Extended Self-Similarity in Deterministic Diffusion
(決定論的拡散における
Extended Self-Similarity に類似したスケーリング則)

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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 \( \tau \). 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 an-
alytically 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 pro-
cesses have also been studied, and are characterized by the temporal evolution of the
MSD as

\[
\langle r^2 \rangle(t) \propto t^\zeta,
\]

\[0 < \zeta < 1 \quad \text{anomalous subdiffusion},\]

\[\zeta = 1 \quad \text{normal diffusion},\]

\[1 < \zeta < 2 \quad \text{anomalous superdiffusion},\]

\[\zeta = 2 \quad \text{ballistic motion}.
\]

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. In such systems, there are crossover phenomena between anomalous and
normal diffusion, which are characterized by 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 (GESSS)\textsuperscript{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\textsuperscript{5-8} and to superdiffusion in oscillating convection flows.\textsuperscript{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 $\phi$ 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 $\phi$ 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) $\psi(t) = \exp(-t/\tau)/\tau$, 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)\textsuperscript{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,\textsuperscript{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 $\psi(r, t) = \psi(t)\lambda(r)$, known as the jump model, or the coupled case $\psi(r, t) = p(r|t)\psi(t)$, 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. For this model, $\psi(t)$ 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 location $r$ at time $t$ in a single motion event. $\Psi(r, t)$ is given by

$$\Psi(r, t) = p(r|t) \int_0^\infty dt' \int_0^\infty dr' \psi(r', t').$$

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:

$$Q(r, t) = \int dr' \int_0^t dt' Q(r - r', t - t')\psi(r', t') + \delta(r)\delta(t).$$
In the Fourier \((r \rightarrow k)\) and Laplace \((t \rightarrow s)\) spaces we have
\[
Q(k, s) = \frac{1}{1 - \psi(k, s)},
\]
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
\[
P(r, t) = \int dq' \int dt' Q(r - r', t - t')\psi(r', t').
\]
Finally in the Fourier and Laplace spaces we have
\[
P(k, s) = \frac{\psi(k, s)}{1 - \psi(k, s)}.
\]
The corresponding \(2m\)-th moments are given in the Laplace space by
\[
\langle r^{2m} \rangle(s) = \frac{\partial^2 P(k, s)}{\partial (ik)^2} \bigg|_{k=0}.
\]
Some supplements to the above descriptions are mentioned below. In the one-dimensional case, usually it is assumed that:
\[
p(r | t) = \frac{1}{2} [\delta(r - vt) + \delta(r + vt)],
\]
where the first and second terms describe the uniform motion with positive constant velocity \(v\) and with negative constant velocity \(-v\). Thus, the key functions \(\psi(r, t)\), \(\psi(k, s)\) and \(\Psi(k, s)\) are explicitly given by
\[
\psi(r, t) = \frac{1}{2}[\delta(r - vt) + \delta(r + vt)],
\]
\[
\psi(k, s) = \frac{1}{2}[\psi(s - ikv) + \psi(s + ikv)],
\]
\[
\Psi(k, s) = \frac{1}{2} \left[ \frac{1 - \psi(s - ikv)}{s - ikv} + \frac{1 - \psi(s + ikv)}{s + ikv} \right].
\]
Therefore, substituting Eqs. (9) and (10) into Eq. (5) and Eq. (6) with \(m = 1\), we obtain the corresponding MSD in the Laplace space, \(\langle r^2 \rangle(s)\), as
\[
\langle r^2 \rangle(s) = 2v^2 \left( s^2 \frac{d}{ds} + 1 - \psi(s) \right) \frac{1}{s^3(1 - \psi(s))}.
\]
It is also convenient to introduce the following two functions
\[
\psi_+(k, s) = \psi(s + ikv) + \psi(s - ikv),
\]
\[
\psi_-(k, s) = \psi(s + ikv) - \psi(s - ikv),
\]
so that we have
\[
P(k, s) = \frac{s}{s^2 + k^2 v^2} + \frac{ikv}{s^2 + k^2 v^2} \frac{\psi_-(k, s)}{2 - \psi_+(k, s)}.
\]
§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 \( \psi(t) \). We assume the following PDF

\[
\psi(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right),
\]

where \( \tau \) 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

\[
\psi(s) = \frac{1}{1 + \tau s}.
\]

