in the case that the waiting time distributions are of the form $p(z)=p\nu(z)$ and $q(z)=(1-p)\nu(z)$ (although this restriction is by no means necessary). In this case the functions $\phi(2mz)$ and $\phi((2m+1)z+ik)$, as occurring in (5.10), (5.22), and (5.24), must be replaced by $[\nu(z)]^{2m}$ and $[\nu(z)]^{2m+1}M(k)$, respectively, where $M(k)$ is the Fourier transform of $\mu(x)$ as defined in (4.12). The eigenvectors Ψ^T and Ψ^S become identical, both having components $\Psi_m^T=\Psi_m^S=[\nu(z)X]^m$, with X defined in (4.5). The action of the matrices $\mathbf{Q}$ upon Ψ^T, as occurring in (5.23), reduces to a multiplication by $[X+M(k)][1-\nu(z)]/z$ or by $[X+M(k)]\nu(z)[1-\nu(z)]/z$ for the matrices standing in front of and behind $\mathbf{S}(1-\mathbf{S})^{-1}$, respectively. The eigenvalue s^0 reduces to

$$s^0=M(k)(1-p)\nu(z)/[1-p\nu(z)X].$$

Instead of (5.11), one finds

$$\phi^{++}(m)=[\phi^{--}(m)]^*=\nu^{2m-1}(z)\{[1-\nu(z)]/z\}^2M(k)$$

and

$$\phi^{+-}(m)=\nu^{2m}(z)\{[1-\nu(z)]/z\}^2.$$

The quantity $G^{00}(k,z)$ finally must be replaced by $s_0+[M(k)+M(-k)]\{[1-\nu(z)]/z\}^2/2\tau$, where s_0 is defined in (4.3b) and the second term results from processes in which precisely one jump occurs. If one inserts all this into (5.23), he recovers the result (4.11) for $G(k,z)$.

A comparison between the analysis for the waiting time Lorentz model and the stochastic Lorentz gas reveals that the difference in behavior of $U^{(2)}(z)$ for the two models is entirely due to the following feature: In the stochastic Lorentz gas the probability for return to the initial interval is on the average proportional to $(1+\Delta^2/l^2)$, as can be seen from (5.9), (5.23), and (5.29). This is simply understood: At both the initial and final times the unconditional probability of finding the light particle on a given interval of length x is proportional to x, and the probability of finding the light particle both initially and finally on the same interval of length x is therefore roughly proportional to x^2. In the waiting time Lorentz models, on the other hand, the probability of a return to the origin is completely independent of the interval lengths. It is the appearance of the factor $(1+\Delta^2/l^2)$ in a few places in the expression for $G(k,z)$ for the stochastic Lorentz gas that cancels the term proportional to $(z\tau)^{1/2}$ in the numerator of (4.23a).

If one just looks at the mathematics, it even seems surprising that the coefficient of the $(z\tau)^{1/2}$ term in $U^{(0)}(z)$ is the same for both models. On physical grounds, however, this is entirely plausible. Indeed, the intuitive derivation of the long-time tail in the vaf given in Sec. I has to be revised slightly for these one-dimensional models: For a fixed configuration of scatterers it is not true that the probability density $P(x,t)$ of finding the light particle at position x at time t is described even on a microscopic scale by the solution of the diffusion equation. Instead, one finds that the probability density $P(n,t)$ of arriving at scatterer n at time t is described to leading order in t by the solution of the regular random walk, or, alternatively, by the solution of a diffusion equation as a function of the discrete variable n, both in the waiting time Lorentz models and in the stochastic Lorentz gas. For example, in the case of isotropic scattering ($p=\frac{1}{2}$) one finds for a light particle starting off on the interval x_0 with positive velocity that asymptotically for large times

$$P(1,t)-P(0,t)\approx\frac{vl^2}{8(Dt)^{3/2}\sqrt{\pi}} .$$

From this one readily obtains the asymptotic result (3.7) or (4.25b) for the vaf.

VI. DISCUSSION

A. Summary of results

In this paper I have investigated the transport properties of one-dimensional stochastic Lorentz models in fairly large detail. For the waiting time Lorentz models discussed in Secs. III and IV the Green's function $G(k,z)$ was calculated explicitly, and from this all equilibrium time correlation functions and generalized transport coefficients could be obtained. For the stochastic Lorentz gas $G(k,z)$ was obtained in Sec. V in the form of an expansion in powers of kl and $(z\tau)^{1/2}$. Only the first few terms in this expansion were obtained, but at least in principle this expansion could be extended to any required order.

For both classes of models the diffusion coefficient was proven to exist and to be equal to the diffusion coefficient for a random walk on the corresponding regular lattice. For both classes of models, also, the velocity autocorrelation function exhibits a long-time tail proportional to $t^{-3/2}$ with a coefficient that in all cases is the same function of the diffusion coefficient and the variance Δ^2 of the interval length. The predictions for the vaf from kinetic theory (Ernst and Weyland, 1971; Grassberger, 1980) and fluctuating hydrodynamics (Dorfman *et al.*, 1981) were found to be correct. Furthermore, it was shown that the long-time tail indeed results from those dynamical processes that one expects intuitively to be responsible for it (see Sec. I and the discussion at the end of Sec. V).

A remarkable difference between the waiting time Lorentz models and the stochastic Lorentz gas appears in the low-frequency behavior of the higher-order transport coefficients. The coefficient $U^{(2)}(z)$ diverges as $(z\tau)^{-1/2}$ as $z\to 0$ for the waiting time models, it is convergent in the same limit for the stochastic Lorentz gas. The coefficients $U^{(2n)}(z)$ with $n>1$ diverge as $(z\tau)^{-n/2}$ for the waiting time Lorentz models, for the stochastic Lorentz gas their low-frequency behavior is yet to be calculated, but it is at least less divergent than for the waiting time Lorentz models and it may even be convergent for all n. The convergence of $U^{(2)}(z)$ provides a partial confirmation in the case of the one-dimensional stochastic Lorentz gas of the conjecture of Alley and Alder (1979) that all coefficients $U^{(2n)}(z)$ are convergent in the limit $z\to 0$. Alley and Alder base their conjecture on computer evidence and on the assumption that the Lorentz gas is effectively equivalent to a Montroll-Weiss waiting time model (Montroll and Weiss, 1965) with a waiting time distribution having a long-time tail. It can be shown, however (Ernst and Van Beijeren, 1981), that such a model cannot reproduce the long-time tail found in the vaf for the Lorentz models. Furthermore, at least at low densities no physical grounds seem to exist for an equivalence of the Lorentz gas to a Montroll-Weiss waiting time model.

