Anomalous diffusion in periodic potentials under self-similar colored noise

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We present numerical studies of anomalous diffusion in periodic potentials by simulating a generalized Langevin equation. It is proved that the particle driven by a thermal colored noise with the spectral density vanishing at zero frequency allows superdiffusive motion. It is found that the system subjected to sub- or superohmic damping exhibits two motion modes in a corrugated plane: running oscillated state and mixed running and oscillating states, respectively. Induced, the anomalous power can be enhanced up twice for the latter case and thus a wide range of diffusive regimes is observed with changing titled force.

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Diffusion processes of atoms, molecules, and clusters of molecules in periodic structures have been subjects of research for many decades due to their intrinsic interest and technological importance [1,2]. As a consequence, the temperature-dependent effective diffusive coefficient calculated by the mean square displacement (MSD) divided by time is exponentially smaller than that of free diffusion. Two simple approaches for giant enhancing diffusion were proposed, such as the periodic potential is either titled [3] or rocked [4]. The mechanism is that the optimal matching of the external driving force and internal noise drives the probability peaks up to the potential hills, which are scattered at the potential tops and smashed into small pieces. Chaos induced by a deterministically rocked asymmetrical periodic potential including of finite inertia can mimic the role of noise [5]. All those studies open interesting perspectives, e.g., to manipulate reaction-diffusion systems. Most of the models, so far, deal with regular Brownian motion cases.

The diffusion and mobility of a particle in a titled periodic potential, i.e., a corrugated plane, provides a simple example of a phase transition between a located state and a running state [1,6]. Very recently, the fractional (sub-) diffusion in titled periodic potential was studied by numerically solving a fractional Fokker-Planck equation [7]. The diffusive and transport behaviors of a superdiffusing system are far more complex and should exhibit richer dynamical phenomena. The nature of anomalous diffusion in periodic potentials, is still not completely understood. In the present state, analytical result for the underdamped case is not available, so more extensive numerical calculations with various parameters are necessary.

In this paper, we focus on the variation of diffusive behavior of a particle in periodic potentials. Here we show that the problem of a particle driven by a thermal colored noise with the spectral density vanishing at zero frequency in the periodic potential also belongs to the class of superdiffusive motions. A generic case for a particle subjected to a nonohmic friction environment is addressed; the mixing oscillated state and running state in the corrugated plane is found to bring results.

The motion of a particle with mass m is described by a generalized Langevin equation (GLE)

$$m\dot{v}(t) = -m\int_0^t \gamma(t-t')v(t')dt' - U'(x) + \varepsilon(t), \qquad (1)$$

where $\gamma(t)$ is the memory friction kernel and $\varepsilon(t)$ is of vanishing mean and its stationary correlation satisfies the fluctuation-dissipation theorem: $\langle\varepsilon(t)\varepsilon(t')\rangle = mk_BT\gamma(t-t')$. Here, k_B is the Boltzmann constant and T is the temperature of the heat bath.

We consider a simple colored noise with the spectral density vanishing at zero frequency, which is called the harmonic velocity noise (HVN) $\varepsilon(t)$ [8] obeying the Langevin equations: $\dot{\sigma}=\varepsilon$, $\dot{\varepsilon}=-\Gamma\varepsilon-\Omega^2\sigma+\xi(t)$, where $\xi(t)$ is Gaussian white noise of vanishing mean with $\langle\xi(t)\xi(t')\rangle = 2\eta\Gamma^2 k_BT\delta(t-t')$, η is the damping coefficient, Γ and Ω denote the damping and frequency parameters of noise, respectively. The spectral density of $\varepsilon(t)$ is given by

$$S_\varepsilon(\omega) = \frac{2\eta\Gamma^2 k_BT\omega^2}{(\omega^2-\Omega^2)^2+\Gamma^2\omega^2}. \qquad (2)$$

Such thermal noise leads to a vanishing effective friction, i.e., the Laplace transform of the damping kernel vanishes at zero frequency [$\hat{\gamma}(0)=\int_0^\infty \gamma(t)dt=0$]. The particle allows asymptotical ballistic diffusive behavior in the absence of potential [9]. Similar thermal fluctuations are relevant to many physical systems, for instance, the coupling of a particle to low frequency modes of a heat bath is weak, as optical-like phonons [9,10]. Other situations that come to mind involve the vortex diffusion in magnetic fields [11], or diverse other open dynamics with an inherent velocity-dependent system-bath coupling [12]. Note also a typical solid-state Drude bath spectrum, thus yielding as well a vanishing, zero-frequency friction [10,13].

