Anomalous transport in a one-dimensional Lorentz gas model

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Employing the generalized master equation proposed in [R. Friedrich et al., Phys. Rev. Lett. 96, 230601 (2006)], we derive a kinetic equation for a random kick model. For a particular choice of the time evolution kernel, a fractional master equation is obtained, which can be related to a Lévy walk. In one dimension, we use this model to describe a stochastic Lorentz gas with an annealed disorder. Exact moment relations are obtained in Laplace space, and the long-time behavior of the moments is discussed. The results are compared to those of related models. © 2008 American Institute of Physics. [DOI: 10.1063/1.2953318]

I. INTRODUCTION

Since the seminal work of Einstein,1 the concept of diffusion has been present throughout physics in the past century. Diffusion processes are observed in almost all complex systems and can be modeled on a microscopic level within the framework of stochastic processes. One important class of the latter is called stochastic Lorentz models.2 Here, one considers a binary gas mixture, where the mass of one kind of molecules is assumed to be much greater than the second one such that the mutual collisions of the latter can be neglected, compared with their encounters with the heavy molecules.3,4 Lorentz models became popular as simple but yet nontrivial models where the ideas of kinetic theory could be checked. Many different Lorentz models can be found in the literature.2 One example is the stochastic Lorentz gas, where one light particle moves with a constant velocity and is scattered with probability $S (0 \leq S \leq 1)$ at the heavy particles, whereas otherwise it passes. Another example of this class is the waiting time Lorentz model where the light particle undergoes instantaneous jumps between the scatterers after random waiting times. In some Lorentz gas models the heavy particles or scatterers are fixed while in others they are moving. In the present paper, we will consider a Lorentz gas model with randomly moving scatterers. It serves as a simple kinetic model to study analytically transport properties in dilute binary gas mixtures for which the Lorentz approximation can be applied.

The starting point of our discussion is a generalized master equation describing the diffusion of inertial weakly damped particles that has been proposed in Refs. 5 and 6. This master equation is considered in one dimension and is altered such that the absolute value of the velocity is conserved throughout the process like in the Lorentz gas models. The time between two successive scattering events is assumed to be random in this model.

In other words, we analyze a situation where the diffusing particle moves ballistically at a constant velocity for a random time before it is scattered. So it is evident that the transport properties in this model are mainly characterized by the distribution of the free flight times. These processes have been called Lévy walk models for power-law distributions of the random times between the kicks.7–9 In the present work, we will mainly focus on this type of waiting time distributions. The Lévy walk is one example of a stochastic process that can exhibit anomalous diffusion, which is defined by $\langle \Delta x^2 \rangle \sim t^\delta$, with $\delta \neq 1$. Such behavior has been found in a large variety of systems ranging from chaotic10 to biological systems.11

The random kick model that underlies the stochastic annealed Lorentz gas presented here is to be based on a continuous time random walk (CTRW) model12 in velocity space, and we will bridge this gap by means of fractional equations and Lévy walks. An application of our model could be Knudsen diffusion (at very low pressures) inside porous media, as has been suggested by Levitz.13

The present article is organized as follows. First, we introduce the random kick model and derive a one-dimensional fractional master equation that describes the annealed stochastic Lorentz gas. Then we explicitly consider the behavior of this model for long times. Finally, we compare our models to related ones found in the literature and discuss our results.

II. A GENERALIZED MASTER EQUATION FOR ANOMALOUS DIFFUSION OF INERTIAL PARTICLES

In order to describe anomalous diffusion of particles in complex systems where inertial effects of the diffusing particles cannot be neglected, a model has been proposed in Ref. 5. In this section, we want to briefly review some of the aspects of this model that are important for the annealed Lévy–Lorentz gas.