B. Comparison with kinetic theory

A comparison of the available results from kinetic theory (Grassberger, 1980) for the stochastic Lorentz gas with the rigorous results obtained in Sec. V is reassuring. Both the diffusion coefficient and the long-time tail in the vaf follow exactly from kinetic theory. In his surprising calculations Grassberger shows that for a Poisson distribution of scatterers the only nonvanishing contributions to the diffusion coefficient are the Lorentz-Boltzmann contribution and a simple-ring correction. For the calculation of the long-time behavior of the vaf the ring term must be renormalized, that is, the light-particle-propagator inside the ring operator may not be approximated simply by the Lorentz-Boltzmann propagator any more. It turns out to be sufficient, however, to use the simplest possible renormalization, i.e., adding to the Boltzmann propagator a propagator containing one simple-ring event. The assumption that is usually made in kinetic theory (Dorfman and Cohen, 1970, 1972, 1975; Pomeau, 1971; Résibois *et al.*, 1970, 1976; Ernst and Weyland, 1971), that the dominant long-time behavior of, e.g., the vaf is determined entirely by a single-ring term, possibly containing renormalized one-particle propagators therefore is fully supported for the one-dimensional stochastic Lorentz gas. For the higher-order diffusion coefficients $U^{(2n)}(z)$ the information available from kinetic theory thus far is restricted. The contributions from the ring term to $U^{(2n)}(z)$ can be shown to be convergent in the limit $z \to 0$ (Ernst and Van Beijeren, 1981). This again is well in agreement with the rigorous result for $U^{(2)}$. A comparison of the limiting value $U^{(2)}(z=0)$ as obtained from kinetic theory and from the method described in Sec. V still is to be made.

C. Quantum-mechanical models

A remarkable difference seems to exist between the character of the long-time tails for classical Lorentz models and those for comparable quantum-mechanical models. For the case of quantum-mechanical motion in a random potential in d dimensions it is claimed by several authors (Oppermann and Wegner, 1979; Götze *et al.*, 1979; Prelovsek, 1981) that the velocity autocorrelation function decays as $t^{-d/2}$ for long times, contrary to the $t^{-(d/2+1)}$ behavior expected for the corresponding classical systems. A simple explanation of this phenomenon does not seem to be available.

On the other hand, Maleev and Toperverg (1975) obtained for genuine quantum-mechanical Lorentz models a long-time tail in the vaf proportional to $t^{-(d/2+1)}$, just like in the classical case. Their methods do not allow for a simple comparison of coefficients, however. Moreover, they claim that these long-time tails are typically of a quantum-mechanical nature and would vanish in the classical limit.

D. The percolation transition

Another interesting statement, concerning the classical Lorentz gas, is made by Götze, Leutheuser, and Yip (1981). They use a self-consistent mode-coupling theory to calculate the vaf for a Lorentz gas with overlapping scatterers. At the percolation density, where diffusion gets blocked, they find an asymptotic long-time tail proportional to $t^{-3/2}$ in both two and three dimensions (no other dimensions were considered), whereas for a density range below the percolation density they find that the asymptotic $t^{-(d/2+1)}$ behavior is preceded by a power-law decay with a density dependent exponent. These results are consistent with molecular dynamics results in two dimensions (Alder and Alley, 1978; Alder, 1978; Alley, 1979); for three dimensions no computer results are available. An interesting thought is that the quasi-one-dimensional result at the percolation density could be due to the ramified structure of the available large open spaces at this density (Domb and Stoll, 1977); on the other hand, it is rather hard to imagine how the fairly drastic approximations made by Götze *et al.* could incorporate the effects of such geometric subtleties.

E. Some special cases

For the waiting time Lorentz models I considered several cases of special interest, such as the symmetric case (equal waiting time distributions for forward and backward jumps), exponential waiting time distributions, Poisson distributions of scatterers, and combinations of these possibilities. In the symmetric case it is of interest that the spatial fluctuations of the interval lengths introduce a frequency dependence into the z-dependent diffusion coefficient $U^{(0)}(z)$. This frequency dependence is such that from $U^{(0)}(z)$ the waiting time distribution can be calculated directly. Furthermore the fluctuations in the interval lengths enhance the high-frequency limit of the diffusion coefficients by a factor $(1+\Delta^2/l^2)$, but this phenomenon is common to all waiting time Lorentz models discussed here.

F. Computer results

Any real experiments to which the theory discussed here may be compared are not available to my knowledge. It may not be simple to find real systems that behave sufficiently one-dimensionally and which in addition may be represented by one of the models discussed here. For the stochastic Lorentz gas some computer simulations have been performed (Grassberger, 1980; Erpenbeck, 1980; Dümcke, 1980). The results obtained for diffusion coefficient, velocity autocorrelation function, and mean-square displacement are generally in good agreement with the theory of Sec. V. A somewhat unexpected result is the occurrence of oscillations in the vaf that persist for fairly long times. The frequency of these oscillations decreases with time and my expectation is that for sufficiently long times the oscillations will disappear. A theoretical explanation for them is lacking so far, but it is noteworthy that Weyland (1974) obtained similar oscillations in an approximate calculation for the deterministic one-dimensional Lorentz gas.

G. Sinai's fluctuations

Another class of problems one may study in detail are finite-system effects, such as those occurring in systems with periodic boundary conditions or in systems of finite length supporting a steady diffusion current. In Sec. III this was done for the special case of a symmetric exponential waiting time Lorentz model. Another subject of investigation, suggested by Sinai, are time correlation functions in systems with a fixed configuration of scatterers and given initial conditions on the light-particle distribution. For instance, the velocity autocorrelation function in this case is a stochastic variable with respect to the distribution of the intervals. Its typical magnitude depends on the initial light-particle distribution. In the worst case it is of order $t^{-3/4}$ for large t, e.g., for a fixed initial position and velocity of the light particle. It may simply be reduced to be of order $t^{-5/4}$ by choosing the initial distribution to be symmetric in the two velocity directions. In the waiting time Lorentz models a simple trick even allows for a reduction of the magnitude of the fluctuating vaf to order $t^{-3/2}$—that is, the same order as was found for the average of the vaf—but whether a similar trick for the stochastic Lorentz model will bring an equally strong reduction of this order is not yet known. From the viewpoint of computer simulations it seems very interesting that a judicious choice of the initial light-particle distribution would allow for a strong reduction of fluctuations in the vaf.