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

\[
\psi_+(k, s) = \frac{2(1 + \tau s)}{(1 + \tau s)^2 + (kv\tau)^2},
\]

\[
\psi_-(k, s) = \frac{-2i kv\tau}{(1 + \tau s)^2 + (kv\tau)^2}.
\]

Therefore, substituting Eqs. \( (17) \) and \( (18) \) into Eq. \( (5) \), we obtain \( P(k, s) \) as

\[
P(k, s) = \frac{1}{2v} \sqrt{\frac{1 + \tau s}{\tau s}} \frac{2 \sqrt{\tau s(1 + \tau s)}}{k^2 + \left(\frac{\sqrt{\tau s(1 + \tau s)}}{kv}\right)^2}.
\]

Equation \( (11) \) yields the corresponding MSD in the Laplace space

\[
\langle r^2 \rangle(s) = \frac{2\tau v^2}{s^2(1 + \tau s)},
\]

whose inverse Laplace transform yields the following scaling form

\[
\frac{\langle r^2 \rangle(t)}{2Dt} = \tilde{\phi}(\frac{t}{2\tau}),
\]

with the diffusion constant

\[
D = \tau v^2,
\]

and the scaling function

\[
\tilde{\phi}(z) = 1 - \frac{1}{2z} (1 - \exp(-2z)).
\]

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

From Eq. \( (6) \) we have

\[
\langle r^{2m} \rangle(s) = \tau \Gamma(2m + 1)(\tau v)^{2m} \frac{1}{\tau s} \left\{ \frac{1}{\tau s(1 + \tau s)} \right\}^m.
\]
For the sake of simplicity, we rescale time as

$$\tau s \rightarrow s \quad \left( \frac{t}{\tau} \rightarrow t \right),$$  \hspace{1cm} (25)

which implies that the time $t$ is normalized by $\tau$, so that we have

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

For large $m$, the inverse Laplace transform can be estimated by use of the saddle-point method as \cite{13}

$$\mathcal{L}^{-1}\left[ \frac{1}{s} \left( \frac{1}{s(1+s)} \right)^m \right] = \frac{1}{2\pi i} \int_{s_{\ast} - i\infty}^{s_{\ast} + i\infty} e^{st - m \log(s(1+s)) - \log s} ds,$$

$$= e^{f(s_{\ast})} \left[ 2\pi f''(s_{\ast}) \right]^{-1/2},$$

$$= (2\pi)^m g\left( \frac{t}{2m} \right) \left[ \frac{t}{2m} \right]^m,$$  \hspace{1cm} (27-29)

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

$$f(s) = st - m \log(s(1+s)) - \log s,$$

$$s_{\ast}(t, m) = s_{\ast} \left( \frac{t}{2m} \right) = \frac{1}{2} \left( -1 + \frac{2m}{t} + \sqrt{1 + \left( \frac{2m}{t} \right)^2} \right),$$

$$\hat{t}(z) = z \phi(z),$$

$$\phi(z) = \frac{\sqrt{1 + z^2} - 1}{z} \exp \left( -z + \sqrt{1 + z^2} \right),$$

$$g(z) = \frac{z + 1 + \sqrt{1 + z^2}}{\sqrt{1 + z^2 + \sqrt{1 + z^2}}},$$  \hspace{1cm} (30-34)