Consider a particle that is subjected to a series of random kicks such that its motion is ballistic most of the time but changes abruptly from time to time. To be more concrete, let $W(\tau)$ be the probability distribution for a velocity change to occur in the time interval $[\tau, \tau+d\tau]$, and let $F(\mathbf{u}; \mathbf{u}')d\mathbf{u}$ be the probability that the particle’s velocity ends up in the ve-
velocity space element $du$ about $u$ when the velocity before the change was $u'$. In Ref. 5 it was shown that such a process is described by the master equation

$$\left[ \frac{\partial}{\partial t} + u \cdot \nabla \right] f(x,u,t) = \int_0^t dt' \int du' f(u';u') \Phi(t-t')$$

$$\times f(x-u'(t-t'),u',t') - \int_0^t dt' \Phi(t-t')$$

$$\times f(x-u(t-t'),u,t').$$

(1)

Here, $\Phi(t-t')$ is a time evolution kernel that is related to the waiting time distribution $W(\tau)$. Before we explain this important point in more detail, we want to give a short interpretation of Eq. (1). The left-hand side describes an ensemble of particles moving ballistically, i.e., with constant velocity and zero acceleration. The right-hand side can be interpreted as a collision operator that consists of a source term and a sink term. The phase space density at $(x,u)$ is increased at time $t$ by particles starting from $x-u'(t-t')$ at time $t'$ with velocity $u'$ and making a transition to $u$ at time $t$ and position $x$. On the other hand, $f(x,u,t)$ is decreased by particles making a transition from velocity $u$ to some other velocity. Equation (1) is obviously nonlocal in time (due to the time kernel) as well as in space (due to the retardation in the probability density). We would like to note in passing that for a transition probability density $F(u;u')$ depending only on the velocity difference $u-u'$, Eq. (1) is invariant with respect to Galilean transformations, as demanded by the Lorentz models.

Let us now return to the definition of the time kernel in Eq. (1). To understand its meaning, we have to introduce an additional distribution $w(\tau)$, which denotes the probability that in the time interval $[0, \tau]$ no random velocity change happens. For this distribution, the relation

$$w(\tau) = 1 - \int_0^\tau dt W(t)$$

holds. In Ref. 5, the equation

$$\frac{\partial}{\partial t} w(t) = - \int_0^t dt' \Phi(t-t') w(t')$$

was obtained, which identifies $\Phi(t-t')$ as the kernel determining the time evolution of $\omega(t)$. It is evident from Eq. (3) that $\Phi(t)$ imposes a memory in the evolution of the waiting times. Consequently the whole process is non-Markovian. Only for the choice of $\Phi(t-t') \sim \delta(t-t')$ a Markov process is recovered since then the waiting times are Poisson distributed. In Laplace space, we have for $\Phi(\lambda)$ the relations

$$\Phi(\lambda) = \frac{\lambda W(\lambda)}{1 - \lambda W(\lambda)} = \frac{\lambda W(\lambda)}{\lambda w(\lambda)}.$$  

(4)

For a detailed description see Ref. 6. A possible choice for the time evolution kernel used in the remainder of this article is

$$\Phi(\lambda) = \lambda^{1-\delta},$$  

(5)

with $0<\delta<1$. The reason for this choice will be explained in the following. Inserting this kernel into the first equation on the right-hand side in Eq. (4), one obtains for the waiting time distribution between the kicks the equation

$$W(\lambda) = \frac{1}{1 - \lambda^\delta} = 1 - \lambda^\delta + \cdots$$  

(6)

in Laplace space. This class of waiting time distributions lacks a finite first moment in the time domain and is in the attraction range of the one-sided Lévy stable probability densities $L_\delta$ whose Laplace transform is given by $L_\delta(\lambda) = \exp(-\lambda^\delta)$. In other words, the probability distribution of the scaled sum of $N$ random numbers drawn from a probability density with power-law tails like Eq. (6) converges to a Lévy distribution for $N \to \infty$. This is a result of the generalized central limit theorem. For a detailed account of Lévy stable distributions, see the book by Feller.13 In the time domain, probability densities of the form Eq. (6) have power-law tails $W(\tau) \sim \tau^{-1-\delta}$ and are called Mittag-Leffler residence time distributions. They bridge the gap from this model to Lévy walks. If we consider, on the other hand, the case $\delta=1$ in Eq. (5), a finite first moment exists.

