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Extended Scaling Laws in the Crossover between Ballistic and Normal Diffusion

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Abstract—Crossover between ballistic motion and normal diffusion is studied based on the continuous-time random walk (CTRW) approach in order to analyze universal properties of strongly correlated motion and the decay process of correlation in deterministic diffusion. There exists a characteristic time scale τ. For the time region $t \ll \tau$, ballistic motion is observed, which is followed by normal diffusion for $t \gg \tau$. Higher-order moments are analytically obtained using the saddle-point method, and it is found that they obey scaling relations that are reminiscent of extended self-similarity (ESS) and generalized extended self-similarity (GESS) found in turbulent systems.

1. Introduction

Diffusion processes are commonly observed in many fields in physics, chemistry and biology, and have been studied both theoretically and experimentally. Normal diffusion such as Brownian motion is characterized by mean square displacement (MSD) that increases linearly with time, $\langle r^2\rangle(t) \propto t$. Other types of diffusion processes have also been studied, and are characterized by the temporal evolution of the MSD as $\langle r^2\rangle(t) \propto t^\zeta$ with $0 < \zeta < 1$ (anomalous subdiffusion), with $1 < \zeta < 2$ (anomalous superdiffusion), and with $\zeta = 2$ (ballistic diffusion). The last case, ballistic motion, is observed in the diffusion caused by thermal noise for the time scale shorter than the mean free time.

Based on the viewpoint of deterministic diffusion[1], diffusion is caused by chaotic dynamics in a dynamical system. The invariant sets relevant to the chaotic dynamics in the phase space suffer bifurcations when the control parameter is changed. Long correlations occur in the vicinity of the bifurcation point, leading to anomalous diffusion. There exists a characteristic time τ, which corresponds to the mean free time in the case of the diffusion caused by thermal noise. Unlike the mean free time, this characteristic time τ may diverge in the vicinity of the bifurcation point. Tangent bifurcation is an example. Thus, it is important to characterize crossover phenomena between anomalous and normal diffusion observed respectively for $t \ll \tau$ and for $t \gg \tau$ by use of various scaling properties, as is also the case for turbulent phenomena [2]. We attempted to find scaling laws that hold from the anomalous subdiffusion region into the normal diffusion region as a whole, and compare them with generalized scaling laws, like extended self-similarity (ESS) and generalized extended self-similarity (GESS), [3, 4] which were introduced to describe turbulence at intermediate Reynolds numbers. Miyazaki et al. succeeded in finding such scaling laws related to modulational intermittency[5, 6, 7, 8] and to superdiffusion in oscillating convection flows.[9]

These kinds of scaling laws are expected to be widely observed for various systems exhibiting crossover phenomena of concern. We will introduce the scaling function ϕ related to the moments of position and the curved time scale $\hat{t}$ characterizing the crossover between strongly correlated motion such as anomalous diffusion or ballistic motion and uncorrelated normal diffusion.

Here, we derive the scaling function ϕ and the curved time scale $\hat{t}$ for a simple system where a particle moves with uniform velocity on the line for a time which is distributed according to an exponential probability density function (PDF) $\varphi(t) = \exp(-t/\tau)/\tau$, and randomly changes its direction. The corresponding MSD shows a crossover between ballistic motion ($t \ll \tau$) and normal diffusion ($t \gg \tau$). For this purpose, we use a continuous-time random walk (CTRW)[10, 11] velocity model, which describes motion consisting of uniform motion and instantaneous changes of direction.

This paper is organized as follows. In §2, we describe the implementation of the CTRW velocity model. We derive the scaling properties characterizing crossover between ballistic motion and normal diffusion in §3. The final section is devoted to concluding remarks.

