Time-dependent diffusion in a random correlated potential

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(Received 26 October 2005; published 7 March 2006)

Diffusive behavior of a particle in a two-dimensional random correlated potential with Gaussian distribution and exponential correlation is investigated via Langevin simulation. Our results show that superdiffusion appears only in the early period of the time of evolution and there does not exist an intermediate time for the occurrence of the whole issue from subdiffusion to superdiffusion. Whether the asymptotic situation of the particle could be arrived before the simulation stops is strongly influenced by the finite-size effect of the random correlated potential simulated. By applying the random correlated potential to the decay of a metastable system, we find that the escape rate of a particle is decreased by hill effect of the random potential.

DOI: 10.1103/PhysRevE.73.031103 PACS number(s): 05.40.−a, 68.35.Fx, 68.43.Jk

In recent years, there has been great interest in anomalous diffusion which was observed in many situations [1]. The motion of a particle is affected by the dissipative influence of a disordered heat bath. The mean square displacement (MSD) of the force-free particle is characterized by $\langle x^2(t)\rangle \sim t^\alpha$ at long times, where α is a phenomenological power exponent taking the values $0<\alpha<2$. For normal diffusive behavior, MSD increases linearly with time, it grows sublinearly with time for subdiffusion and grows superlinearly with time for superdiffusion. Recently, Sancho *et al.* [2,3] showed that the nature of intermediate-time diffusive behavior for Langevin dynamics on a two-dimensional (2D) random correlated potential (RCP) surface with Gaussian distribution varies as the friction coefficient changes. The subdiffusion occurs for high friction and the superdiffusion occurs for low friction. These are significant results, especially since they may explain the apparent "Lévy flight" results observed in recent experiments and simulations. It should be an interesting and largely uncharted territory, if it is true. Nevertheless, the argument still remains on the intermediate time when the superdiffusion occurs [4,5].

An excellent experiment was reported on the effect of bacterial motion on micron-scale beads in a freely suspended soap film [6]. The MSD of the particle shows ballistic diffusion in short time and normal diffusion is recovered in the long time limit. This is a result of the transient formation of coherent structures in the bacterial bath. It is known that the MSD of a particle driven by a Gaussian white noise always shows an increasing behavior with time faster than the linear law at the early time, and approaches asymptotically normal diffusion. An instant approach [7] was developed for calculations of various correlation functions describing the statistical behavior of the elastic string in the two-dimensional random potential. However, in the present state, the analytical result for the damping RCP is not available, so more extensive numerical simulations with various parameters are necessary. Anyway, the generation of the RCP with a large spatial scale is required to simulate the motion of the particle during a long period of time especially in the case of weak friction, because the simulation will be stopped once a particle reaches one boundary of the potential.

Diffusion and transport in the presence of the RCP has been applied to investigate many microscopic phenomena in molecular biology. In the process of the protein sliding along the DNA activated by thermal noise, the energy of the protein has a random correlated component. During the transport of the DNA through the nanopore, the potential energy of the DNA is randomly correlated too. These examples of application have been discussed in detail in Ref. [8].

In this paper, we are aiming at identifying time-dependent diffusive behavior of an underdamped particle in a two-dimensional random correlated potential with Gaussian distribution and exponential correlation. The characteristic quantity is the MSD divided by time. It will be shown from our simulations with a larger spatial scale that the asymptotic diffusive behavior of the particle in the 2D RCP that we considered here is subdiffusion for various parameters. Furthermore, we consider a particle escaping out of a metastable potential well in the presence of a random correlated potential and calculate the time-dependent escape rate.

The equation of motion of a 2D diffusing particle reads

$$m\ddot{\mathbf{x}} = -\nabla V(\mathbf{x}) - \gamma\dot{\mathbf{x}} + \xi(t), \tag{1}$$

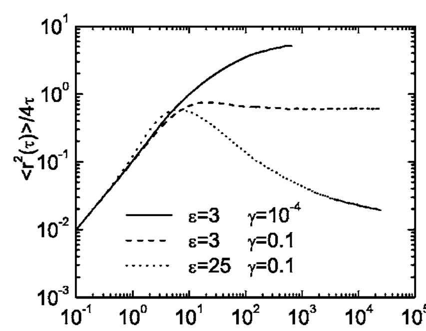

FIG. 1. $\langle r^2(t)\rangle/4\tau$ for three sets of values of the random potential intensity g_0 and the damping coefficient γ. All the parameters are the same as Ref. [5] and $\epsilon=2\pi\lambda^2 g_0$, $\langle r^2(\tau)\rangle=\langle[x(\tau)-x(0)]^2/\lambda^2\rangle+\langle[y(\tau)-y(0)]^2/\lambda^2\rangle$. τ has been defined in Ref. [2].

