Environment-dependent continuous time random walk*

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A generalized continuous time random walk model which is dependent on environmental damping is proposed in which the two key parameters of the usual random walk theory: the jumping distance and the waiting time, are replaced by two new ones: the pulse velocity and the flight time. The anomalous diffusion of a free particle which is characterized by the asymptotical mean square displacement $\langle x^2(t)\rangle \sim t^\alpha$ is realized numerically and analysed theoretically, where the value of the power index α is in a region of $0 < \alpha < 2$. Particularly, the damping leads to a sub-diffusion when the impact velocities are drawn from a Gaussian density function and the super-diffusive effect is related to statistical extremes, which are called rare-though-dominant events.

Keywords: continuous time random walk, environment-dependent, rare-though-dominate events, anomalous diffusion

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1. Introduction

In connection with the growing interest in the physics of complex systems, anomalous diffusion properties and their descriptions have received considerable attention. Among the different frameworks for describing anomalous diffusion, the continuous time random walk (CTRW) theory was introduced by Montroll and Weiss,[1] and Scher and Montroll[2] separately. In the model, two powerful schemes have been established to account for the typical features of anomalous diffusion: Lévy statistics and non-Gaussian propagates. The diffusion process of a random walker is considered to contain two independent steps: jumping with a length and waiting for a period of time between two successive jumps, which are respectively drawn from their own probability distribution functions (PDFs). The CTRW can realize anomalous diffusion with the power index $0 < \alpha < 2$, as a result, the mean square displacement (MSD) of a free particle in a long-time limit satisfies: $\langle x^2(t)\rangle \sim t^\alpha$. It is called sub-diffusion for $0 < \alpha < 1$ due to the divergence of the mean waiting time and the finiteness of the second moment of jump distribution and super-diffusion for $1 < \alpha < 2$ due to the finiteness of the mean waiting time and the divergence of the second moment of jump distribution.

Unlike the generalized Langevin equation (GLE), the CTRW is not based on the dynamical process of a particle but on the viewpoint of observation. In recent years, the CTRW has been greatly developed and successfully used to investigate diffusion and transport behaviour of a system in external potentials.[3−10] The fractional Langevin equation (FLE) and the fractional Fokker–Planck equation (FFPE) have been used to describe anomalous diffusion by CTRW tools,[11,12] and several experiments such as blinking quantum dots and motion in rotating flow[13] have been successfully performed. Nevertheless, the original CTRW, where the jump of the walker does not require time, can take neither the environment-damping influence nor the dynamics in a jump process into account easily and conveniently.

The purpose of the present work is to generalize the CTRW "jump model" by including the damping and potential, so the new model is named as "the environment-dependent CTRW". In the model, the jumping distance and the waiting time are replaced by the pulse velocity and the flight time, both of which are random variables and obey different PDFs in different types of diffusions. In the model, the walker will no longer "jump" but "fly" and in the flight process, the motion of the walker is determined by the Newton second law. The rest of the present paper is organized as follows. In Section 2, the environment-dependent CTRW and its numerical sim-

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ulating algorithm are presented in detail and the effect of rare-though-dominate events in super-diffusion is also shown. In Section 3, the theoretical analysis of diffusion behaviour is performed. A summary is drawn in Section 4.

2. Environment-dependent continuous time random walk model

2.1. Molecular dynamics combined with random flight

In the usual CTRW model, the motion of a particle is divided into being of two processes: jump and wait. However, in the present model, the two processes mentioned above have been reformed as one process: flight. The random walker starts one flight process when it is affected by a stochastic pulse velocity. As the walker undergoes the flight process, the motion of the walker is described by the molecular dynamics, i.e., the Newton second law as

$$\dot{x} = v(t), \quad m\dot{v} = -\gamma v(t) + f(x(t)), \tag{1}$$

where $f(x(t)) = -U'(x)$, with $U(x)$ being the external potential. In the meantime, how long the flight process will continue is controlled by another stochastic parameter: the flight time, which should be determined before the flight process starts, too. When the current flight process ends, the walker will be affected by another pulse velocity and start another flight process, thus another flight time is drawn.

Here the randomness is introduced by two factors: (i) a random pulse velocity δv is added to the current velocity of the particle at position $x(t)$ and time t when a flight process is going to start, i.e., $v(t+0) = v(t) + \delta v$; (ii) the flight time τ of particle with the starting velocity $v(t+0)$ is stochastic, too. Then in the flight process, the particle is subjected to the damping and the potential via Eq. (1). A new pulse velocity is drawn and added to the velocity of particle $v(t+\tau)$ again to start a new flight when the current flight time is up.