H. Generalizations

In which directions could the results obtained in this paper be generalized? In the one-dimensional case the most interesting generalization seems to be that to random mixtures of different types of scatterers; this may have a bearing on superionic conductors (Bernasconi *et al.*, 1979), and it may provide a means of studying the cage effect (Alder and Alley, 1978) that appears to be quite important in higher dimensions at high densities of scatterers. For a study of these mixtures an extension of the methods discussed in Sec. V seems to be the most appropriate. Bernasconi and co-workers (Alexander *et al.*, 1981) have developed closely related methods, but thus far they have only discussed the leading low-frequency behavior of $U^{(0)}$.

Most interesting from a physical point of view certainly would be a generalization to higher-dimensional lattices. However, the waiting time Lorentz models lose their triviality in higher dimensions: Consider the case that all lattice points have independent but equal probability to be occupied by a scatterer. Then, because it is possible to return to the origin along a path that is different from the path along which one has left it, the length of the jumps made is no longer irrelevant for the probability of a return to the origin. For instance, a long first jump will increase the average number of jumps required to return, and a short first jump will make this number smaller. Similarly, for the stochastic Lorentz gas the method sketched in Sec. V cannot be used any more.

Furthermore, the diffusion coefficient will no longer be the same as that for a random walk on a regular lattice with the same scattering probabilities and a fixed lattice spacing, equal to the average jump length on the stochastically occupied lattice. This is especially transparent in the case where the probability for occupation of a lattice site by a scatterer is very small and backscattering of the light particle is not allowed. In this case the diffusion process can be described by a lattice Lorentz-Boltzmann equation (this may also be viewed as a regular random walk with a stochastically distributed jump length), and the diffusion coefficient becomes proportional to $l^2+\Delta^2$. Of course, the opposite limit (occupation probability $=1$) is just the regular lattice.

For small—respectively, large—occupation probability one may attack the problem by means of perturbation expansions. In the first case one must expand about the Lorentz-Boltzmann result in orders of the density of scatterers. This may be considered a lattice version of Ehrenfest's wind tree model (Hauge and Cohen, 1968, 1969; Gates, 1972). In the case that backscattering is allowed the possibility of retracing events offers an extra complication, which is well known for the wind tree model. The complication looks less harmful here, however, because the probability for these events decreases roughly exponentially with the length of the path retraced. In the case of large occupation probability one may expand about the regular random walk in orders of the density of vacancies. The first term in this expansion can be related to a lattice with just one vacancy, and has been investigated by Aizenman (1980, private communication). A classification of the next-order terms and of the dynamical processes contributing to these is not yet available. Work in both limiting areas is currently being done, with emphasis on the density dependence of the diffusion coefficient and the long-time behavior of the velocity autocorrelation function.

In the region of intermediate occupation probability at present no systematic expansion parameter seems available. One may feel somewhat optimistic, however, that a combination of the intuitive ideas developed in Sec. I with the known results for regular random walks may provide a good approximation for the vaf in this regime.

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APPENDIX A: NORMAL SOLUTIONS OF THE LORENTZ-BOLTZMANN EQUATION

If the density of scatterers is sufficiently low, the time evolution of the distribution function for the light particles in a Lorentz model can be described by a Lorentz-Boltzmann equation (McKean, 1967; Hauge, 1970; 1974). For the case of isotropic scattering in d dimensions this equation assumes the form

$$\begin{aligned}\frac{\partial}{\partial t}f(\mathbf{r},\mathbf{v},t)+\mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v},t)&=B^{\mathrm{LB}}f(\mathbf{r},\mathbf{v},t)\\&=\nu\left\{\frac{\delta(v-v_0)}{\Omega_d v_0^{d-1}}\int d\mathbf{v}'f(\mathbf{r},\mathbf{v}',t)-f(\mathbf{r},\mathbf{v},t)\right\}\\&\equiv\nu\{\phi(v)\rho(\mathbf{r},t)-f(\mathbf{r},\mathbf{v},t)\}\;.\end{aligned} \tag{A1}$$

Here v_0 is the fixed speed of the light particles, ν is the collision frequency, $\rho(\mathbf{r},t)$ is the number density of light particles at time t, and Ω_d is the surface area of the d-dimensional unit sphere. The Lorentz-Boltzmann operator B^{LB} is linear. Its action upon $f(\mathbf{r},\mathbf{v},t)$ is defined in the last two lines of (A1). The only collisional invariant of this operator is the unit function, the average of which is just $\rho(\mathbf{r},t)$. Now, applying the Chapman-Enskog method (Chapman and Cowling, 1970), we may look for normal solutions of the form

$$f(\mathbf{r},\mathbf{v},t)=f^{(0)}(\mathbf{r},\mathbf{v},t)+f^{(1)}(\mathbf{r},\mathbf{v},t)+\cdots\;, \tag{A2}$$

where the ordering is in powers of the gradient of the density field. The zeroth order contribution has to satisfy the equation

$$B^{\mathrm{LB}}f^{(0)}(\mathbf{r},\mathbf{v},t)=0\;. \tag{A3}$$

The only solutions to this are of the form

$$f^{(0)}(\mathbf{r},\mathbf{v},t)=\varphi(v)\rho(\mathbf{r},t)\;. \tag{A4}$$

As usual, we impose the requirement that $\rho(\mathbf{r},t)$ is the actual light-particle density at position $\mathbf{r}$ and time t. The next contribution has to be found from the equation

$$\begin{aligned}B^{\mathrm{LB}}f^{(1)}(\mathbf{r},\mathbf{v},t)&=\left[\frac{\partial^{(1)}}{\partial t}+\mathbf{v}\cdot\nabla\right]f^{(0)}(\mathbf{r},\mathbf{v},t)\\&=\frac{\delta(v-v_0)}{\Omega_d v_0^{d-1}}\left[\frac{\partial^{(1)}}{\partial t}+\mathbf{v}\cdot\nabla\right]\rho(\mathbf{r},t)\;.\end{aligned} \tag{A5}$$

Integration of both sides of this equation over the velocity yields the compatibility condition

$$\frac{\partial^{(1)}}{\partial t}\rho(\mathbf{r},t)=0\;, \tag{A6}$$

which can be interpreted as the diffusion equation to first order in the gradient. Since $\rho(\mathbf{r},t)$ is determined completely by $f^{(0)}(\mathbf{r},\mathbf{v},t)$, one has

$$\int d\mathbf{v}\,f^{(1)}(\mathbf{r},\mathbf{v},t)=0\;, \tag{A7}$$

and it follows from (A1) that the action of B^{LB} on $f^{(1)}(\mathbf{r},\mathbf{v},t)$ simply amounts to a multiplication by $-\nu$. Hence $f^{(1)}$ takes the form

$$f^{(1)}(\mathbf{r},\mathbf{v},t)=-\nu^{-1}\varphi(v)(\mathbf{v}\cdot\nabla)\rho(\mathbf{r},t)\;. \tag{A8}$$