In Fig. 1, we plot typical trajectories of a regular Brownian particle (left panel) and that subjected to a thermal HVN $\varepsilon(t)$ (right panel) in the two-dimensional separable periodic potential: [$U(x,y)=-U_0(\cos x+\cos y)$]. The initial position is $x(0)=y(0)=0$ and the initial velocity obeys a Gaussian velocity distribution of zero mean with variance k_BT/m. Of interest to us is the possibility that jumps of the particle driven by HVN belong to superdiffusive motion. This is clearly observed for intermediate heights of the potential barrier (or equivalent to intermediate temperatures). These inho-

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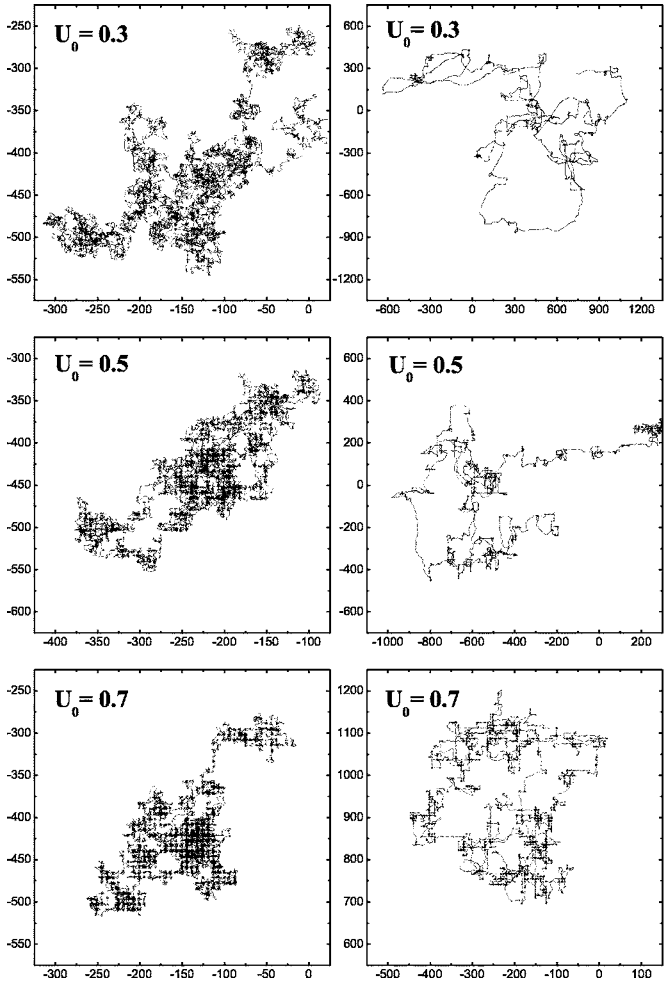

FIG. 1. Comparison of the trajectories in two-dimensional periodic potential. Left: White noise induced. Right: Harmonic velocity noise induced. The parameters used are $m=1.0$, $k_BT=1.0$, $\eta=1.0$, $\Gamma=1.0$, and $\Omega=1.0$.

mogeneous jumps exist in this case, because the particle should jump a long distance with several periods when a particle of this kind with a strong velocity memory rather than its position surmounts up the potential top. This is in agreement with the distinct feature of the superdiffusion being the hierarchical clustering of the trajectory [14]. This phenomenon was also proved in the random correlated potential at intermediate times [15], but subdiffusion at long times [16]. The present result also differs with Lévy statistics in a Hamiltonian system [17]. We assert that a special assumption for the distribution of noise is not necessary in order to realize superdiffusion.

Time evolution of MSD of the HVN-driven particle moving in the one-dimensional periodic potential $[U(x)=-U_0\cos x]$ is shown in Figs. 2(a) and 2(b) at fixed temperature $k_BT=1.0$ for various U_0. The comparison with the white noise case is performed in Fig. 2(c). The power α, calculated over the time variation of MSD in Figs. 2(a) and 2(b), is plotted in Fig. 2(d), as a function of U_0. Upon inspection, we find a prominent result: There is a gradual change in the power α starting from two which tends to $\alpha=1$ only for very large values of barrier height. This behavior depends explicitly on the parameters of the present colored noise. With a large U_0, the particle undergoes a noise activated escape event and performs a hopping process from one well to the neighboring ones, and thus shows normal diffusion at long times.