Importantly, the flight time τ and the pulse velocity δv are two independent random variables, which are sampled from the PDFs selected in Subsection 2.2. The second-order Runge–Kutta algorithm with a small time step Δt ($\Delta t \ll \tau$) is used to numerically integrate Eq. (1). Because the flight trajectory of the particle is determined by the dynamical equation, the dependence of the generalized CTRW on the environment is natural and accurate. As a result, the present model can be conveniently applied to the transport of an anomalous diffusive system with power index $0 < \alpha < 2$ in a complicated potential. Finally, it is necessary to explain that, similar to the usual CTRW, the randomness of the generalized CTRW is introduced externally rather than by internal noise, so the relation between the dissipation and the fluctuation needs not to be restricted by the fluctuation–dissipation theorem.

2.2. Distributions of flight time and pulse velocity

Three cases are distinguished: sub-diffusion, normal diffusion and super-diffusion and the PDFs of the pulse velocity and the flight time are determined respectively.

In the case of sub-diffusion ($0 < \alpha < 1$), the PDF of the flight time can be defined by the Mittag–Leffler density function as

$$\psi(\tau) = -\frac{\mathrm{d}}{\mathrm{d}\tau} E_\alpha(-(\tau/\tau_0)^\alpha), \tag{2}$$

where $E_\alpha(-(\tau/\tau_0)^\alpha)$ is the Mittag–Leffler function and given by

$$E_\alpha(-(\tau/\tau_0)^\alpha) = \sum_{n=1}^{\infty} \frac{[-(\tau/\tau_0)^\alpha]^n}{\Gamma(1+n\alpha)}. \tag{3}$$

In fact, the above Mittag–Leffler function can be numerically calculated as follows:[14]

$$E_\alpha(-\xi) \approx \sum_{n=1}^{N} \frac{(-\xi)^n}{\Gamma(1+n\alpha)}, \tag{4}$$

if $\xi < \xi_0$; and

$$E_\alpha(-\xi) \approx -\sum_{n=1}^{M} \frac{(\xi)^{-n}}{\Gamma(1-n\alpha)}, \tag{5}$$

if $\xi > \xi_0$. Here suitable values of N, M and ξ_0 need to be chosen.[9]

In order to make numerical simulation easier and save computing time, the Pareto density function[9] is used as an approximation for the Mittag–Leffler density function, which is determined by

$$\psi(\tau) = -\frac{\mathrm{d}}{\mathrm{d}\tau} P_\alpha(\tau/\tau_0) \tag{6}$$

with the survival probability

$$P_\alpha(\tau/\tau_0) = \frac{1}{[1+\Gamma(1-\alpha)^{1/\alpha}(\tau/\tau_0)]^\alpha}. \tag{7}$$

For the pulse velocity, a Gaussian function is chosen as being its PDF,

$$\lambda(\delta v) = \frac{1}{\sqrt{4\pi\sigma^2}} \exp\left[-\frac{(\delta v)^2}{4\sigma^2}\right]. \quad (8)$$

In the case of super-diffusion ($1 < \alpha < 2$), the Poissonian function is considered to be the PDF of the flight time,

$$\psi(\tau) = \frac{1}{\tau_0} \exp\left(-\frac{\tau}{\tau_0}\right). \quad (9)$$

The Lévy distribution is chosen as the PDF of the pulse velocity, which has a power law asymptotic tail,[15−17]

$$\lambda(\delta v) = \sigma^{\mu} \frac{\Gamma(1+\mu)\sin(\pi\mu/2)}{\pi|\delta v|^{1+\mu}} \quad (\mu = 2/\alpha). \quad (10)$$

For the normal diffusion, the Gaussian function (Eq. (8)) and the Poissonian function (Eq. (9)) are respectively chosen as the PDFs of the pulse velocity and the flight time.

2.3. Numerical results

First, for the super-diffusion in the CTRW model, the width of distribution of the particle coordinates is measured rather than its variance because of the divergence of the MSD,[18,19] which is determined by

$$\langle x^2(t)\rangle_L = \frac{1}{N}\sum_{n=1}^{N} x_n^2, \quad \text{for} \quad x_n \in [-Lt^{\alpha/2}, Lt^{\alpha/2}]. \quad (11)$$

This implies that the above cut-off is time dependent and the imaginary box spans the spatial interval $\Delta(t) = 2Lt^{\alpha/2}$ which increases with time. This gives a measure that a finite portion of the probability is gathered within a given interval $\Delta(t)$.