The next-order equation becomes

$$\begin{aligned}B^{\mathrm{LB}}f^{(2)}(\mathbf{r},\mathbf{v},t)&=\frac{\partial^{(2)}}{\partial t}f^{(0)}(\mathbf{r},\mathbf{v},t)\\&\quad+\left[\frac{\partial^{(1)}}{\partial t}+\mathbf{v}\cdot\nabla\right]f^{(1)}(\mathbf{r},\mathbf{v},t)\;.\end{aligned} \tag{A9}$$

Integration over the velocity and use of (A7) and (A8) yields a second compatibility condition

$$\frac{\partial^{(2)}}{\partial t}\rho(\mathbf{r},t)=\frac{v_0^2}{\nu d}\nabla^2\rho(\mathbf{r},t)\;. \tag{A10}$$

If one truncates at this order, the compatibility conditions (A6) and (A10) combine into Fick's law,

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t)=D\nabla^2\rho(\mathbf{r},t)\;, \tag{A11}$$

with $D=v_0^2/(\nu d)$. One may substitute the solution (1.2) of this equation, for a density that starts off as a δ function at the origin, into (A4) and (A8). The resulting distribution function is just the one given by (1.26).

APPENDIX B: DISTRIBUTION OF NUMBER OF SCATTERERS IN AN INTERVAL

Let $P_L(N)$ denote the probability of finding N scatterers on an interval of given length L; let $P(n,x)$ denote the probability density of finding scatterer n at position x, given that scatterer 0 is located at the origin; and let $Q(x)$ denote the probability of finding no scatterer in the interval (O,x), given that scatterer 0 sits at the origin. Then $P_L(N)$ can be expressed as

$$P_L(N)=\frac{1}{l}\int_0^L dx\,P(N-1,L-x)\times\int_0^x dy\,Q(y)Q(x-y)\;. \tag{B1}$$

Here $1/l$ is the unconditional probability density of finding a scatterer at position y; $Q(y)$ is the probability that this scatterer is the first scatterer beyond $x=0$; then $P(N-1,L-x)$ is the probability density of finding the Nth scatterer at $L-x+y$, and $Q(x-y)$ is the probability of finding no scatterers between the Nth one and $x=L$. The probability $Q(y)$ can be expressed in terms of $\mu(x)$ as

$$Q(y)=\int_y^\infty dx\,\mu(x)\;. \tag{B2}$$

The Fourier transforms of $Q(y)$ and $P(N,x)$ are given as

$$\hat{Q}(k)=\frac{1-M(k)}{ik}\;, \tag{B3}$$

$$\hat{P}(N,k)=M^N(k)\;, \tag{B4}$$

where $M(k)$ is the Fourier transform of $\mu(x)$. Hence a Fourier transform of (B1) with respect to L yields

$$\hat{P}_k(N)=\frac{-1}{lk^2}[1-M(k)]^2M^{N-1}(k)$$
$$=-\frac{e^{Na}}{lk^2}(e^a+e^{-a}-2)\;, \tag{B5}$$

with

$$a=\sum_{n=1}^\infty\frac{(-ik)^n}{n!}\langle x^n\rangle_c\;, \tag{B6}$$

provided all moments of x with respect to $\mu(x)$ exist. Substituting (B6) into (B5) and expanding about a Gaussian distribution in k, one obtains

$$\hat{P}_k(N)=le^{-iNkl-N\Delta^2k^2/2}\left[1-\frac{ik\Delta^2}{l}-k^2\left[\frac{\langle x^3\rangle_c}{3l}+\frac{\Delta^4}{4l^2}+\frac{l^2}{12}\right]+\frac{ik^3N\langle x^3\rangle_c}{6}+\frac{k^4N}{6}\left[\frac{\langle x^4\rangle_c}{4}+\frac{\langle x^3\rangle_c\Delta^2}{l}\right]\right.$$
$$\left.-\frac{k^6N^2}{72}\langle x^3\rangle_c^2+O(k^3)+O(k^5N)+O(k^7N^2)+\cdots\right]\;. \tag{B7}$$

The inverse Fourier transform yields

$$P_x(N)=\frac{l}{\Delta\sqrt{2\pi N}}\left[1-\frac{\Delta^2}{l}\frac{d}{dx}+\left[\frac{\langle x^3\rangle_c}{3l}+\frac{\Delta^4}{4l^2}+\frac{l^2}{12}\right]\frac{d^2}{dx^2}\right.$$
$$\left.-\frac{N\langle x^3\rangle_c}{6}\frac{d^3}{dx^3}+\frac{N}{6}\left[\frac{\langle x^4\rangle_c}{4}+\frac{\langle x^3\rangle_c\Delta^2}{l}\right]\frac{d^4}{dx^4}+\frac{N^2}{72}\langle x^3\rangle_c^2\frac{d^6}{dx^6}+\cdots\right]\exp-\frac{(x-Nl)^2}{2N\Delta^2}$$
$$=\frac{l}{\Delta\sqrt{2\pi N}}\exp-\frac{(x-Nl)^2}{2N\Delta^2}\left[1+\frac{1}{N}\left[\frac{\langle x^3\rangle_c}{6l\Delta^2}-\frac{\Delta^2}{4l^2}-\frac{l^2}{12\Delta^2}+\frac{\langle x^4\rangle_c}{8\Delta^4}-\frac{5\langle x^3\rangle_c^2}{24\Delta^6}\right]+\frac{(x-Nl)}{Nl}\left[1-\frac{\langle x^3\rangle_c l}{2\Delta^4}\right]\right.$$
$$+\frac{(x-NL)^2}{(NL)^2}\left[\frac{-2\langle x^3\rangle_c l}{3\Delta^4}+\frac{1}{4}+\frac{l^4}{12\Delta^4}-\frac{\langle x^4\rangle_c l^2}{4\Delta^6}+\frac{5\langle x^3\rangle_c^2 l^2}{8\Delta^8}\right]$$
$$+\frac{(x-Nl)^3}{(NL)^2}\frac{\langle x^3\rangle_c l^2}{6\Delta^6}+\frac{(x-NL)^4}{(NL)^3}\left[\frac{\langle x^4\rangle_c l^3}{24\Delta^8}+\frac{\langle x^3\rangle_c l^2}{6\Delta^6}-\frac{5\langle x^3\rangle_c^2 l^3}{24\Delta^{10}}\right]$$
$$\left.+\frac{(x-Nl)^6}{(NL)^4}\frac{\langle x^3\rangle_c^2 l^4}{72\Delta^{12}}+\cdots\right]\;. \tag{B8}$$