2. Implementation of the CTRW velocity model

Following the description of Zumofen and Klafter[12], we review the general framework of the CTRW theory. In the CTRW framework the random-walk process is entirely specified by $\psi(r, t)$, the probability density to move a distance r in time t in a single motion event. $\psi(r, t)$ can be either the decoupled case $\psi(r, t) = \varphi(t)\lambda(r)$, known as the *jump model*, or the coupled case $\psi(r, t) = p(r|t)\varphi(t)$, called the *velocity model*, where $\lambda(r)$ is the PDF to move a distance r in a single motion event and $p(r|t)$ is the conditional probability to move a distance r in time t. Here, we focus only on the velocity model, and we assume in the following:

$$p(r|t) = \frac{1}{2}\left[\delta(r - vt) + \delta(r + vt)\right], \tag{1}$$

where the first and second terms describe the uniform motion with positive constant velocity v and with negative constant velocity $-v$. For this model, $\varphi(t)$ is the PDF to go straight in one direction up to time t, 'the flight duration'. The probability density $P(r,t)$ to be at location r at time t will be calculated in terms of $\psi(r,t)$. In order to obtain $P(r,t)$ we define $\Psi(r,t)$, the probability to pass at location r at time t in a single motion event. $\Psi(r,t)$ is given by

$$\Psi(r,t) = \frac{1}{2}\left[\delta(r - vt) + \delta(r + vt)\right] \int_t^\infty dt'\, \varphi(t'). \tag{2}$$

In order to derive recursive expressions for $P(r,t)$, we consider $Q(r,t)$, the probability to arrive at r exactly at time t and to stop before randomly choosing a new direction. Irrespective of which model we choose, the following recursive relation holds:

$$Q(r,t) = \int dr' \int_0^t dt'\, Q(r-r', t-t')\psi(r',t') + \delta(r)\delta(t). \tag{3}$$

In the Fourier ($r \to k$) and Laplace ($t \to s$) spaces we have

$$Q(k,s) = \frac{1}{1 - \psi(k,s)}, \tag{4}$$

where we introduce for the Fourier and/or Laplace transforms the convention that the arguments indicate the space in which the function is defined, e.g., $Q(k,s)$ is the Fourier-Laplace transform of $Q(r,t)$. Moreover the probability density $P(r,t)$ is related to $Q(r,t)$ by

$$P(r,t) = \int dr' \int_0^t dt'\, Q(r - r', t - t')\Psi(r', t'). \tag{5}$$

Finally in the Fourier and Laplace spaces we have

$$P(k,s) = \frac{\Psi(k,s)}{1 - \psi(k,s)}. \tag{6}$$

The corresponding $2m$-th moments are given in the Laplace space by

$$\langle r^{2m}\rangle(s) = \left.\frac{\partial^{2m} P(k,s)}{\partial(ik)^{2m}}\right|_{k=0}. \tag{7}$$

Some supplements to the above descriptions are mentioned below. The key functions $\psi(r,t)$, $\psi(k,s)$ and $\Psi(k,s)$ are explicitly given by

$$\psi(r,t) = \frac{1}{2}\left[\delta(r - vt) + \delta(r + vt)\right] \varphi(t), \tag{8}$$

$$\psi(k,s) = \frac{1}{2}\left[\varphi(s - ikv) + \varphi(s + ikv)\right], \tag{9}$$

$$\Psi(k,s) = \frac{1}{2}\left[\frac{1 - \varphi(s - ikv)}{s - ikv} + \frac{1 - \varphi(s + ikv)}{s + ikv}\right]. \tag{10}$$

Therefore, substituting Eqs. (9) and (10) into Eq. (6) and Eq. (7) with $m = 1$, we obtain the corresponding MSD in the Laplace space, $\langle r^2\rangle(s)$, as

$$\langle r^2\rangle(s) = \frac{2v^2\left(s\frac{d\varphi(s)}{ds} + 1 - \varphi(s)\right)}{s^3(1 - \varphi(s))}. \tag{11}$$