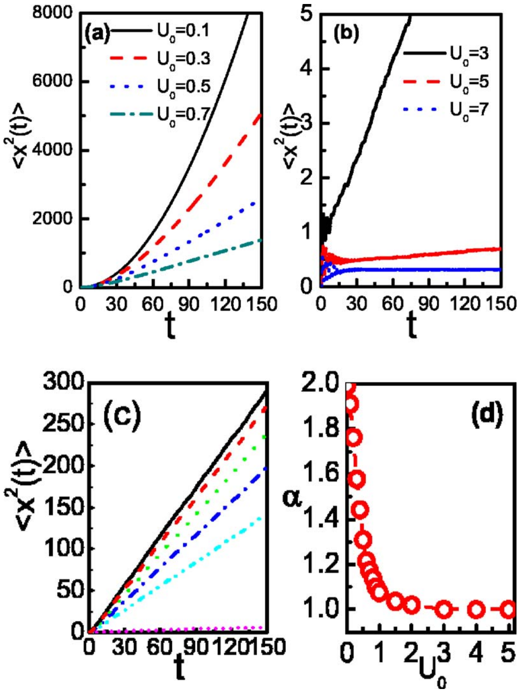

FIG. 2. (Color online) The mean square displacement of the particle subjected to a thermal HVN vs time for versus potential barriers in (a) and (b); the white noise case for $U_0=0.1, 0.3, 0.5, 0.7, 1.0, 3.0$ from top to bottom is compared in (c). The power α appearing in $\langle x^2(t)\rangle=2D_\delta t^\alpha$ of (a) and (b) as a function of U_0 is plotted in (d). The parameters used are the same in Fig. 1.

Next, let us consider a generic model leading to a rich variety of different diffusion regimes, namely, a particle subjected to a nonohmic damping environment [18]. The time-dependent damping kernel is deduced from the spectral density of environmental oscillators, i.e.,

$$\gamma(t)=\frac{2}{m\pi}\int_0^\infty d\omega\frac{J(\omega)}{\omega}\cos(\omega t) \tag{3}$$

with $J(\omega)=\gamma_\delta(\omega/\tilde{\omega})^{\delta-1}f_c$, where f_c is a high frequency cutoff function, $\tilde{\omega}$ denotes a reference frequency allowing for the friction constant $m\gamma_\delta$ to have the dimension of a viscosity of any δ. A smooth cutoff function is chosen to be $f_c=\exp(-\omega/\omega_c)$, $m=1.0$, $\gamma_\delta=4.0$, $\omega_c=4.0$, and $\tilde{\omega}=1.0$ are used in the forthcoming calculations.

The case of particle modeled by the GLE (1) subject to both a nonohmic memory damping (3) and a potential is a much more difficult problem, because the GLE cannot be transferred into a set of Markovian LEs and the corresponding colored noise cannot be simulated directly yet. Here we develop a numerical technique for solving GLE with the nonohmic memory friction, which is realized by using the Fourier transform technique to generate noise [19] and the stochastic Runge-Kutta method [20] to solve the whole equa-

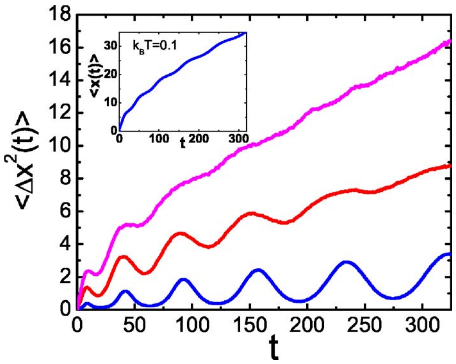

FIG. 3. (Color online). Time-dependent mean square displacement of a subohmic damping particle ($\delta=0.6$) at fixed $F=5.0$ and $k_BT=1.0$, 0.5, 0.1 from top to bottom. The mean displacement of $k_BT=0.1$ case is also plotted in the inset.

tion. This approach is very successful as shown in Ref. [21], which has been compared with several solvable examples.

In Fig. 3, we plot the MSD of a subohmic damping particle with $\delta=0.6$ as a function of time in the titled periodic potential $[U(x)=-U_0\cos x-Fx$ with $U_0=1.0]$ at fixed F and for various temperatures; the MD is also plotted in the inset of this figure. It is seen that the MSD and MD of the particle show quasiperiodic synchronization, namely, the MSD allows maximal or minimal when the particle arrives at the maximal or minimal position of the original potential, respectively. This state is called the *running oscillated state* and will disappear with the increase of temperature.

Figure 4 shows time-dependent MSD of a superohmic damping particle with $\delta=1.7$. The most interesting finding is: The power α appearing in the fitted MSD function $[\langle\Delta x^2(t)\rangle\sim t^{\alpha}]$ is a nonmonotonous function of the tilted force and $\alpha=\delta$ when $F>1$ (local potential minima disappear). Near $F_c=0.75$, the value of α yields maximum and is about 3.34. In particular, this behavior of diffusion is induced by the mixing of two separated velocity modes: *oscillating* state and *running* state. The dimensionless backward and forward barriers are $U_1=2\sqrt{1-F^2}+2F\arcsin F+F\pi$ and $U_2=2\sqrt{1-F^2}+2F\arcsin F-F\pi$ at $x_0=\arcsin(F)$. At low-temperature $k_BT=0.1$, $k_BT<U_2\ll U_1$, the particle oscillates around a potential minimum with a large probability. Never-