As a check on this equation we may consider the normalization. From (B1) and (B2) it follows that

$$\int_0^\infty dx\,P_x(N)=l\;. \tag{B9}$$

One can easily check that (B8) satisfies this relation through order $1/N$. Furthermore, one may check (B8) for the Poisson distribution, for which one has

$$P_x(N)=\frac{e^{-x/l}}{N!}\left[\frac{x}{l}\right]^N\;. \tag{B10}$$

A Taylor expansion of $\log P_x(N)$ about the point $x=Nl$ leads to

$$P_x(N)=\frac{e^{-N}N^N}{N!}\exp\left[-\frac{(x-Nl)^2}{2Nl^2}+\frac{(x-Nl)^3}{3N^2l^3}-\frac{(x-Nl)^4}{4N^3l^4}+\cdots\right] \tag{B11a}$$

$$=\frac{1}{\sqrt{2\pi N}\left[1+\frac{1}{12N}+\cdots\right]}\exp\left[-\frac{(x-Nl)^2}{2Nl^2}\right]\left[1+\frac{(x-Nl)^3}{3N^2l^3}-\frac{(x-Nl)^4}{4N^3l^4}+\frac{(x-Nl)^6}{18N^4l^6}+\cdots\right]$$

$$=\frac{1}{\sqrt{2\pi N}}\exp\left[-\frac{(x-Nl)^2}{2Nl^2}\right]\left[1-\frac{1}{12N}+\frac{(x-Nl)^3}{3N^2l^3}-\frac{(x-Nl)^4}{4N^3l^4}+\frac{(x-Nl)^6}{18N^4l^6}+\cdots\right]. \tag{B11b}$$

The cumulant moments for the Poisson distribution are found from

$$\langle e^{-ikx}\rangle=\frac{1}{l}\int_0^\infty dx\, e^{-x/l}e^{-ikx}=\frac{1}{1+ikl}=\exp\left[\sum_{n=1}^{\infty}\frac{1}{n}(-ikl)^n\right]. \tag{B12}$$

Hence

$$\langle x^n\rangle_c=(n-1)!l^n\,. \tag{B13}$$

Substitution of this result into (B8) reproduces (B11b).

Next (B8) must be expanded in powers of $(N-n_0)$ about the Gaussian

$$(1/\Delta)(2\pi n_0)^{-1/2}\exp\left[\frac{-l^2(N-n_0)^2}{2\Delta^2 n_0}\right],$$

where $n_0=x/l$ is the average number of scatterers on an interval of length x. The expansion is straightforward, and the result reads

$$\begin{aligned}P_x(N)=\frac{l}{\Delta}\,\frac{\exp\left[-\frac{(N-n_0)^2l^2}{2\Delta^2n_0}\right]}{\sqrt{2\pi n_0}}\Bigg[1&+\frac{1}{n_0}\left[\frac{\langle x^3\rangle_c}{6l\Delta^2}-\frac{\Delta^2}{4l^2}-\frac{l^2}{12\Delta^2}+\frac{\langle x^4\rangle_c}{8\Delta^4}-\frac{5\langle x^3\rangle_c^2}{24\Delta^6}\right]+\frac{N-n_0}{n_0}\left[-\frac{3}{2}+\frac{l\langle x^3\rangle_c}{2\Delta^4}\right]\\&+\frac{(N-n_0)^2}{n_0^2}\left[\frac{17}{8}-\frac{17l\langle x^3\rangle_c}{12\Delta^4}+\frac{l^4}{12\Delta^4}-\frac{l^2\langle x^4\rangle_c}{4\Delta^6}+\frac{5l^2\langle x^3\rangle_c^2}{8\Delta^8}\right]\\&+\frac{(N-n_0)^3}{n_0^2}\left[\frac{l^2}{2\Delta^2}-\frac{l^3\langle x^3\rangle_c}{6\Delta^6}\right]\\&+\frac{(N-n_0)^4}{n_0^3}\left[-\frac{5l^2}{4\Delta^2}+\frac{5l^3\langle x^3\rangle_c}{6\Delta^6}+\frac{\langle x^4\rangle_c l^4}{24\Delta^8}-\frac{5l^4\langle x^3\rangle_c^2}{24\Delta^{10}}\right]\\&+\frac{(N-n_0)^6}{n_0^4}\left[\frac{\langle x^3\rangle_c^2}{72}+\frac{l^4}{8\Delta^4}-\frac{l^5\langle x^3\rangle_c}{12\Delta^8}\right]+\cdots\Bigg],\end{aligned} \tag{B14}$$

which is identical to (3.33). Again, one may check for the Poisson distribution. For the latter the expansion in powers of $(N-n_0)$ about the Gaussian leads to

$$P_x(N)=\frac{1}{\sqrt{2\pi n_0}}\exp\left[-\frac{(N-n_0)^2}{2n_0}\right]\left[1-\frac{1}{12n_0}-\frac{(N-n_0)}{2n_0}+\frac{3(N-n_0)^2}{8n_0^2}+\frac{(N-n_0)^3}{6n_0^2}-\frac{(N-n_0)^4}{6n_0^3}+\frac{(N-n_0)^6}{72n_0^4}+\cdots\right] \tag{B15}$$

This is reproduced if one substitutes (B13) into (B14).

APPENDIX C: RANDOM WALK PROBABILITIES

What is the probability for a random walk with reflection probability p, starting on the interval x_0 with given velocity V_0, to arrive in the interval x_f with given velocity V_f, traversing each of the intervals x_i just n_i times as specified in Sec. V? This is equivalent to asking for the weight of a linear multigraph (Essam and Fisher, 1970), where the vertices correspond to the scatterers, the bonds correspond to traversals of an interval, and each different way of traversing the graph, starting at the vertex labeled $\frac{1}{2}[1-sg(V_0)]$ and ending at the vertex labeled $(f+\frac{1}{2}[1+sg(V_f)])$, contributes $p^{n_r}(1-p)^{n_{tr}}$, with n_r the number of reflections and n_{tr} the number of transmissions at a vertex. The total weight of a given graph can be found as a product of weight factors for all the vertices. The weight factor of a single vertex j, with n_{j-1} and n_j bonds to the left and to the right of it, respectively, is found by enumerating all allowed ways of traversing these bonds and by then attributing the proper weight factors to them.