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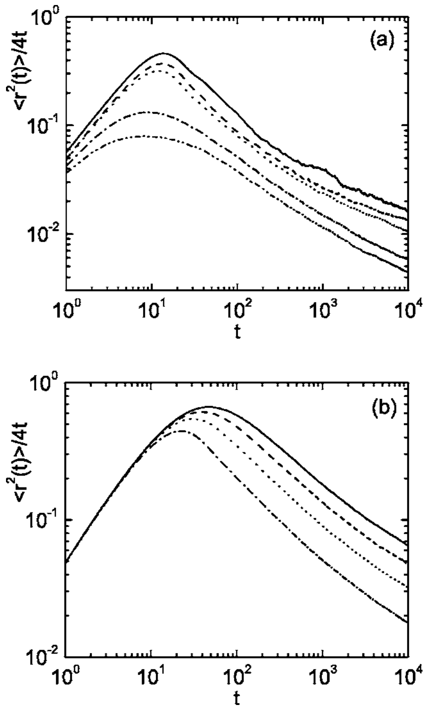

FIG. 2. Mean square displacements of the particle in the 2D RCP at fixed $k_BT=0.1$. (a) $g_0=0.16$, $\lambda=5.0$, $\gamma=0.0005$, 0.005, 0.05, 0.5, and 1.0 from top to bottom. (b) $g_0=0.2$, $\gamma=0.1$, $\lambda=25$, 20, 15, and 10 from top to bottom.

where γ is the coefficient of friction, $\xi(t)$ denotes the Gaussian white noise with zero mean and obeys the fluctuation-dissipation relation

$$\langle \xi_i(t)\xi_j(t')\rangle = 2\gamma k_B T \delta_{ij}\delta(t-t'), \tag{2}$$

where k_B is the Boltzmann constant and T is the absolute temperature. The 2D RCP $V(\mathbf{x})$ has a Gaussian distribution with zero mean and exponential correlation function

$$\langle V(\mathbf{x})V(\mathbf{x}')\rangle = g_0 \exp[-|\mathbf{x}-\mathbf{x}'|^2/(2\lambda^2)]. \tag{3}$$

Two basic parameters which characterize the RCP are the correlation length λ and the potential intensity g_0.

The Brownian motion of noninteracting particles in the RCP has been extensively presented in Refs. [9,10]. The overdamped diffusion in the short ranged RCP was investigated in Ref. [11]. By means of the algorithm of Refs. [11,12], the RCP with any spatial correlation can be generated. In our simulations, the one-dimensional (1D) RCP is generated on a linear grid of size $L_1=2^{22}$ and the 2D RCP is constructed on a square grid of size $L_2\times L_2$ where $L_2=2^{13}$ except for Fig. 1. The linear size of the cell is $\delta x=1.0$ and $k_BT=0.1$ in the forthcoming simulations except for Fig. 1. Note that the size of 2D RCP in this paper is twice as large as that in Refs. [2,3], which allows us to treat the diffusion of the test particles for a longer period of time. At the initial time, the particles are uniformly randomly located in a line section in the 1D case or a square in the 2D case, with a Maxwellian velocity distribution. The stochastic Runge-Kutta algorithm [13,14] is used to numerically solve the Langevin equation (1) discretized in time.

TABLE I. The coefficients of fitting function $A+Bt^{\alpha}$ for MSD vs λ.

λ	α	β
5	0.627	0.37
10	0.625	1.04
15	0.647	1.53
20	0.658	2.08
25	0.631	3.70
30	0.613	5.75
40	0.636	6.87

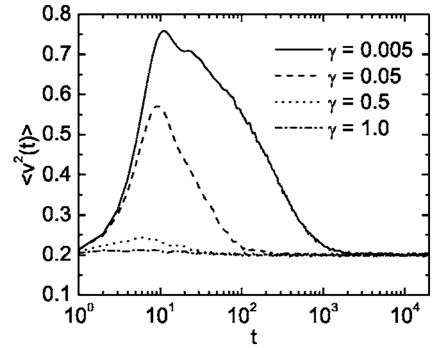

FIG. 3. Mean square velocity of the particle in the 2D RCP for various $\gamma=0.005$, 0.05, 0.5, and 1.0 from top to bottom. The parameters used are $k_BT=0.1$, $g_0=0.16$, and $\lambda=5.0$.

