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Discrete velocity random motion in an external field

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We consider the effects of an external constant force on the one-dimensional transport of a particle whose velocity stochastically fluctuates between two fixed values, $\pm v$. Transport in the presence of a single trap is analyzed in detail. It is found that in the long time limit the trapping probability is decreased compared to that for the overdamped diffusion by the factor $1/(1+v_d/v)$ where v_d is the average drift velocity.

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Discrete velocity kinetic models have been studied intensively in recent years because they provide a convenient framework for both numerical simulations and analytical treatment of complex phenomena. In the simplest one-dimensional model a ''particle'' has the velocity fluctuating with a characteristic relaxation time τ between two values v and $-v$. This is the continuous-space version of a persistent random walk leading to the telegrapher's equation [1]. The model has been applied in many different fields including thermodynamics [2], solid state physics [3,4], diffusion of light in turbid media [5], quantum mechanics [6], tunneling diffusion [7], and dispersion of particles suspended in fluid [8]. A subject of recent interest was transport in the presence of traps. In continuous phase space the problem is very difficult to solve for arbitrary damping. Enormous literature on the trapping problem addresses mainly the case of Brownian motion in the strong damping limit, when inertial effects are completely washed out, and the reduced distribution function (for position only) is governed by the Smoluchowski equation. This approximation leads to underestimated results for the survival probability since it implies that a particle is trapped whenever it reaches a trapping site, while a more general absorbing boundary condition involves only particles moving with the appropriate velocity. Discretization of the velocity space leads to a couple of evolution equations which are more suitable for analytical treatment than the underlying Fokker-Planck equation while preserving the essential features of the problem. Probably the first exactly solvable model of transport with traps in discrete velocity space has been analyzed by Weiss [9]. More recently, Masoliver *et al.* [10] gave a detailed analysis of the telegrapher's equation subject to a variety of boundary conditions including the absorbing one. Bicout and Szabo [11] found the first passage time distribution as a function of initial velocity and discussed also a generalized model with more than two velocity states. In all these studies only unbiased transport without external forces had been considered. The possible way to incorporate external potential into the model is to assume that the external field induces additional transitions between two velocity states in such a way that the momentum and the field at any point would be connected by Newton's second law. This is a particular case of the more general model, explored by Masoliver and Weiss [12], in which a particle spends more time in one of the states than in the other. The scheme has been used recently in Ref. [3] in the specific context of the problem about stationary response in a weak alternating field. The aim of the present paper is to analyze nonstationary solutions of this model for the cases of transport on an unbounded line and on a semi-infinite line in the presence of a single trap located at the origin.

The basic equations of the two velocity model with external potential are the following:

$$\frac{\partial f^+}{\partial t}=-v\,\frac{\partial f^+}{\partial x}-\frac{f^+-f^-}{2\tau}+\frac{F}{2mv}f, \tag{1}$$

$$\frac{\partial f^-}{\partial t}=v\,\frac{\partial f^-}{\partial x}+\frac{f^+-f^-}{2\tau}-\frac{F}{2mv}f. \tag{2}$$

Here $f^{\pm}(x,t)$ are the probability densities of the particle at *x*, at time *t*, with velocity $\pm v$, $f(x,t)=f^++f^-$ is the total probability density, and $F(x)$ is an external force which is assumed to be time independent. The second terms in the right-hand sides of Eqs. (1) and (2) describe stochastic transitions between two velocity states with the rate constant $1/2\tau$. It will be shown that τ is exactly the momentum relaxation time, and therefore parameter $1/\tau$ plays in the model essentially the same role as the damping constant in the Langevin equation and in the corresponding Klein-Kramers equation. The last terms represent the field induced transitions $(df^{\pm}/dt)_F=\pm Ff/(2mv)$. It can be derived under the assumption that the local momentum density $p(x,t)=mv(f^+-f^-)$ satisfies Newton's equation $(dp/dt)_F=mv[(df^+/dt)_F-(df^-/dt)_F]=Ff$, and taking into account that $(df^+/dt)_F=-(df^-/dt)_F$. The relation with the model of Masoliver and Weiss [12] is evident from the fact that the