Consider first the case $j>f$, with $n_{j-1}=2m$ and $n_j=2n$. In the language of the random walk the first time the light particle reaches scatterer j it comes from the left, and the last time it leaves scatterer j it goes off to the left. Now, how many ways does this leave to the light particle to traverse the two intervals with a number of transmissions equal to $2l$? First note that the number of transmissions from left to right and from right to left must be equal to l, because in both intervals the number of passages of the light particle to the right equals the number of passages to the left (reflections automatically respect this property). Each time the light particle approaches scatterer j from the left it is free to choose between a transmission or a reflection until it has reached the maximal number of either one. This provides a total number of possibilities $m!/l!(m-l)!$. When the particle approaches scatterer j from the right for the last time, it must be transmitted, because it has to end up at the left (unless $n=0$, when no approach from the right ever occurs). The other $n-1$ times it approaches scatterer j from the right it is free to choose again, as long as both options are available. This provides a number of possibilities $(n-1)!/(l-1)!(n-l)!$, with $l\geq 1$, provided $n>0$. With the convention $p!/(-1)!=\delta_{p,-1}$, this describes also the case $n=0$ correctly if one allows for the value $l=0$. Multiplying by the weight factor $(1-p)^{2l}p^{n+m-2l}$, and summing over l, one obtains the result (5.2) for t_{mn}. The same result is obtained for $j<0$. For $0<j<f$ one must consider a vertex with $2m+1$ bonds to the left and $2n+1$ bonds to the right. Now there are $2m+1$ approaches of the vertex from the left, the last one of which must result in a transmission, and there are $2n$ approaches from the right, all of which are in principle free to choose between a transmission or a reflection. For $2l+1$ transmissions this yields a combinatorial factor

$$\frac{n!}{(n-l)!l!}\frac{m!}{(m-l)!l!}\,,$$

and multiplication by the weight factor $(1-p)^{2l+1}p^{n+m-2l}$ and summation over l leads to (5.3).

Equation (5.5) may be derived as follows:

$$\sum_{n=0}^{\infty} t_{mn}x^n$$
$$=\sum_{n=0}^{\infty}\sum_{l=0}^{\min(m,n)}\frac{m!}{(m-l)!l!}\frac{(n-1)!}{(n-l)!(l-1)!}p^{n+m-2l}(1-p)^{2l}x^n$$
$$=\sum_{l=0}^{m}\sum_{j=0}^{\infty}\frac{m!}{(m-l)!l!}\frac{(j+l-1)!}{j!(l-1)!}(px)^j p^{m-l}[(1-p)^2x]^l$$
$$=\sum_{l=0}^{m}\frac{m!}{(m-l)!l!}(1-px)^{-l}p^{m-l}[(1-p)^2x]^l$$
$$=\left[\frac{p+(1-2p)x}{1-px}\right]^m,$$

where I put $n-l=j$. Equation (5.6) follows in a similar way.

REFERENCES

Aizenman, M., 1980 (private communication).

Alder, B. J., 1978, Computer results on transport properties, in Stochastic Processes in Nonequilibrium Systems, edited by L. Garrido, P. Seglar, and P. J. Shepherd, Lecture Notes in Physics (Springer, Berlin), Vol. **84**, p. 168.

Alder, B. J., and W. E. Alley, 1978, J. Stat. Phys. **19**, 341.

Alder, B. J., D. M. Gass, and T. E. Wainwright, 1970, J. Chem. Phys. **53**, 3813.

Alder, B. J., and T. E. Wainwright, 1970, Phys. Rev. A **1**, 18.

Alexander, S., J. Bernasconi, W. R. Schneider, and R. Orbach, 1981, Rev. Mod. Phys. **53**, 175.

Allan, G. A. T., and D. D. Betts, 1968, Can. J. Phys. **46**, 15.

Allan, G. A. T., and D. D. Betts, 1969, J. Phys. Soc. Jpn. **26**, Suppl., 163.

Alley, W. E., 1979, Studies in molecular dynamics of the friction coefficient and the Lorentz gas, Ph.d thesis, University of California, Davis.

Alley, W. E., and B. J. Alder, 1979, Phys. Rev. Lett. **43**, 653.

Anshelevich, V. V., and A. V. Vologodskii, 1981, J. Stat. Phys. **25**, 419.

Bedeaux, D., and P. Mazur, 1974a, Physica **73**, 431.

Bedeaux, D., and P. Mazur, 1974b, Physica **75**, 79.

Bernasconi, J., H. U. Beyeler, S. Strässler, and S. Alexander, 1979, Phys. Rev. Lett. **42**, 819.

Brandt, U., and K. Jacoby, 1976, Z. Phys. B **25**, 181.

Brandt, U., and K. Jacoby, 1977, Z. Phys. B **26**, 245.

Bruin, C., 1974, Physica **72**, 261.

Bunimovich, L. A., 1972, Dokl. Akad. Nauk SSSR **204**, 778.

Bunimovich, L. A., 1974, Theory Probab. Its Appl. **19**, 65.

Bunimovich, L. A., 1979, Commun. Math. Phys. **65**, 295.

Bunimovich, L. A., and Ya. G. Sinai, 1973, Mat. Sb. **90**, 415.

Bunimovich, L. A., and Ya. G. Sinai, 1981, Commun. Math. Phys. **78**, 247, 479.

Büttiker, M., and R. Landauer, 1980, J. Phys. C **13**, L325.

Case, K. M., and P. F. Zweifel, 1967, *Linear Transport Theory* (Addison-Wesley, Reading, Mass.).

Chandrasekhar, S., 1943, Rev. Mod. Phys. **15**, 1.