Another important aspect is that the choice $\Phi(\lambda)=\lambda^{1-\delta}$ leads to fractional equations. This is because in the time domain, $\Phi(\tau)$ has the asymptotic behavior

$$\Phi(t-t') \sim \frac{1}{(t-t')^{2-\delta}},$$  

(7)

which can be verified by inverse Laplace transform. For the correspondence

$$\int_0^t dt' \Phi(t-t') f(t') \to D_1^{1-\delta} f(t),$$  

(8)

a regularization procedure has to be applied due to the divergence for $t \to t'$. For a detailed description of this procedure see Ref. 6. The case $\delta=1$ corresponds to the choice of a $\delta$-function for the time evolution kernel. Inserting this kernel into the master equation [Eq. (1)] yields the fractional master equation

$$\left[ \frac{\partial}{\partial t} + u \cdot \nabla \right] f(x,u,t) = \int du' F(u;u') D_1^{1-\delta} f(x,u',t')$$

$$- D_1^{1-\delta} f(x,u,t'),$$  

(9)

where $D_1^{1-\delta}$ is the Riemann–Liouville fractional substantial derivative of order $1-\delta$.

$$D_1^{1-\delta} f(x,u,t) = \frac{1}{\Gamma(\delta)} \left[ \frac{\partial}{\partial t} + u \frac{\partial}{\partial x} \right]$$

$$\times \int_0^t (t-t')^{1-\delta} e^{-(t-t')\partial(\delta;\partial t)} f(x,u,t').$$  

(10)

This generalized fractional operator was introduced in Ref. 6. The particularity of this derivative will be explained later. For a general account on fractional operators, see Refs. 15 and 16. In this way, one obtains a fractional master equation.
Thus this case, we can write for the velocity transition amplitude

$$F(u;u') = T\delta(u-u') + (1-T)\delta(u+u').$$

(11)

Thus $|u|$ is conserved throughout the whole process. This leads us to the one-dimensional master equation

$$\left[\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right)f(x,u,t)\right]_0^T = \int_0^T \Phi(t-t')dt' (1-T)$$

$$\times \{f(x+u(t-t'),-u,t') - f(x-u(t-t'),u,t')\}. \tag{12}$$

We use nonequilibrium initial conditions; i.e., in our model, the particle dynamics always starts with a kick event. Otherwise, the first waiting time would follow from a different probability distribution than those between the flights. To become more concrete, we let the particle start at time $t=0$ at position $x(t=0)=0$. The velocity of the particle shall be $u$ or $-u$, respectively, each with probability $\frac{1}{2}$.

The evolution equations for the moments of second order are obtained in a straightforward manner,

$$\frac{\partial}{\partial t} \langle u^2 \rangle(t) = 0. \tag{13}$$

$$\frac{\partial}{\partial t} \langle ux \rangle(t) = \langle u^2(t) \rangle - 2(1-T)$$

$$\times \int_0^T \Phi(t-t')dt' \langle \langle ux \rangle(t') + \langle u^2(t') \rangle(t-t') \rangle. \tag{14}$$