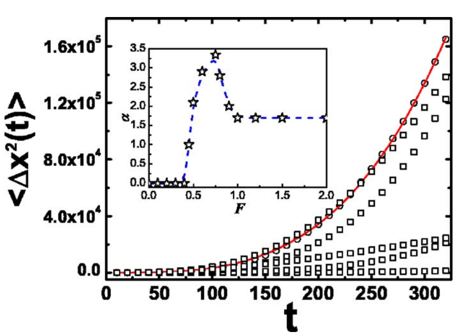

FIG. 4. (Color online) Time-dependent mean square displacement of a superohmic damping particle ($\delta=1.7$) at fixed $k_BT=0.1$ and $F=0.8$, 0.7, 0.9, 0.6, 0.5 (open squares) from top to bottom. Here open circles are $F=0.75$ and the solid line is their fitting curve. The power α fitted as a function of F is also plotted in the inset.

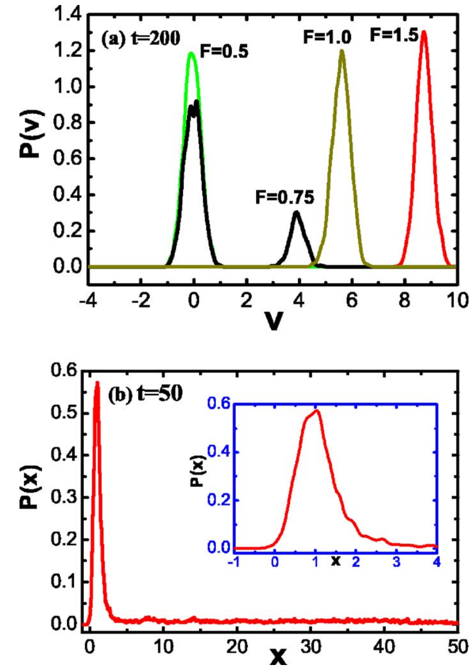

FIG. 5. (Color online) (a) The distributions of velocity at $t=200$ for various titled forces; notice that the velocity presents a coexistence of two bells shaped when $F=0.75$. (b) The position distribution at $t=50$ for $F=0.75$. Here $\delta=1.7$ and $k_BT=0.1$.

theless, once the particle climbs over its forward barrier it will transfer into the running state.

In Figs. 5(a) and 5(b), we plot the probability distributions of velocity and position of the particle with $\delta=1.7$, respectively. It is seen that the velocity distribution in the oscillating state approximately obeys the Maxwellian one for small F. As long as the particle escapes from a potential well it is easy to pass over the array of potential barriers. The relative velocity between the running state and the oscillating state increases inhomogeneities with time, thus the distribution of the particle position has a long tail shown in Fig. 5(b).

Note that the velocity distribution presents a two-bell shape, corresponding to the small oscillation and moving particles: this is a *coexistence regime* of the running and oscillating states. At time t, we assume that the oscillating mode including of $N_1(t)$ text particles with $\langle x_b(t)\rangle\approx 0$; the running mode having $N_2(t)$ test particles and reads $\langle x_d(t)\rangle \approx at^{\tilde{\alpha}}$, where a is a constant and $\tilde{\alpha}=1.627$ found in our simulation. We have $\langle x(t)\rangle\approx\langle x_d(t)\rangle N_2(t)/N\propto t^{\tilde{\alpha}}$ and

$$\langle\Delta x^2(t)\rangle = N^{-1}\left[\sum_{j=1}^{N_1(t)}(x_{b,j}(t)-\langle x(t)\rangle)^2 + \sum_{j=1}^{N_2(t)}(x_{d,j}(t)-\langle x(t)\rangle)^2\right]\propto t^{2\tilde{\alpha}}, \qquad (4)$$

where $N_1(t)+N_2(t)=N$. Then the power is yielded as $2\tilde{\alpha}=3.25$ which is consistent with the previous fitting result of 3.34. The variation of α with F is actually due to the configuration of velocity distribution being either split or united.

In conclusion, we have explored the diffusive behavior of a particle in periodic potentials described by a generalized Langevin equation. There exhibits a wide range of diffusive regimes. This behavior, is much richer than that of the regular Brownian motion. When the temperature is sufficiently large, the particle driven by a thermal colored noise with the spectral density vanishing at zero-frequency exhibits a superdiffusive motion. A sub- or superohmic damping particle moving in a titled periodic potential allows either a running oscillated state or a mixing of the two states. Indeed, the power of superdiffusing system characterized by the mean square displacement as a function of time is enhanced twice near a critical titled force, because the velocity distribution presents a coexistence of two-bell shaped, corresponding to oscillating and moving particles, and the position distribution has a long tail. This implies that a wide anomalous diffusion with the power from zero to four can be realized in a titled periodic potential. The present result, a periodic structure not only enhances the diffusion constant but also changes the diffusive behavior of a system, and will open future studies.

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