Chapman, S., and T. G. Cowling, 1970, *The Mathematical*

Theory of Non-Uniform Gases, 3rd ed. (Cambridge University Press, Cambridge, England).
Cramèr, H., 1951, *Mathematical Methods of Statistics* (Princeton University Press, Princeton, N. J.).
de Schepper, I. M., 1975, Generalized hydrodynamics for the diffusion process, Ph.D. thesis (Nijmegen).
de Schepper, I. M., and E. G. D. Cohen, 1978, Phys. Lett. A **68**, 308.
de Schepper, I. M., and M. H. Ernst, 1979, Physica A **98**, 189.
de Schepper, I. M., H. van Beijeren, and M. H. Ernst, 1974, Physica **75**, 1.
Domb, C., and E. Stoll, 1977, J. Phys. A **7**, 1141.
Dorfman, J. R., and E. G. D. Cohen, 1970, Phys. Rev. Lett. **25**, 1257.
Dorfman, J. R., and E. G. D. Cohen, 1972, Phys. Rev. A **6**, 776.
Dorfman, J. R., and E. G. D. Cohen, 1975, Phys. Rev. A **12**, 292.
Dorfman, J. R., M. H. Ernst, J. Machta, and H. van Beijeren, 1981 (unpublished).
Drude, P., 1900, Ann. Phys. **1**, 566; **3**, 369.
Dufty, J. W., and J. A. McLennan, 1974, Phys. Rev. A **9**, 1266.
Dümcke, R., 1980 (unpublished).
Dürr, D., S. Goldstein, and J. L. Lebowitz, 1981, Commun. Math. Phys. **78** 507.
Einstein, A. 1905, Ann. Phys. **17**, 549.
Elliott, R. J., J. A. Krumhansl, and P. L. Leath, 1974, Rev. Mod. Phys. **46**, 465.
Ernst, M. H., B. Cichocki, J. R. Dorfmann, J. Sharma, and H. van Beijeren, 1978, J. Stat. Phys. **18**, 237.
Ernst, M. H., E. H. Hauge, and J. M. J. van Leeuwen, 1970, Phys. Rev. Lett. **25**, 1254.
Ernst, M. H., E. H. Hauge, and J. M. J. van Leeuwen, 1971, Phys. Rev. A **4**, 2055.
Ernst, M. H., E. H. Hauge, and J. M. J. van Leeuwen, 1976, J. Stat. Phys. **15**, 1,7.
Ernst, M. H., and H. van Beijeren, 1981, J. Stat. Phys., to appear.
Ernst, M. H., and A. Weyland, 1971, Phys. Lett. A **34**, 39.
Erpenbeck, J. J., 1980 (unpublished).
Essam, J. W., and M. E. Fisher, 1970, Rev. Mod. Phys. **42**, 272.
Fedele, P. D., and Y. W. Kim, 1980, Phys. Rev. Lett. **44**, 691.
Fedders, P. A., 1978, Phys. Rev. B **17**, 40.
Feller, W., 1968, *An Introduction to Probability Theory and its Applications,* 2nd ed. (Wiley, New York), Vol. 2.
Feller, W., 1971, *An Introduction to Probability Theory and its Applications,* Vol. 2, 2nd ed. (Wiley, New York).
Foch, J. D., Jr., and G. W. Ford, 1970, "The dispersion of sound in monoatomic gases," in *Studies in Statistical Mechanics V,* edited by J. de Boer and G. E. Uhlenbeck (North-Holland, Amsterdam), Part B., p. 101.
Forster, D., D. Nelson, and M. J. Stephen, 1976, Phys. Rev. Lett. **36**, 867.
Gallavotti, G., 1969, Phys. Rev. **185**, 308.
Gallavotti, G., 1972, Rigorous theory of the Boltzmann equation in the Lorentz gas, Nota Interna No. 358, Istituto di Fisica, Universita di Roma.
Gallavotti, G., 1975, "Lectures on the Billiard," in Dynamical Systems, Theory and Applications, edited by J. Moser, Lecture Notes in Physics (Springer, Berlin), Vol. 38, p. 236.
Gates, J. D., 1972, J. Math. Phys. **13**, 1005, 1315.
Götze, W., E. Leutheusser, and S. Yip, 1981, Phys. Rev. A **24**, 1008.
Götze, W., P. Prelovsek, and P. Wölfle, 1979, Solid State Commun. **30**, 369.
Gradshteyn, I. S., and I. M. Ryzhik, 1965, Table of Integrals, Series and Products (Academic, New York).
Grassberger, P., 1980, Physica A **103**, 558.
Green, M. S., 1952, J. Chem. Phys. **20**, 1281.
Green, M. S., 1954, J. Chem. Phys. **22**, 398.
Gunther, L., and Y. Imry, 1980, Phys. Rev. Lett. **44** 1225.
Haan, S. W., and R. Zwanzig, 1977, J. Phys. A **10**, 1547.
Harris, T. E., 1965, J. Appl. Prob. **2**, 323.
Hauge, E. H., 1970, Phys. Fluids **13**, 1201.
Hauge, E. H., 1974, "What can one learn from Lorentz models?" in *Transport Phenomena,* edited by G. Kirczenow and J. Marro, Lecture Notes in Physics (Springer, Berlin), Vol. 31, p. 337.
Hauge, E. H., and E. G. D. Cohen, 1968, Det Fysiske Seminar i Trondheim, No. 7., Inst. Theor. Phys. N. T. H. Trondheim.
Hauge, E. H., and E. G. D. Cohen, 1969, J. Math. Phys. **10**, 397.
Haus, J. W., and K. W. Kehr, 1979, J. Phys. Chem. Solids **40**, 1019.
Hemmer, P. C., 1959, Det Fys. Sem. i Trondheim, No. 2., Inst. Theor. Phys., N. T. H., Trondheim.
Holley, R., 1969, Trans. Am. Math. Soc. **144**, 253.
Jepsen, D. W., 1965, J. Math. Phys. **6**, 405.
Kawasaki, K., 1970, Phys. Lett. A **32**, 379.
Kawasaki, K., 1971, Phys. Lett. A **34**, 12.
Kawasaki, K., and J. D. Gunton, 1973, Phys. Rev. A **8**, 2048.
Kehr, W., R. Kutner, and H. van Beijeren, 1981, to appear.
Keyes, T., and J. Mercer, 1979, Physica A **95**, 473.
Keyes, T., and I. Oppenheim, 1973, Physica **70**, 100.
Kirkpatrick, S., 1973, Rev. Mod. Phys. **45**, 574.
Knops, H. J. F., 1970 (private communication).
Kubo, R., 1957, J. Phys. Soc. Jpn. **12**, 570.
Lagar'kov, A. N., and A. K. Sarychev, 1975, Zh. Eksp. Teor. Fiz. **68**, 641 [Sov. Phys.—JETP **41**, 317 (1975)].
Lagar'kov, A. N., and V. M. Sergeev, 1978, Usp. Fiz. Nauk **125**, 409 [Sov. Phys.—Usp. **21**, 566 (1979)].
Landauer, R., 1978, *Electrical Conductivity in Inhomogeneous Media in Electrical Transport and Optical Properties of Inhomogeneous Media,* edited by J. C. Garland and D. B. Tanner (American Institute of Physics, New York), p. 2.
Lanford, O. E., III, 1976a, Time evolution of large classical systems, in *Dynamical Systems, Theory and Applications,* edited by J. Moser, Lecture Notes in Physics (Springer, Berlin), vol. 38, p. 1.
Lanford, O. E., III, 1976b, On the derivation of the Boltzmann equation, Soc. Math. de France, Astérisque **40**, 117.
Lebowitz, J. L., and J. Percus, 1967, Phys. Rev. **155**, 122.
Lebowitz, J. L., and H. Spohn, 1978, J. Stat. Phys. **19**, 633.
Lewis, J. C., and J. A. Tjon, 1978, Phys. Lett. A **66**, 349.
Lorentz, H. A., 1905, Proc. Roy. Acad. Amst. **7**, 438, 585, 684.
Maleev, S. V., and B. P. Toperverg, 1975, Zh. Eksp. Teor. Fiz. **69**, 1440 [Sov. Phys.—JETP **42**, 734 (1975)].
Mazur, P., and E. Montroll, 1960, J. Math. Phys. **1**, 70.
McCoy, B. M., E. Barouch and D. Abraham, 1971, Phys. Rev. A **4**, 2331.
McKean, H. P., Jr., 1967, J. Math. Phys. **8**, 547.
McLennan, J. A., 1973, Phys. Rev. A **8**, 1479.
Montroll, E. W., and G. H. Weiss, 1965, J. Math. Phys. **6**, 167.
Montroll, E. W., and B. J. West, 1979, in *Fluctuation*