III. THE ANNEALED ONE-DIMENSIONAL STOCHASTIC LORENTZ GAS

Let us now consider a Lorentz gas model in which the scatterers are not fixed but are moving randomly. One may call this an annealed version of the Lorentz gas in contrast to the usual Lorentz gas, which we will call quenched. To have fully elastic kicks, the absolute value $|u|$ of the diffusing particle has to be conserved. Due to this constraint, the dimensionality of the transition amplitude density $F(u;u')$ is reduced—e.g., in two dimensions, a random angle is sufficient. In two dimensions, this corresponds to a kind of Pearson random walk with variable jump lengths. To connect this model to the stochastic Lorentz gas, we generalize the model. We assume that with a probability $T$ the particle is not scattered and retains its current velocity, while it is scattered with probability $1-T$. In the following, we would like to consider the simplest case, i.e., a one-dimensional model. In this case, we can write for the velocity transition amplitude

$$F(u;u') = T\delta(u-u') + (1-T)\delta(u+u').$$

Thus $|u|$ is conserved throughout the whole process. This leads us to the one-dimensional master equation

$$\left[\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right)f(x,u,t)\right]_0^T = \int_0^T \Phi(t-t')dt' (1-T)$$

$$\times \{f(x+u(t-t'),-u,t') - f(x-u(t-t'),u,t')\}. \tag{12}$$

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$$\times \int_0^T \Phi(t-t')dt' \langle \langle ux \rangle(t') + \langle u^2(t') \rangle(t-t') \rangle. \tag{14}$$

$$\frac{\partial}{\partial t} \langle x^2 \rangle(t) = 2\langle ux \rangle(t). \tag{15}$$

Due to the conservation of the moment of the particle, one has $\langle u^2 \rangle(t)=\langle u^2 \rangle(t=0)=A$. This system of equations can be solved exactly in Laplace space,

$$\langle u^2 \rangle(\lambda) = A \frac{1 - 2(1-T) \frac{\partial}{\partial \lambda} \Phi(\lambda)}{\lambda(\lambda + 2(1-T)\Phi(\lambda))}, \tag{16}$$

$$\langle x^2 \rangle(\lambda) = 2A \frac{1 - 2(1-T) \frac{\partial}{\partial \lambda} \Phi(\lambda)}{\lambda^2(\lambda + 2(1-T)\Phi(\lambda))}. \tag{17}$$

Let us now consider the aforementioned class of time evolution kernels that lead to Lévy walks and fractional equations,

$$\langle u^2 \rangle(\lambda) = A \frac{1 - 2(1-T)(1-\delta)\lambda^{-\delta}}{\lambda(\lambda + 2(1-T)\lambda^{1-\delta})}, \tag{18}$$

$$\langle x^2 \rangle(\lambda) = 2A \frac{1 - 2(1-T)(1-\delta)\lambda^{-\delta}}{\lambda^2(\lambda + 2(1-T)\lambda^{1-\delta})}. \tag{19}$$

Unfortunately, it is not possible to transform these equations back analytically for $0<\delta<1$, but we can obtain the behavior of the second order moments in the long-time limit. This is achieved with the help of the Tauberian theorems, which connect the behavior of small $\lambda$ with that for large $t$. For a general account on the link between the asymptotic behavior of probability densities and their characteristic functions, see Ref. 14.

If we consider the limit $\lambda \to 0$ in Eqs. (17) and then transform the equations back, we obtain the following for the long-time behavior of the second order moments:

$$\langle u^2 \rangle(t) = A(1-\delta)t, \tag{18}$$

$$\langle x^2 \rangle(t) = A(1-\delta)t^2. \tag{19}$$

This indicates that the diffusion in such a system with power-law waiting times between the kicks is always ballistic for long times.

On the other hand, for $\delta=1$, where a finite first moment of the waiting distribution exists, we obtain for the mean square displacement in Laplace space the expression

$$\langle x^2 \rangle(\lambda) = \frac{2}{\lambda(\lambda^2 + 2(1-T)\lambda)}, \tag{20}$$

which can be transformed back exactly. For $0 \leq T < 1$, we obtain

$$\langle x^2 \rangle(t) = A \frac{2t(1-T) + e^{-2(1-T)} - 1}{2(1-T)^2}, \tag{21}$$

and for $T=1$, we get

$$\langle x^2 \rangle(t) = A t^2. \tag{22}$$

This result states that for waiting times with a finite first moment, the particle first diffuses in a nonanomalous fashion
for long periods of time. This is an exact result and corresponds to the findings of the theory of CTRW, where waiting time distributions with a finite first moment lead to normal Fickian diffusion. The time scale after which the asymptotic behavior \((x^2)(t) \sim t\) is reached crucially depends on \(T\). The smaller \((1-T)\) gets, i.e., the less probable it becomes that the diffusing particle is actually scattered, the longer a period of superdiffusion dominates at the beginning. Clearly, if \(T=1\), no scattering event happens at all, and the diffusion is ballistic at any time.