First, we carry out simulations for the time-dependent diffusion of the particle in the 2D RCP with the size of lattice $L_2=16\,382$ which is four times as much as that of Ref. [5]. The 2D MSD of the particle $\langle r^2(\tau)\rangle$ is plotted in Fig. 1. It is seen that our results are the same as that of Ref. [5] before the time when their simulations are stopped, displaying diffusive and subdiffusive regimes. However, there does not exist superdiffusive behavior for a 2D diffusing system after the time $\tau=5\times10^2$. It is clear that the particle becomes free when the temperature is very high comparing with the barrier height of the RCP, for instance, the maximal value of g_0 is about 0.03 and the temperature is $k_BT=0.2$ as used in Ref. [5]. This implies that the test particles have sufficient thermal

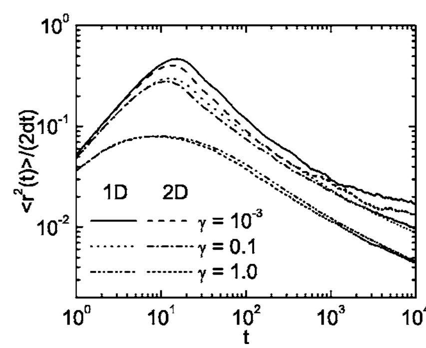

FIG. 4. Comparison of the 1D MSD with the 2D MSD for several values of γ. The parameters used are $k_BT=0.1$, $g_0=0.16$, and $\lambda=5.0$.

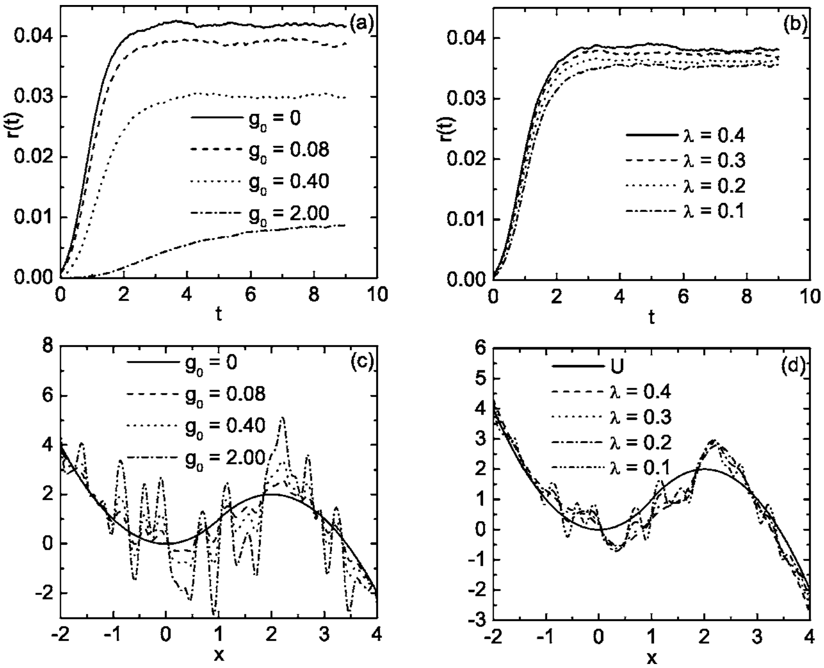

FIG. 5. Time-dependent escape rate for various g_0 at γ=0.1 in (a) and for various λ at g_0 =0.2 in (b). The temperature is k_BT=0.1 and the number of text particles 5×10^5. The total potential for various g_0 is plotted in (c) and various λ in (d).

energy to overcome the barrier of the RCP, so the asymptotic diffusion of the particle seems to be normal in this case.

Figures 2(a) and 2(b) show the time-dependent 2D MSD for various frictions γ and correlation lengths λ of the RCP. For early times, the test particles, which are located on barriers at the initial time, slide down quickly and show superdiffusion. Nevertheless, the asymptotic behavior of the particle becomes the subdiffusion at long times, because the friction and the RCP dissipate the kinetic energy of the particle. Superdiffusion only exits in the early time of evolution, but the transient superdiffusion of this kind cannot be regarded as the characteristic behavior of the system. Indeed, the diffusive behavior of the particle appears to be a nonmonotonic varying with time and the transient time corresponding to the curve peak comes later when the friction decreases or the correlation length of the RCP increases.

Let us discuss the role of the correlation length of the RCP in detail. We assume that the MSD is written as a function of time, i.e., $\langle r^2(t)\rangle = A + Bt^{\alpha}$ at long times, and present some fitting results in Table I. It is seen that the value of B increases monotonously with λ. The particle diffuses more quickly for a larger value of λ, because the distance between the two adjacent barriers of the RCP increases and the potential becomes flatter. The previous work has pointed out that the exponent α is only determined by g_0 and k_BT in the overdamped regime [11]. In the case of finite friction, our results show that the dispersion of α is small enough to be considered as the statistical uncertainty, then the exponent α does not depend on λ when the values of k_BT, g_0, and γ are fixed. This is in agreement with the results of Ref. [11].