The movement trajectory, MSD and mean square velocity (MSV) of a free particle with three different values of α are shown in Fig. 1, where the dimensionless parameters used are $m = 1.0$, $\gamma = 2.0$, $\tau_0 = 0.2$, $\sigma = 0.2$ and $L = 10.0$ and 5×10^4 test particles are used to describe the statistical behaviour of a single particle. Figure 1(a) shows that the generalized CTRW approach also presents a picture of trajectory similar to the dynamical evolution.

In Fig. 1(b), $\ln\langle x^2(t)\rangle$ is plotted as a function of $\ln t$. If the asymptotic MSD of the particle has the form of $\langle x^2(t)\rangle \sim t^{\alpha}$, the slope of the linear curve is equal to the power index α. Various power indexes $\alpha = 0.6$, 1.0 and 1.6 are respectively chosen

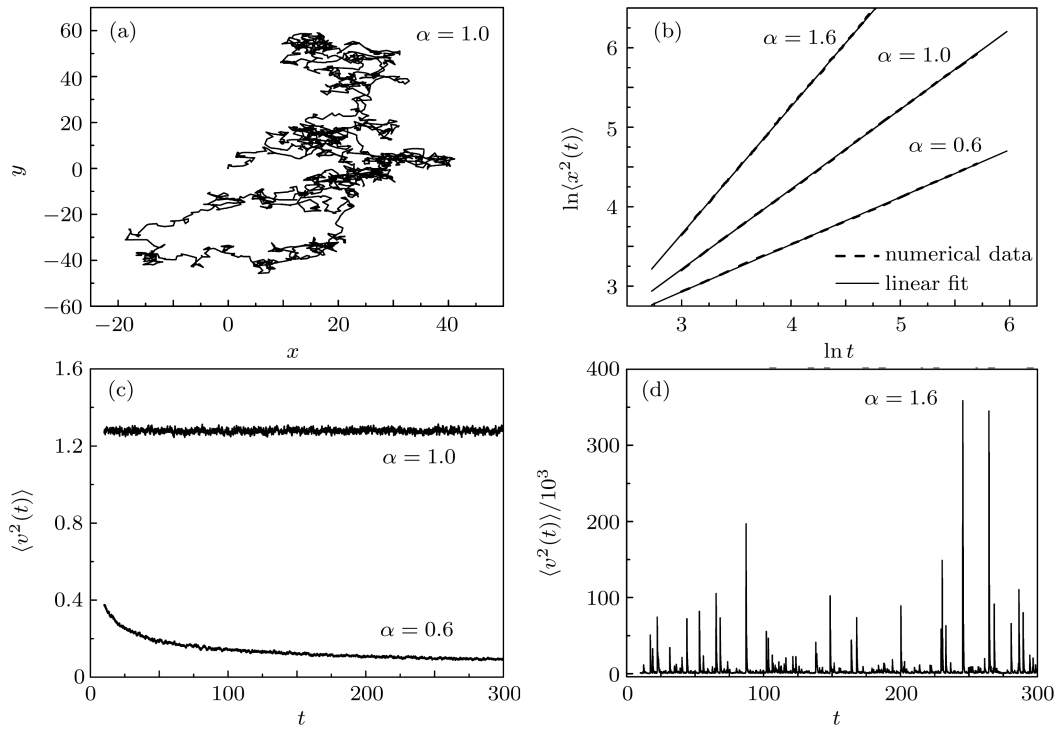


Fig. 1. (a) A two-dimensional trajectory of a free particle undergoing normal diffusion process; (b) Plots of $\ln\langle x^2(t)\rangle$ versus $\ln t$ for different power indexes. (c) Variations of mean square velocity $\langle v^2(t)\rangle$ with time for normal diffusion ($\alpha = 1.0$) and sub-diffusion ($\alpha = 0.6$); (d) Variation of mean square velocity with time for supper-diffusion ($\alpha = 1.6$).

as the representations of sub-, super- and normal diffusion and they are simulated with the environment-dependent CTRW. The linear fittings show that the slopes of the numerical results are respectively equal to 0.59513, 1.00548 and 1.6024, which are in very good agreement with the expected values.

In the present environment-dependent CTRW model, both the fluctuation of velocity of the particle and its distribution are the central quantities. We plot the MSVs of a particle in the cases of sub- and normal diffusion in Fig. 1(c) and in the case of super-diffusion in Fig. 1(d). It is surprising that unlike the normal diffusion and the sub-diffusion, the MSV of the particle does not approach to a constant value in the case of super-diffusion; on the contrary, it diverges at some times. This phenomenon will be explained and used to comprehend the mechanism of super-diffusion in the next section.