IV. COMPARISON TO RELATED MODELS FOUND IN THE LITERATURE

In the present section, we would like to compare our results to those obtained in the framework of two similar models found in the literature. The first one is by Barkai et al., who considered a model that they called “one-dimensional stochastic Lévy–Lorentz gas.” They considered the diffusion of a particle that moves with a constant velocity among point scatterers arranged randomly on a line. The spacings between the scatterers were assumed to be distributed with the same distribution as in Eq. (6). Accordingly, for constant velocities, this model is the quenched version of the model presented in this article. They performed numerical simulations and found lower bounds for the long-time behavior of the mean square displacement which are in line with our results. It is easy to see that the power-law decay of the ballistic peaks at \(x = \pm ut\) that they found in their investigations holds for our model as well. However, one has to be careful in comparing the two models since in contrast to our model, their scatterers are fixed.

A second model related to ours was proposed by Sokolov and Metzler in Ref. 18. They introduced a two-state Markovian process in one dimension where a particle moves with a velocity \(v\) to the right with probability \(P_r\), and to the left with probability \(P_l\). They generalized their model with the (ad hoc) introduction of what they called a “fractional material” derivative. Thus they introduced a model that behaves very similarly to the deterministic \((T=0)\) version of our model. They obtained the same long-time behavior for the mean square displacement like we do in Eq. (19) for what they called the ballistic regime. In contrast to the ad hoc introduction of their fractional material derivative, the introduction of the fractional substantial derivative Eq. (10) in Ref. 6 is microscopically justified and stems from a CTRW process in velocity space. Moreover, it is straightforward to include external potentials in Eq. (10) and thus to construct biased Lévy walks.\(^{5,19}\) Furthermore, we should mention that the coordinate-time representation of the fractional material derivative introduced in Ref. 18 is only valid for the “primal” fractional derivative \(D^\alpha_t\). However, one has to be careful with the construction of the “descendants” of this derivative, \(D^{1-\delta}_t, D^{2-\delta}_t, \ldots\). For the usual fractional derivative, these are constructed via

\[
D^{1-\delta}_t = -\frac{\partial}{\partial t} D^\delta_t. \tag{23}
\]

For fractional substantial derivatives, this method no longer holds. The correct form is

\[
D^{1-\delta}_t = \left[ -\frac{\partial}{\partial t} + u \cdot \nabla_x \right] D^\delta_t. \tag{24}
\]

For a detailed account on this subtle problem, see Ref. 6. This is an important point since in the model by Sokolov and Metzler as well as in our model, descendant fractional derivatives are used.

V. SUMMARY AND CONCLUSIONS

In the present paper, we have derived a one-dimensional annealed Lorentz gas model from the generalized master equation introduced in Ref. 5. This model describes a particle that moves with a constant velocity \(v\) for a random time \(\tau\) and then arrives at a scattering point where it is either scattered with probability \((1-T)\) or left through with probability \(T\). We found that for waiting time distributions with an infinite first moment, the diffusion of the particle is ballistic in the long-time limit, independent of the choice of the parameter \(T\). On the other hand, when the waiting time distribution between the kicks possesses a finite first moment, the diffusion becomes normal after an intermediate ballistic period whose length depends crucially on the parameter \(T\). This behavior is in line with that described by the Cattaneo equation.\(^{20}\)

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