In Fig. 3, we plot the mean square velocity of the particle for various γ, which is used to check whether the system has arrived at the stationary state. The initial velocity of the particle obeys a Maxwellian distribution: $P(\vec{v}_0) = (2\pi k_BT)^{-d/2}\exp[-|\vec{v}_0|^2/(2k_BT)]$, where d is the dimension of the space. It is seen from this figure that the value of $\langle|\vec{v}(t)|^2\rangle$ approaches dk_BT in a long time limit. At the initial time, some test particles are located at the barrier tops of the 2D RCP and then their potential energies are transferred into kinetic energies in the early stages of time, however, the friction makes the motion of the particle slower. Thus the mean square velocity of the particle during the transient period is larger than its equilibrium value. After a long time, the particle approaches the equilibrium state in the velocity space. This implies that the motion of the particle is not in the asymptotic or stationary state before the value of $\langle|\vec{v}(t)|^2\rangle$ arrives at dk_BT.

The comparison of the 2D results with the 1D results for various frictions is plotted in Fig. 4. It is seen that the diffusive behavior of the particle in the 2D RCP is similar to that in the 1D RCP, because the two degrees of freedom are independent. In fact, the particle does not experience a descend force anywhere. It always needs to climb over a ridge of the RCP and remains for a longer time interval in a deeper well. Namely, there is no way to make the asymptotic diffusive behavior of the particle surpass normal diffusion in this kind of RCP. We think that only subdiffusion appears in a long time limit in this RCP at low temperatures, because the diffusive mechanism of the classical particle is a process of random barrier crossing. In the overdamped regime, the MSD has the form $\langle x^2(t)\rangle \sim t^{z_{\mathrm{eff}}}$ according to the renormalization group calculations [9,11], where z_{eff} is the effective subdiffusive exponent less than the unity. It is found from our simulations that the particle with finite friction can arrive at the asymptotic state before the simulation is stopped if the size of the RCP is large enough. It is concluded that the asymptotical behavior of the particle in the present RCP is either subdiffusion at a low temperature or normal diffusion at a high temperature.

As an application, we consider the time-dependent escape rate of a particle in a one-dimensional metastable potential adding a RCP, which is determined numerically by

$$r(t) = -\frac{1}{N(t)}\frac{\Delta N(t)}{\Delta t}. \tag{4}$$

The bare metastable potential consists of an inverse harmonic potential linking smoothly with a harmonic potential, where the barrier height is equal to 2.0, the position of the saddle point is $x_b=2.0$, the coordinate of the link point is $x_c=1.0$, and the two well curvatures are $\omega_0=\omega_b=1.0$. In Eq. (4), $N(t)$ denotes the number of test particles that have not undergone an escape at time t and $\Delta N(t)$ is the number of test particles that have undergone an escape from the saddle point of the bare metastable potential within a time interval $t\to t+\Delta t$. In the simulations, Δt is chosen to be much larger than the interval between the two successive escapes [15,16].

Figures 5(a) and 5(b) show the time-dependent escape rate of the particle for various g_0 and λ. Here the case of $g_0=0$ corresponds to the usual barrier escape induced by a Gaussian white noise. It is seen that the escape rate of the particle in a metastable potential combining with a RCP is less than that in a bare metastable potential. This can be understood from the total potential plotted in Figs. 5(c) and 5(d). There exist many hills before the saddle point in the 1D potential, thus the particle needs sufficient thermal energy to overcome each potential barrier so it can arrive at the exit point. The increase of g_0 leads to the hill being deeper and the number of hill increases when the correlation length of RCP decreases. Both are not propitious to diffusion and escape.

From the above simulations of the diffusion in the RCP and the escape process in the metastable potential, we have found that the effect of the random correlated potential on the diffusion is always negatively biased. The larger the intensity g_0 or the shorter the correlation length λ, the more difficult the diffusion is, so that the asymptotical diffusive behavior of the particle in the present random correlated potential cannot surpass normal diffusion.

In summary, we have identified time-dependent diffusive behavior of a particle in a random correlated potential with Gaussian distribution and exponential correlation through many simulations with a larger system. A translation of the particle motion from initially superdiffusion to asymptotic subdiffusion has been observed and the superdiffusion only exists in the early stages of time. The friction indeed characterizes the time scale of the system approaching the stationary state, namely, diffusion arrives slowly at the asymptotic state when the friction decreases. We have emphasized the importance of the size of the random correlated potential simulation, because the simulation will be stopped once a particle arrives at a boundary of the random correlated potential. In the case of very little friction, the size of the random correlated potential needs to be large enough, otherwise the asymptotic behavior for a long amount of time cannot be observed before the motion of the test particle is stopped. It might be expected that the asymptotic behavior of a particle in the random correlated potential with Gaussian distribution and exponential correlation is normal diffusion at a very high temperature, which is subdiffusion at a low temperature and finite friction.

This work was supported by the Specialized Research Fund for the Doctoral Program of Higher Education under Grant No. 20050027001 and the National Natural Science Foundation of China under Grant No. 10235020.

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