It is also convenient to introduce the following two functions

$$\psi_+(k,s) = \varphi(s + ikv) + \varphi(s - ikv), \tag{12}$$

$$\psi_-(k,s) = \varphi(s + ikv) - \varphi(s - ikv), \tag{13}$$

so that we have

$$P(k,s) = \frac{s}{s^2 + k^2v^2} + \frac{ikv}{s^2 + k^2v^2}\,\frac{\psi_-(k,s)}{2 - \psi_+(k,s)}. \tag{14}$$

3. Crossover between ballistic motion and normal diffusion

We derive the crossover between anomalous ballistic motion and normal diffusion by using the CTRW velocity model. As mentioned in the preceding section, to calculate MSD, firstly we must obtain $\varphi(t)$. We assume the following PDF

$$\varphi(t) = \frac{1}{\tau}\exp(-\frac{t}{\tau}), \tag{15}$$

where τ corresponds to a characteristic time scale of the crossover, which is equal to the average flight duration. The Laplace transform of Eq. (15) is given by

$$\varphi(s) = \frac{1}{1 + \tau s}. \tag{16}$$

Substituting Eq. (16) into Eqs. (12) and (13), we have

$$\psi_+(k,s) = \frac{2(1 + \tau s)}{(1 + \tau s)^2 + (kv\tau)^2}, \tag{17}$$

$$\psi_-(k,s) = \frac{-2ikv\tau}{(1 + \tau s)^2 + (kv\tau)^2}. \tag{18}$$

Therefore, substituting Eqs. (17) and (18) into Eq. (6), we obtain $P(k,s)$ as

$$P(k,s) = \frac{1}{2v}\sqrt{\frac{1 + \tau s}{\tau s}}\,\frac{2\frac{\sqrt{\tau s(1+\tau s)}}{\tau v}}{k^2 + \left(\frac{\sqrt{\tau s(1+\tau s)}}{\tau v}\right)^2}, \tag{19}$$

which coincides with the result derived by Zumofen and Klafter [12]. Equation (11) yields the corresponding MSD in the Laplace space

$$\langle r^2\rangle(s) = \frac{2\tau v^2}{s^2(1 + \tau s)}, \tag{20}$$

whose inverse Laplace transform yields the following scaling form

$$\frac{\langle r^2\rangle(t)}{2Dt} = \bar{\phi}(\frac{t}{2\tau}), \tag{21}$$

with the diffusion constant

$$D = \tau v^2, \tag{22}$$

and the scaling function

$$\bar{\phi}(z) = 1 - \frac{1}{2z}\left(1 - \exp(-2z)\right). \tag{23}$$

We have $\bar{\phi}(z) \sim z$ for $z \ll 1$, and $\bar{\phi}(z) \sim 1$ for $z \gg 1$.

From Eq. (7) we have

$$\langle r^{2m}\rangle(s) = \tau\Gamma(2m+1)(\tau v)^{2m}\frac{1}{\tau s}\left\{\frac{1}{\tau s(1+\tau s)}\right\}^m. \tag{24}$$

For the sake of simplicity, we rescale time as

$$\tau s \to s \qquad (\frac{t}{\tau} \to t), \tag{25}$$

which implies that the time t is normalized by τ, so that we have

$$\langle r^{2m}\rangle(t) = \Gamma(2m+1)(\tau v)^{2m}\mathcal{L}^{-1}\left[\frac{1}{s}\frac{1}{(s(1+s))^m}\right]. \tag{26}$$

For large m, the inverse Laplace transform can be estimated by use of the saddle-point method as[13]

$$\begin{aligned}
&\mathcal{L}^{-1}\left[\frac{1}{s}\frac{1}{(s(1+s))^m}\right] \\
&= \frac{1}{2\pi i}\int_{s_*-i\infty}^{s_*+i\infty} e^{st-m\log(s(1+s))-\log s}\,ds, && (27)\\
&= e^{f(s_*)}\left[2\pi f''(s_*)\right]^{-1/2}, && (28)\\
&= (2e)^m g(\frac{t}{2m})\left[\hat{t}\left(\frac{t}{2m}\right)\right]^m, && (29)
\end{aligned}$$