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last two terms in Eqs. (1) and (2) can be written in the form $\mp f^{+}/2\tau_{+} \pm f^{-}/2\tau_{-}$, where $1/2\tau_{\pm} = 1/2\tau \mp F/2mv$. We will demonstrate below that this is a reasonable way to incorporate dynamics into the two velocity model (see also Ref. [3]). At this point, however, one can see that the model has an inherent restriction because the above derivation implies that both of the states are not empty. It is easy to guess that this condition does not hold automatically. In fact, in our simplified scheme, field-induced transitions, tending to deplete one of the states, are proportional to the total local density rather than to the population of particular states. Therefore, one must worry that sooner or later the force will completely deplete one of the states. On the other hand, stochastic transitions tend to equate the populations of states, and one can anticipate that the state populations will always be positive if the frequency of stochastic transitions $1/\tau$ is sufficiently large. Throughout the paper the inequality

$$\xi \equiv \frac{|F|\tau}{mv} < 1 \tag{3}$$

will be assumed to hold. It will be shown that at least for a linear potential this condition guarantees the positiveness of distribution functions $f^{\pm}(x,t)$, provided that initially both states are filled with the same probabilities. We will show that in the case of large damping $1/\tau \gg |F|/mv$ ($\xi \ll 1$) the model leads in the long time limit to the same result as the Smoluchowski equation. Fortunately, inequality (3) does not put constraints that are too strong, but cover also the more interesting regime of moderate damping (ξ is less but comparable with 1) when inertial effects cannot be ignored.

It is easy to obtain from Eqs. (1) and (2) the following equation for the total distribution function $f = f^{+} + f^{-}$:

$$\frac{\partial^2 f}{\partial t^2} + \frac{1}{\tau}\frac{\partial f}{dt} = v^2 \frac{\partial^2 f}{\partial x^2} - \frac{\partial}{\partial x}\left(\frac{F}{m} f\right), \tag{4}$$

which reduces to the telegrapher's equation if $F = -dU/dx = 0$. In the stationary state the solution of this equation is given by the Boltzmann distribution $f = f_0 \exp[-U(x)/(kT)]$ if we identify v with the thermal velocity $v_{th} = \sqrt{kT/m}$.

Using the transformation

$$f(x,t) = \varphi(x,t) \exp\left(-\frac{t}{2\tau} + \frac{1}{2mv^2}\int_{x_0}^{x} dx F(x)\right), \tag{5}$$

Eq. (4) can be somewhat simplified:

$$\frac{\partial^2 \varphi}{\partial t^2} = v^2 \frac{\partial^2 \varphi}{\partial x^2} + g(x)\varphi, \tag{6}$$

$$g(x) = \frac{1}{4\tau^2} - \frac{F^2}{4m^2v^2} - \frac{1}{2m}\frac{dF}{dx}. \tag{7}$$

For many physical applications the appropriate initial conditions can be written in the form

$$f^{\pm}(x,0) = \frac{1}{2}\delta(x - x_0), \tag{8}$$

$$\frac{\partial f^{\pm}(x,0)}{\partial t} = \mp \frac{v}{2}\frac{d\delta(x-x_0)}{dx} \pm \frac{F(x_0)}{2mv}\delta(x - x_0). \tag{9}$$

Here the first equation reflects the assumption that initially the particle is located at x_0 with equal probability to be in each of two states. The second equation follows from the first one and the requirement that the functions $f^{\pm}(x,t)$ initially satisfy Eqs. (1) and (2). The initial conditions for the total distribution function $f(x,t)$ and for the function $\varphi(x,t)$ will be, respectively, the following:

$$f(x,0) = \delta(x - x_0), \quad \frac{\partial f(x,0)}{\partial t} = 0, \tag{10}$$

$$\varphi(x,0) = \delta(x - x_0), \quad \frac{\partial \varphi(x,0)}{\partial t} = \frac{1}{2\tau}\delta(x - x_0) \tag{11}$$

[we identify the arbitrary lower limit of the integral in Eq. (5) with the initial coordinate x_0 of the particle].

