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• Letter to the Editor •

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A quenched trap model for non-Gaussian diffusion

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Dear Editors,

Brownian motion is well-known for its linear growing mean-square displacement (MSD)

$$\left\langle \Delta x^2 \right\rangle = 2Dt^{\alpha}, \qquad \alpha = 1, \tag{1}$$

and the Gaussian-shaped displacement distribution

$$P(x,t) = (4\pi Dt)^{-1/2} \exp(-x^2/4Dt), \tag{2}$$

where D is the diffusion coefficient. In the past thirty years, various deviations from the original Brownian motion have been intensively studied, including sub-diffusion with $\alpha < 1$ due to crowding or freezing [1], super-diffusion with $\alpha > 1$ due to active transport [2, 3]. Bae et al. [4] observed another class of anomalous diffusion, which is still Fickian with $\alpha = 1$ while the displacement distribution is non-Gaussian. It was speculated the "Fickian, but non-Gaussian" phenomena arise from limited duration of observation [5], which is usually not sufficient for particles to sample the whole heterogeneous environment. Deviations from Gaussian distribution may hence arise. Recent molecular dynamics (MD) simulation [6] and *in vivo* experiment [7] observed non-Gaussian displacement distribution. The non-Gaussian phenomena in the models of disordered oscillator chain were also reported [8]. Several theoretical studies (see eg. ref. [9]) concerning fluctuating and correlated diffusivity were performed. But it is still not clear how the non-Gaussian behavior arises from heterogeneous environment. In this work, we introduce a quenched energy landscape, which is short-range correlated. Our simulation shows that the non-Gaussian behavior naturally appears on the correlated energy landscape.

The correlated energies $\{V_i\}$ on lattice are generated by a two-step scheme. We first construct an uncorrelated energy landscape $\{U_i\}$, which follows the exponential distribution

$$P(U) = U_0^{-1} \exp(-U/U_0), \qquad U < 0. \tag{3}$$

An extreme landscape $\{V_i\}$ is then introduced by setting the value of V_i by the deepest trap of $\{U_j\}$ in its r_c-neighbourhood:

$$V_i = \min\{U_j | r_{ij} < r_c\}. \tag{4}$$

The landscape $\{V_i\}$ is hence composed by basins $\{C_k\}$ of local minima $\{\tilde{V}_k\}$. The spatial correlation is strictly constrained to the size of the basins, which gives the correlation length $\xi \sim 2r_c$.

The trap dynamics [10, 11] is adopted to describe the diffusion on the landscape. In trap dynamics, the hopping rate from site i to its nearest-neighbour site j is purely determined by V_i,

$$W_{i\to j} = W_0 \exp(V_i). \tag{5}$$

The random walk is hence equivalent to a continuous time random walk with site-dependent diffusivity $D_i = W_0 \exp(V_i) a^2/2$ with a as the lattice constant. It can be shown that, on the landscape $\{V_i\}$ generated by the above scheme, the diffusivity $\{D_i\}$ follows exponential distribution

$$P(D) = D_0^{-1} \exp(-D/D_0). \tag{6}$$

Kinetic Monte Carlo simulation was performed to study the random walk on one-dimensional quenched landscape

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with periodic boundary condition. The size of the landscape is up to $L = 10^5$ while the correlation length $r_c = 100$, where we set the lattice constant $a = 1$. The trap depth is controlled by $U_0 = 1$. The dynamic rate is chosen as $W_0 = 1$. As shown in Figure 1, the distribution of diffusivity follows eq. (6) with $D_0 = 0.0025$. The displacement distribution is extracted from long trajectories of 10^{10} hoppings, which span over the whole lattice. Figure 2 shows the distribution of displacement over time intervals. One can clearly read the exponential tail for short time interval and the crossover to Gaussian tail for longer time intervals, as what have been observed in experiments and MD simulations.

We briefly elucidate the origin of the anomalous phenomena. The spatially correlated diffusivity is introduced in the model by the basins of local minima. In the short-time regime, the random walk is governed by the local diffusivity D_k of the initial basin k. The displacement distribution

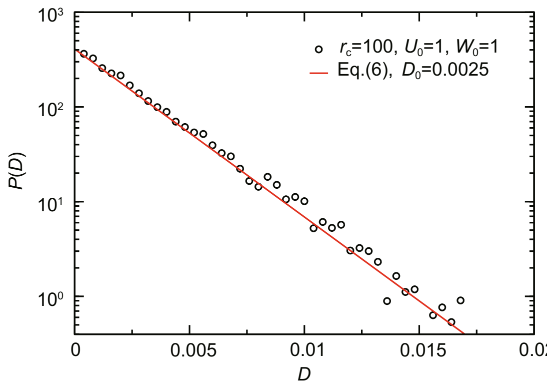

Figure 1 (Color online) The distribution of diffusivity. (Open circles) The normalized histogram of the diffusivity on the generated landscape. (Solid line) Numberical evaluation of eq. (6) with $D_0 = 0.0025$.

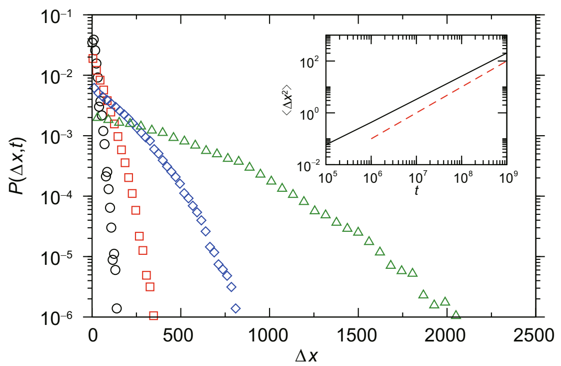

Figure 2 (Color online) The displacement distribution with $t = 10^5$ (black), $t = 10^6$ (red), $t = 10^7$ (blue) and $t = 10^8$ (green). Mean squared displacement (inset). The solid line shows the MSD from simulation. The dash line indicates the linear dependence.

in each basin follows the usual Gaussian form

$$P(x, t|D_k) = (4\pi D_k t)^{1/2} \exp(-x^2/4D_k t), \quad t \ll \xi^2/D_k. \tag{7}$$

Averaging over particles of different local diffusivities, the mean distribution is of the exponential shape (noticing eq. (6) for the distribution of D). In long time limit, on the other hand, most particles visit multi-basins. The diffusivity is thus self-averaged in every wide-spanned trajectory. The displacement distribution from each single self-averaged trajectory converges to the Gaussian one, governed by the unique mean diffusivity $\langle D\rangle$. Hence the mean distribution of displacement becomes Gaussian.

The experiments usually cannot fully arrive at the self-averaging time scale, even if some of the tracers can leave the initial basins. It is thus important to study the crossover from single basin non-Gaussian behavior to multi-basin Gaussian behavior. The crossover depends on complicated properties of the heterogeneous environment, which are not well understood yet. Our simple model focuses on the spatial correlation of the environment, which gives a theoretical framework to investigate the anomalous diffusion in heterogeneous environment. It is still an open question whether the dimensionality of the environment is crucial to the results. To further compare the model with experiments, more detailed investigation is also required.

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