where the argument of the exponential function f, the saddle point s_*, the *curved* time scale $\hat{t}$, and the additional function g are given by

$$\begin{aligned}
f(s) &= st - m\log(s(1+s)) - \log s, && (30)\\
s_*(t,m) &= s_*\left(\frac{t}{2m}\right),\\
&= \frac{1}{2}\left(-1 + \frac{2m}{t} + \sqrt{1 + (\frac{2m}{t})^2}\right), && (31)\\
\hat{t}(z) &= z\,\phi(z), && (32)\\
\phi(z) &= \frac{\sqrt{1+z^2}-1}{z}\exp\left(-z + \sqrt{1+z^2}\right), && (33)\\
g(z) &= \frac{z+1+\sqrt{1+z^2}}{\sqrt{1+z^2+\sqrt{1+z^2}}}. && (34)
\end{aligned}$$

The saddle point $s = s_*(t,m)$ is determined from $f'(s) = 0$, which leads to $t - \frac{m}{s} - \frac{m}{1+s} - \frac{1}{s} = 0$. For $m \gg 1$, the last term can be ignored, so that the saddle point in the convergence domain is given by Eq. (31). As shown in Fig. 1, the smooth, bounded, and monotonically increasing function $g(z)$ given by Eq. (34) satisfies $\sqrt{2} = g(0) \le g(z) \le g(\infty) = 2$ for $z \ge 0$. We have $\phi(z) \propto z$ for $z \ll 1$, and $\phi(z) \sim 1$ for $z \gg 1$, so that $\hat{t}(z) \propto z^2$ for $z \ll 1$, and $\hat{t}(z) \propto z$ for $z \gg 1$. Using Eqs. (26) and (29) and returning to the original time scale ($t \to \frac{t}{\tau}$), we obtain

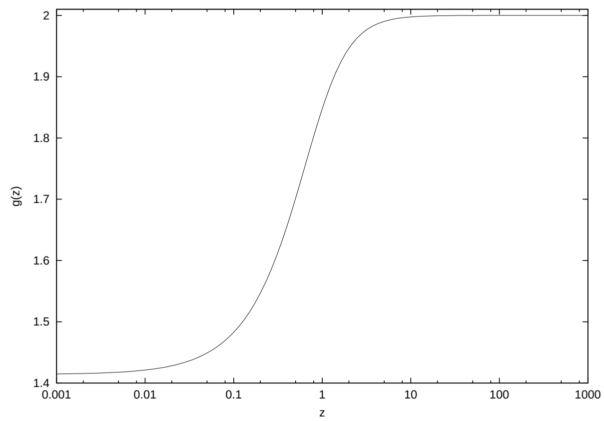

Figure 1: The function $g(z)$ given by Eq. (34) appearing in the scaling law of the $2m$-th moment Eq. (35). Note that this function is nearly constant, except for $z \sim 1$.

$$\langle r^{2m}\rangle(t) = N_m\, g\left(\frac{t}{2m\tau}\right)\left[\hat{t}\left(\frac{t}{2m\tau}\right)\right]^m \tag{35}$$

with $N_m = \Gamma(2m+1)(2e\tau^2 v^2)^m$. Figure 2 depicts $\phi(z)$ (solid line) derived by the saddle-point method. Also plotted is $\bar{\phi}(z)$ (dashed line) given by Eq. (23) appearing in the scaling law of the second moment ($m = 1$) Eq. (21) derived exactly for comparison. Good agreement implies that the results derived by the saddle-point method for $m \to \infty$ hold even for lower-order moments.