Let us consider first the transport in an unbounded one-dimensional space in a field of constant force F. In this case the function $g(x)$ [Eq. (7)] becomes a constant

$$G^2 = \frac{1}{4\tau^2} - \frac{F}{(2mv)^2} = \frac{1 - \xi^2}{4\tau^2}, \tag{12}$$

which is positive due to assumption (3). Then Eq. (6) for $\varphi(x,t)$ has the form of the modified telegrapher's equation whose solution is well known (see, e.g., Ref. [13]). Using boundary conditions (11) and turning back from $\varphi(x,t)$ to the distribution function, we have

$$f(x,t) = \exp\left(-\frac{t}{2\tau} + \frac{FX}{2mv^2}\right)[\varphi_1(X,t) + \varphi_2(X,t) + \varphi_3(X,t)], \tag{13}$$

where

$$\varphi_1(X,t) = [\delta(X - vt) + \delta(X + vt)]/2,$$

$$\varphi_2(X,t) = \frac{1}{4v\tau} I_0\left(\frac{G}{v}\sqrt{v^2t^2 - X^2}\right)\Theta(vt - |X|),$$

$$\varphi_3(X,t) = \frac{Gt}{2\sqrt{v^2t^2 - X^2}} I_1\left(\frac{G}{v}\sqrt{v^2t^2 - X^2}\right)\Theta(vt - |X|), \tag{14}$$

$X = x - x_0$, $I_0(z)$ and $I_1(z)$ are the modified Bessel functions, and $\Theta(z)$ is the Heaviside step function. If the damping is strong ($\xi \ll 1$), the function $f(x,t)$ in the long-time limit ($t \gg \tau, vt \gg X$) behaves asymptotically exactly as a solution of the Smoluchowski equation for diffusion in a field of constant force:

$$f(x,t) \approx \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{(X - V_d t)^2}{4Dt}\right), \tag{15}$$

where $D = \tau v^2$ is the diffusion coefficient, and $V_d = F\tau/m$ is the drift velocity.

It can be seen from Eqs. (1) and (2) that the momentum density $p(x,t)=mv(f^+-f^-)$ is connected with f by the continuity equation $\partial f/\partial t+m^{-1}\partial p/\partial x=0$ and satisfies

$$\frac{\partial^2 p}{\partial t^2}+\frac{1}{\tau}\frac{\partial p}{dt}=v^2\frac{\partial^2 p}{\partial x^2}-\frac{F(x)}{m}\frac{\partial p}{\partial x} \tag{16}$$

as long as the force does not depend on time. Because this equation and Eq. (4) for $f=f^++f^-$ have different forms, generally there is no way to write down uncoupled equations separately for f^+ and f^-. However, for the case $F=\text{const}$ such decomposition is possible:

$$\frac{\partial^2 f^\pm}{\partial t^2}+\frac{1}{\tau}\frac{\partial f^\pm}{dt}=v^2\frac{\partial^2 f^\pm}{\partial x^2}-\frac{F}{m}\frac{\partial f^\pm}{\partial x}. \tag{17}$$

These equation can be solved using relation (5) for the transformation of the functions f^+ and f^- through the new functions φ^+ and φ^-,

$$f^\pm=\varphi^\pm\exp(-t/2\tau+FX/2mv^2), \tag{18}$$

and taking into account that the initial conditions for the functions $\varphi^\pm$ are

$$\varphi^\pm(x,0)=\frac{1}{2}\delta(X),$$

$$\frac{\partial\varphi^\pm(x,0)}{\partial t}=\mp\frac{v}{2}\exp\left(-\frac{FX}{2mv^2}\right)\delta'(X)+\left(\frac{1}{4\tau}\pm\frac{F}{2mv}\right)\delta(X). \tag{19}$$

The corresponding solutions have the following form:

$$f^\pm=\exp(-t/2\tau+FX/2mv^2)(\varphi_1^\pm+\varphi_2^\pm+\varphi_3^\pm),$$

$$\varphi_1^\pm(X,t)=[\delta(X-vt)+\delta(X+vt)]/4, \tag{20}$$

$$\varphi_2^\pm(X,t)=\frac{1}{8v}\left(\frac{1}{\tau}\pm\frac{F}{mv}\right)I_0\left(\frac{G}{v}\sqrt{v^2t^2-X^2}\right)\Theta(vt-|X|),$$

$$\varphi_3^\pm(X,t)=\frac{Gt}{4\sqrt{v^2t^2-X^2}}\left(1\pm\frac{X}{vt}\right)I_1\left(\frac{G}{v}\sqrt{v^2t^2-X^2}\right)\times\Theta(vt-|X|). \tag{21}$$