The saddle point $s = s_{\ast}(t, m)$ is determined from $f'(s) = 0$, which leads to $t - \frac{m}{s_{\ast}} = \frac{m}{t} - \frac{1}{s} = 0$. 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 $\sqrt{2} = g(0) \leq g(z) \leq g(\infty) = 2$ for $z \geq 0$. We have $\phi(z) \propto z$ for $z \ll 1$, and $\phi(z) \sim 1$ for $z \gg 1$, so that $\hat{t}(z) \propto z^{2m}$ for $z \ll 1$, and $\hat{t}(z) \propto z^m$ for $z \gg 1$. Using Eqs. (26) and (29) and returning to the original time scale ($t \rightarrow \frac{t}{\tau}$), we obtain

$$\langle r^{2m} \rangle (t) = N_m g\left( \frac{t}{2m} \right) \left[ \frac{t}{2m} \right]^m,$$  \hspace{1cm} (35)

with $N_m = \Gamma(2m+1)(2e^2v_0^2)^m$. Figure 2 depicts $\phi(z)$ (solid line) derived by the saddle-point method. Also plotted is $\phi(z)$ (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 $m \rightarrow \infty$ hold even for lower-order moments.
Fig. 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 \( z \sim 1 \).

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

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

\[
\langle r^{2n} \rangle(t_n) = N_n g \left( \frac{t}{2\tau} \right) \left[ \hat{t} \left( \frac{t}{2\tau} \right) \right]^n.
\]

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

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

which leads to

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

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

\[
\langle r^{2m} \rangle(t_m) \propto \langle r^{2n} \rangle^{m/n}(t_n),
\]

which is reminiscent of ESS observed in turbulence.\(^3\) We introduce the function

\[
E_{mn}(t) = \frac{d \langle \log \langle r^{2m} \rangle(t_m) \rangle}{d \langle \log \langle r^{2n} \rangle(t_n) \rangle},
\]
Fig. 2. The function $\phi(z)$ (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 $\tilde{\phi}(z)$ (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.

which extracts the power from the scaling law Eq. (40). In the time region where the time dependence of $g(t)$ is ignored, we have

$$E_{mn}(t) = \frac{m}{n},$$  \hspace{1cm} (42)

which holds for $0 < t \ll \tau$ and $t \gg \tau$.

In order to eliminate the function $g(t)$, we rewrite Eq. (39) as

$$\left[ g \left( \frac{t}{2\tau} \right) \right]^{-1} = \left[ \frac{N_m}{N_n} \frac{\langle r^{2n} \rangle^{m/n}(t_n)}{\langle r^{2m} \rangle^{m/n}(t_m)} \right]^{\frac{1}{n-1}} = \left[ \frac{N_K}{N_L} \frac{\langle r^{2L} \rangle^{k/l}(t_L)}{\langle r^{2L} \rangle^{k/l}(t_K)} \right]^{\frac{1}{l-1}},$$  \hspace{1cm} (43)

so that we have

$$G_{m,n}(t) = \frac{N_m}{N_n} \left( \frac{N_l}{N_K} \right)^{\frac{1}{n-1}} [G_{k,l}(t)]^{m-n \over n-1},$$  \hspace{1cm} (44)

where the compensated moment is defined by

$$G_{q,p}(t) = \frac{\langle r^{2q} \rangle^{q/p}(t_q)}{\langle r^{2p} \rangle^{q/p}(t_p)}.$$  \hspace{1cm} (45)

This scaling relation is reminiscent of GESS.\cite{footnote:4} We introduce a function to extract the power from Eq. (44) as

$$D_{m,n,k}(t) = \frac{d (\log G_{m,n}(t))}{d (\log G_{k,l}(t))},$$  \hspace{1cm} (46)
which satisfies

\[ D_{mnkt}(t) = \frac{m - n}{k - l} \]  \hspace{1cm} (47)

for all \( t \).

\section*{§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 system describing crossover ballistic motion and normal diffusion. The theoretical results obtained here can be confirmed, for instance, by numerical simulation of Lorentz gas.

A nonhyperbolic one-dimensional map has been intensively studied through the viewpoint of deterministic diffusion.\textsuperscript{14, 15} Long ballistic motion occurs in the vicinity of tangent bifurcation in this system. In this case, the PDF of flight time duration is replaced by \( \psi(t) \propto 1/t \), which is nothing but the PDF of the laminar time duration of the type I intermittency. Derivation of the scaling functions and the curved time scale as well as numerical confirmation of the theory by use of this one-dimensional map will be studied in the next publication.

\section*{References}