We find that the curved time scale $\hat{t}$ depends on the order of the moment m. However, introducing the time $t_m = mt$, which are the actual time scaled by the inverse of the moment order, $1/m$, we have the $2m$- and $2n$-th moments expressed in terms of $\hat{t}\left(\frac{t}{2\tau}\right)$ as

$$\begin{aligned}
\langle r^{2m}\rangle(t_m) &= N_m g\left(\frac{t}{2\tau}\right)\left[\hat{t}\left(\frac{t}{2\tau}\right)\right]^m, && (36)\\
\langle r^{2n}\rangle(t_n) &= N_n g\left(\frac{t}{2\tau}\right)\left[\hat{t}\left(\frac{t}{2\tau}\right)\right]^n. && (37)
\end{aligned}$$

From Eqs. (36) and (37), we have

$$\hat{t}\left(\frac{t}{2\tau}\right) = \left[\frac{\langle r^{2m}\rangle(t_m)}{N_m g\left(\frac{t}{2\tau}\right)}\right]^{1/m} = \left[\frac{\langle r^{2n}\rangle(t_n)}{N_n g\left(\frac{t}{2\tau}\right)}\right]^{1/n}, \tag{38}$$

which leads to

$$\langle r^{2m}\rangle(t_m) = \frac{N_m}{N_n^{m/n}}\left[g\left(\frac{t}{2\tau}\right)\right]^{1-m/n}\langle r^{2n}\rangle^{m/n}(t_n). \tag{39}$$

Ignoring the time dependence of $g(t)$, we have

$$\langle r^{2m}\rangle(t_m) \propto \langle r^{2n}\rangle^{m/n}(t_n), \tag{40}$$

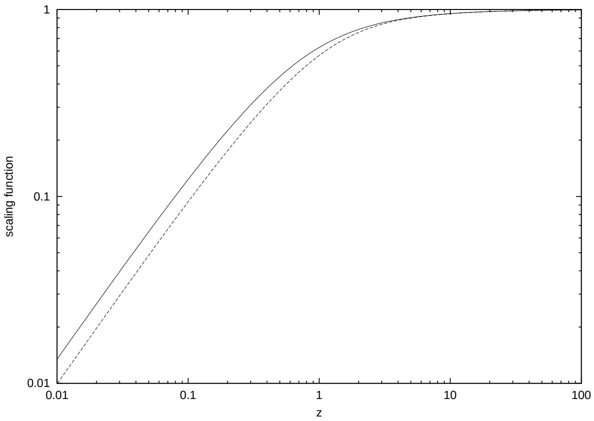

Figure 2: The function $\phi(z)$ (upper solid line) given by Eq. (33) appearing in the scaling law of the $2m$-th moment Eq. (35) derived by the saddle-point method. The function $\bar{\phi}(z)$ (lower dashed line) given by Eq. (23) appearing in the scaling law of the second moment ($m = 1$) Eq. (21) derived exactly for comparison. Good agreement implies that the results derived by the saddle-point method for $m \to \infty$ hold even for lower-order moments.

which holds for $0 < t \ll \tau$ and $t \gg \tau$, and is reminiscent of ESS observed in turbulence [3].

When we consider the moment normalized by the function g

$$\frac{\langle r^{2m}\rangle(t_m)}{g(\frac{t}{2\tau})} \propto \left\{\frac{\langle r^{2n}\rangle(t_n)}{g(\frac{t}{2\tau})}\right\}^{m/n}, \qquad (41)$$

which holds for all t. This scaling relation is an analog of GESS [4].

4. Concluding remarks

A test particle under the influence of deterministic diffusion has strongly correlated motion for the time scale which is much shorter than a characteristic time which is estimated by the correlation time due to the underlying chaotic dynamics causing deterministic diffusion.

General nonhyperbolic dynamical systems found in the realistic world have rich structures of bifurcations. The bifurcation diagram of the logistic map illustrates this situation most clearly. In the vicinity of bifurcation points, the above characteristic time becomes very long, so it is important to analyze universal properties of strongly correlated motion and the decay process of correlation in deterministic diffusion. Based on this idea, the scaling properties of higher order moments were derived for the simple stochastic process, i.e., the CTRW jump model describing crossover between ballistic motion and normal diffusion. It is a future problem to confirm the scaling law (35) for a concrete dynamical system. The climbing sine map [14, 15] is a good candidate.

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