One can see that $f^\pm$ are always positive since we assume $\xi<1$. For the average velocity $V(t)$ we have

$$V(t)=v\int dx[f_+(x,t)-f_-(x,t)]=\frac{F}{4mv}\int_{-vt}^{vt}dX\times\exp\left(-\frac{t}{2\tau}+\frac{FX}{2mv^2}\right)I_0\left(\frac{G}{v}\sqrt{v^2t^2-X^2}\right). \tag{22}$$

Instead of calculating this integral, it is much easier to derive from Eq. (16) the equation

$$V(t)''+(1/\tau)V(t)'=0 \tag{23}$$

and to solve it with initial conditions $V(t=0)=0$, and $V'(t=0)=F/m=V_d/\tau$:

$$V(t)=V_d(1-e^{-t/\tau}). \tag{24}$$

This result can be easily generalized for the case of nonzero initial velocity $V(t=0)=V_0$. The corresponding initial conditions for the functions $f^\pm(x,t)$ are the following:

$$f^\pm(x,0)=a^\pm\delta(x-x_0), \tag{25}$$

$$\frac{\partial f^\pm(x,0)}{\partial t}=\mp a^\pm v\frac{d\,\delta(x-x_0)}{dx}\mp\left(\frac{a^+-a^-}{2\tau}-\frac{F}{2mv}\right)\times\delta(x-x_0), \tag{26}$$

where parameters $a^\pm$ satisfy the relations $a^++a^-=1$ and $a^+-a^-=V_0/v$. Using Eq. (26) one can find the second initial condition for the average velocity: $V'(t=0)=(V_d-V_0)/\tau$. Then the solution of Eq. (23) has the expectable form

$$V(t)=V_d+e^{-t/\tau}(V_0-V_d). \tag{27}$$

Let us consider now the process in the presence of one trapping point located at $x=0$, provided that initially the particle is to the right from the trap, i.e., $x_0>0$. In this case the appropriate boundary condition is

$$f^+(0,t)=0, \tag{28}$$

which implies that there is no reflection from the point $x=0$. As we have seen, in the presence of the external field generally there is no way to obtain uncoupled equations separately for f^+ and f^-. We concentrate here on the case $F=\text{const}$ when such decomposition is possible, and calculations can be carried out in the manner of Masoliver *et al.* [10]. Just as for the case of a freely diffusing particle, one can consider only the equation for f^+ since according to Eq. (1) f^- may be found from f^+ through the relation

$$f^-(x,t)=\left[\frac{\partial f^+}{\partial t}+v\frac{\partial f^+}{\partial x}+f^+\left(\frac{1}{2\tau}-\frac{F}{2mv}\right)\right]\left(\frac{1}{2\tau}+\frac{F}{2mv}\right)^{-1}. \tag{29}$$

Using again transformation (18), we come to the following equations for the one-trap problem:

$$\frac{\partial^2\varphi^+}{\partial t^2}=v^2\frac{\partial^2\varphi^+}{\partial x^2}+G^2\varphi^+, \tag{30}$$

$$\varphi^-=\left(\frac{\partial\varphi^+}{\partial t}+v\frac{\partial\varphi^+}{\partial x}\right)\left(\frac{1}{2\tau}+\frac{F}{2mv}\right)^{-1} \tag{31}$$

with the initial conditions (19) and boundary conditions $\varphi^+(0,t)=0$. Using a combined Fourier-sine and Laplace transform

$$\hat{\varphi}^+(k,s)=\int_0^\infty dx\int_0^\infty dt\,\sin(kx)\exp(-st)\varphi^+(x,t) \tag{32}$$

we get

$$\hat{\varphi}^{+}(k,s)=\frac{(s+R)\sin(kx_0)+kv\cos(kx_0)}{2(s^2+v^2k^2-G^2)},\qquad(33)$$

where G is defined by Eq. (12) and

$$R=\frac{1}{2\tau}+\frac{F}{2mv}.\qquad(34)$$

Making the inverse Fourier transform, one can obtain the Laplace transform $\tilde{\varphi}^{+}(x,s)=\int_0^\infty dt\,\exp(-st)\varphi^{+}(x,t)$:

$$\tilde{\varphi}^{+}(x,s)=\frac{\beta(s)\pm1}{4v}\exp[\pm\varrho(s)(x_0-x)]-\frac{\beta(s)-1}{4v}\exp[-\varrho(s)(x_0+x)].\qquad(35)$$