2.4. Rare-though-dominant events in super-diffusion

The causation of super-diffusion of a free particle subjected to random pulse velocities obeying Lévy distribution of $\alpha = 1.6$ will be investigated numerically in the following. If the absolute value of the pulse velocity is larger than a reference value, for instance, $v_c = 50.0$, it will not be added into the current velocity of the particle and a new one will be sampled from the Lévy distribution. This leads about 0.4% greatly contributive samples to be rejected. Under this restriction, the MSV of the particle (Fig. 2(a)) and its MSD (Fig. 2(b)) are calculated. It shows that the MSV approaches to a stationary value without large fluctuation and thus the MSD has a normal diffusion behaviour.

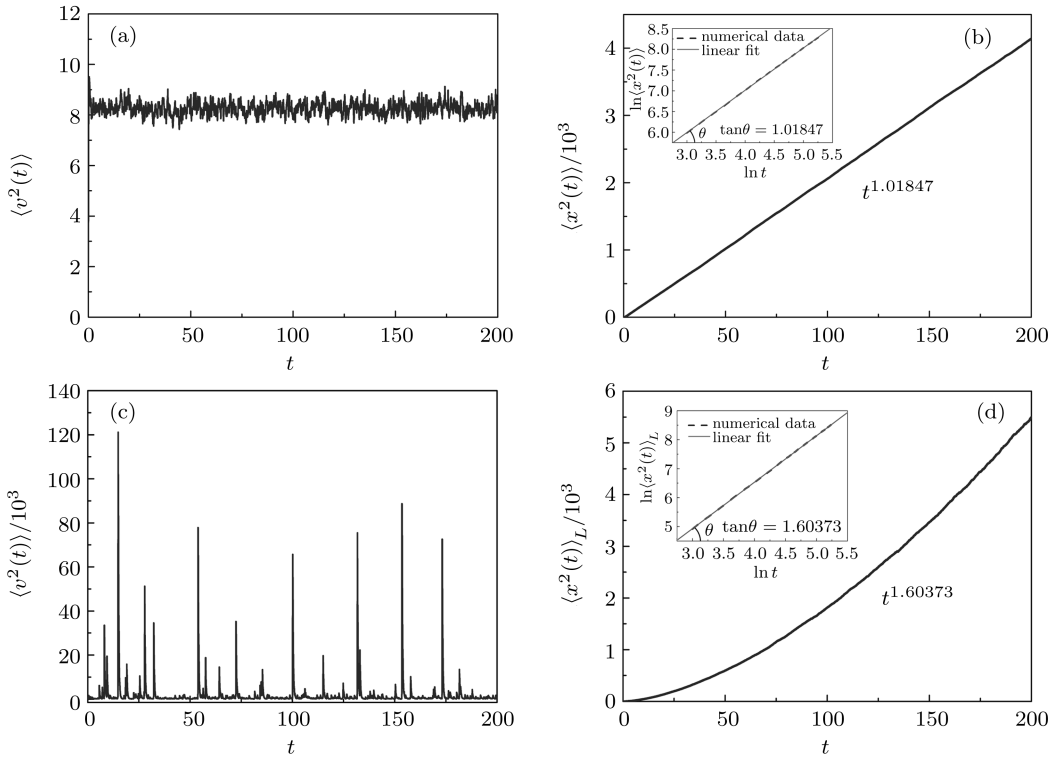


Fig. 2. (a) Calculated mean square velocity without the greatly contributive samples whose absolute values are larger than 50.0, (b) calculated power index of diffusion (corresponding to (a)) $\alpha = 1.01847$, (c) mean square velocity with the contribution of all pulse velocities and (d) calculated power index (corresponding to (c)) $\alpha = 1.60373$, with parameters being $\alpha = 1.6$, $\tau_0 = 0.5$, $\gamma = 2.0$, and $L = 10.0$.

In the next step, we employ all pulse velocity samples to calculate the width of coordinate distribution of particle and a super-diffusion with the expected power index $\alpha = 1.6$ is successfully realized as shown in Figs. 2(c) and 2(d). This result indicates that the rare-though-dominant samples play a greatly contributive role. Under the present parameters, the square values of these samples can be more than 10^3

times larger than the total number of the particles. If several test particles receive greatly contributive samples as the pulse velocity at the same time t, it results in the appearance of a very high peak in the curve of $\langle v^2(t)\rangle$ shown in Fig. 2(c). It is concluded that the cut-off of a fat tail (the pulse velocities with large absolute value and small probability in the present case) leads to the disappearance of the super-diffusion behaviour.