Phenomena, edited by E. W. Montroll and J. L. Lebowitz, Studies in Statistical Mechanics (NHPC, Amsterdam), Vol. VII, p. 61.
Morita, T., and H. Mori, 1976, Prog. Theor. Phys. **56**, 498.
Mott, N. F., and E. A. Davis, 1979, *Electronic processes in non-crystalline materials,* 2nd ed. (Clarendon, Oxford).
Niemeyer, Th., 1967, Physica **36**, 377.
Niemeyer, Th., 1968, Physica **39**, 313.
Onuki, A., 1975, Transport Coefficients of Dense Fluids and Long Range Correlations in Non-equilibrium Gases, Ph.D. thesis (University of Tokyo).
Oppermann, R., and F. Wegner, 1979, Z. Phys. B **34**, 327.
Papanicolao, G. C., and S. R. S. Varadhan, 1980, preprint.
Peierls, Sir R., 1974, "Some simple remarks on the basis of transport theory," in *Transport Phenomena,* edited by G. Kirczenow and J. Marro, Lecture Notes in Physics (Springer, Berlin), vol. 31, p. 1.
Perk, J. H. H., and H. W. Capel, 1977, Physica A **89**, 265.
Perk, J. H. H., and H. W. Capel, 1978, Physica A **92**, 163.
Pfister, G., and H. Scher, 1978, Adv. Phys. **27**, 747.
Pomeau, Y., 1971, Phys. Rev. A **3**, 1174.
Pomeau, Y., and P. Résibois, 1975, Phys. Rep. C **19**, 63.
Prelovsek, P., 1981, Phys. Rev. B **23**, 1304.
Résibois, P., 1970, Physica **70**, 413.
Résibois, P., and Y. Pomeau, 1976, Physica **72**, 47.
Richards, P. M., 1977, Phys. Rev. B **16**, 1393.
Rubin, R. J., 1960, J. Math. Phys. **1**, 309.
Rubin, R. J., 1961, J. Math. Phys. **2**, 373.
Scher, H., and E. W. Montroll, 1975, Phys. Rev. B **12**, 2455.
Schneider, T., and E. Stoll, 1980, Phys. Rev. B **22**, 395.
Shante, V. K. S., and S. Kirkpatrick, 1973. Adv. Phys. **20**, 325.
Shklovskiĭ, B. I., and A. L. Éfros, 1975, Usp. Fiz. Nauk **117**, 401 [Sov. Phys.—Usp. **18**, 845 (1975)].
Sinai, Ya. G., 1970, Russ. Math. Surv. **25**, 137.
Sinai, Ya. G., 1973, "Ergodic theory," in *The Boltzmann Equation,* edited by E. G. D. Cohen and W. Thirring, Acta Phys. Austriaca, Suppl. X (Springer, Vienna), p. 575.
Sinai, Ya. G., 1980, (private communication).
Sinai, Ya. G., 1981, Ergodic and Kinetic Properties of the Lorentz Gas, in *Nonlinear Dynamics,* edited by R. H. G. Helleman, Ann. N. Y. Acad. Sci., Vol. 357.
Spohn, H., 1978, Comm. Math. Phys. **60**, 277.
Spohn, H., 1980, Rev. Mod. Phys. **53**, 569.
Spohn, H., 1981 (private communication).
Theodosopulu, M., and P. Résibois, 1976, Physica A **82**, 47.
Thouless, D. J., 1978, Percolation and Localization, in Ill-condensed Matter, edited by R. Balian, R. Maynard, and G. Toulouse, Les Houches XXXI (North-Holland, Amsterdam), p. 1.
Tunaley, J. K. E., 1974, Phys. Rev. Lett. **33**, 1037.
Vaidya, H. C., and C. A. Tracy, 1978, Physica A **92**, 1.
van Beijeren H., O. E. Lanford, III, J. L. Lebowitz, and H. Spohn, 1980, J. Stat. Phys. **22**, 237.
van Beijeren H., and H. Spohn, 1981, J. Stat. Phys., to appear.
van Leeuwen, J. M. J., and A. Weyland, 1967, Physica **36**, 457.
Wainwright, T. E., B. J. Alder, and D. M. Gass, 1971, Phys. Rev. A **4**, 233.
Weyland, A., and J. M. J. van Leeuwen, 1968, Physica **38**, 35.
Weyland, A., 1974, J. Math. Phys. **15**, 1942.
Widom, A., 1970, Phys. Rev. A **3**, 1394.
Wood, W. W., 1975, "Computer studies on fluid systems of hard core particles," in *Fundamental Problems in Statistical Mechanics III,* edited by E. G. D. Cohen (North-Holland, Amsterdam), p. 331.
Wood, W. W., and F. Lado, 1971, J. Comput. Phys. **7**, 528.
Yamada, T., and K. Kawasaki, 1975, Prog. Theor. Phys. **53**, 111.
Zwanzig, R., 1964, J. Chem. Phys. **40**, 2527.
Zwanzig, R., and M. Bixon, 1970, Phys. Rev. A **2**, 2005.
Zwanzig, R., J. Nordholm, and N. Mitchell, 1972, Phys. Rev. A **5**, 2680.
Zwerger, W., and K. W. Kehr, 1980, Z. Phys. B **40**, 157.