Taking into account relation (29), we find the Laplace transform for the "total" function $\varphi=\varphi^{+}+\varphi^{-}$:

$$\tilde{\varphi}(x,s)=-\frac{1}{2R}\delta(x-x_0)+\frac{\beta(s)\pm1}{4v}\left(1+\frac{s\mp\rho(s)v}{R}\right)\times\exp[\pm\varrho(s)(x_0-x)]-\frac{\beta(s)-1}{4v}\left(1+\frac{s-\rho(s)v}{R}\right)\times\exp[-\varrho(s)(x_0+x)].\qquad(36)$$

In Eqs. (35) and (36) the upper and lower signs correspond to the regions $x>x_0$ and $x<x_0$, respectively, and function $\varrho(s)$ and $\beta(s)$ are defined by

$$\varrho(s)=\frac{1}{v}\sqrt{s^2-G^2},\qquad\beta(s)=\frac{s+R}{\sqrt{s^2-G^2}}.\qquad(37)$$

Using Eq. (5), the Laplace transform for the distribution function $f(x,t)$ can be written as

$$\tilde{f}(x,s)=\exp(FX/2mv^2)\tilde{\varphi}\left(x,s+\frac{1}{2\tau}\right),\qquad(38)$$

where $\tilde{\varphi}(x,s)$ is given by Eq. (36). One can perform inversion of this equation in terms of known functions, but the result is somewhat complicated and is therefore omitted. Instead we concentrate on the analysis of survival probability $P(t)=\int_0^\infty f(x,t)dx$. In contrast with freely diffusing on a line particle, the function $P(t)$ in the presence of an external field has a nonzero long-time limit P_∞ provided the force is directed away from the trap. In this case integration of Eq. (38) gives for the Laplace transform of the survival probability $\tilde{P}(s)$ the following asymptotic form:

$$\tilde{P}(s)=\frac{2\tau}{\xi^2(1+\xi)}\,\frac{1+\xi-\exp[-Fx_0/(mv^2)]}{-1+\sqrt{1+4\tau s/\xi^2}},\qquad(39)$$

which holds for small s. Since $P_\infty=\lim_{s\to0}s\,\tilde{P}(s)$, we finally have

$$P_\infty=1-\frac{\exp[-x_0V_d/D]}{1+\xi},\qquad(40)$$

where, as in Eq. (15), $D=\tau v^2$ and $V_d=F\tau/m$.

In the strong friction limit the problem is reduced to solving the Smoluchowski equation

$$\frac{\partial f}{\partial t}=D\frac{\partial^2 f}{\partial x^2}-V_d\frac{\partial f}{\partial x}\qquad(41)$$

with initial condition $f(x,0)=\delta(x-x_0)$ and the boundary condition $f(0,t)=0$. The corresponding solution is

$$f(x,t)=\exp\left(-\frac{tV_d^2}{4D}+\frac{(x-x_0)V_d}{2D}\right)\times[f_0(x,t|x_0)-f_0(x,t|-x_0)],\qquad(42)$$

where $f_0(x,t|x_0)=(1/\sqrt{4\pi Dt})\exp[-(x-x_0)^2/(4Dt)]$. Respectively, for the escape probability one can find $P_\infty=1-\exp[-x_0V_d/D]$. Comparison of this result with Eq. (40) shows that in the diffusion (overdamped) approximation the probability of trapping $(1-P_\infty)$ is overestimated by the factor $1+\xi=1+v_d/v$, while its dependence on initial position and external field is the same as for the case of two velocities stochastic process at moderate damping.

The presented discrete kinetic model is probably the simplest one to treat random motion in an external field beyond the strong damping approximation. It can be improved and generalized in many different ways (more than two velocity states, two- and three-dimensional space, etc.). An extension of presented consideration on the case of nonlinear potential would be of much interest because it could give more insight into many important problems requiring a solution of the Klein-Kramers equation in the presence of absorbing boundaries (escape from a metastable state, transport in biomolecules, etc.). It is not certain, however, that the condition $\xi<1$ guarantees the positiveness of the state populations for an arbitrary potential. Further work is needed to clarify this question. For the case $\xi>1$ the presented model leads to the modified Klein-Gordon equations for the functions $\varphi^{\pm}(x)$. Its solutions take an unphysical negative values at times $t\gtrsim t_F=mv/F$. One should note, however, that the model can be regarded as a reasonable approximation even in the underdamped regime ($\xi\gg1$) for processes with a characteristic time of less than t_F [3]

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