3. Theoretical analysis of diffusion behaviour

Let N be the number of steps performed by the walker during the time t and the total time t is simply the sum of N flight times encountered, i.e. $t = \sum_{n=1}^{N} \tau_n$. The MSD is thus given by[21]

$$\langle x^2(t)\rangle = \langle l^2(\tau)\rangle N \quad (N \to \infty), \tag{12}$$

where $\langle l^2(\tau)\rangle$ is the mean squared length of a flight. The solution of a length distance is obtained from Eq. (1) in the absence of potential as

$$l(\tau) = \frac{\delta v}{\gamma}\left[1 - \exp(-\gamma\tau)\right]. \tag{13}$$

(i) If the impact velocities are Gaussian and the mean flight time is divergent, it is known that the values of both $\langle \delta v^2\rangle$ and $\langle [1-\exp(-\gamma\tau)]^2\rangle = \int_0^\infty [1 - \exp(-\gamma\tau)]^2 \psi(\tau)\mathrm{d}\tau$ are finite, hence

$$\langle x^2(t)\rangle = \frac{\langle \delta v^2\rangle}{\gamma^2}\langle [1-\exp(-\gamma\tau)]^2\rangle N. \tag{14}$$

If $\psi(\tau)$ is a broad distribution, it leads to

$$\psi(\tau) = \tau_0^\mu \tau^{-(1+\mu)} \quad (\tau \to \infty), \tag{15}$$

with $0 < \mu < 1$ then $\langle\tau\rangle = +\infty$ and t behaves as

$$t \sim \tau_0 N^{1/\mu}, \quad N \sim (t/\tau_0)^\mu. \tag{16}$$

This leads to sub-diffusive behaviour

$$\langle x^2(t)\rangle \sim A_\mu t^\mu \quad (0 < \mu < 1). \tag{17}$$

An interesting point is that the damping leads to a sub-diffusion when the impact velocities are Gaussian, while for ballistic motion between collisions (zero damping), it yields super-ballistic motion for the test particle.[22,23]

(ii) If $\langle\tau\rangle$ is finite, then t behaves typically as $t \sim N\langle\tau\rangle$, or $N \sim t/\langle\tau\rangle$. We obtain the probability density function of a flight distance from the pulse velocity distribution (Eq. (10)) through the Jacobs transform as

$$\begin{aligned} & W(l(\tau)) \\ &= \lambda(\delta v)\frac{\partial \delta v}{\partial l(\tau)} \\ &= \lambda\left(\frac{l(\tau)\gamma}{1-\exp(-\gamma\tau)}\right)\frac{\gamma}{1-\exp(-\gamma\tau)} \\ &= \frac{\sigma^\mu \Gamma(1+\mu)\sin(\pi\mu/2)}{\gamma^{\mu-1}|l|^{1+\mu}}\left(1-\exp(-\gamma\tau)\right)^\mu. \end{aligned} \tag{18}$$

In order to extract the scaling form, one could enclose the walker in an imaginary growing box[19] as described below:

$$\begin{aligned} & \langle x^2(t)\rangle_L \\ &= \langle l^2(\tau)\rangle_L N \\ &= \int_{-Lt^{1/\mu}}^{Lt^{1/\mu}} l^2 W(l)\mathrm{d}l \cdot N \\ &\sim B_\mu t^{2/\mu-1}\cdot\frac{t}{\langle\tau\rangle} \sim \frac{B_\mu}{\langle\tau\rangle}t^{2/\mu} \quad (1<\mu<2). \end{aligned} \tag{19}$$

It shows supper-diffusion behaviour and has been implemented numerically as shown in Fig. 1.

4. Summary

A generalized continuous time random walk model has been proposed, where a test particle undergoes flight process and is randomly kicked. The flight time is described by power law distribution and the impulse velocity also reveals power behaviour. As a result, the environment influence such as damping and potential can be taken into account conveniently, because the motion of particle is described by the molecular dynamics combined with random flights, which is a unique advantage of the present new model. It is interesting that the damping leads to a sub-diffusion when the impact velocities are Gaussian, while for ballistic motion between collisions with zero damping, it yields super-ballistic motion for the test particle. From the viewpoint of rare-though-dominant events, a numerical conclusion can be made that the cut-off of a fat tail leads to the disappearance of anomalous diffusion behaviour.

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