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Diffusion of Brownian particles in a tilted periodic potential under the influence of an external Ornstein–Uhlenbeck noise

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ABSTRACT

The diffusion behaviors of Brownian particles in a tilted periodic potential under the influence of an internal white noise and an external Ornstein–Uhlenbeck noise are investigated through numerical simulation. In contrast to the case when the bias force is smaller or absent, the diffusion coefficient exhibits a nonmonotonic dependence on the correlation time of the external noise when bias force is large. A mechanism different from locked-to-running transition theory is presented for the diffusion enhancement by a bias force in intermediate to large damping. In the underdamped regime and the presence of external noise, the diffusion coefficient is a monotonically decreasing function of low temperature rather than a nonmonotonic function when external noise is absent. The diffusive process undergoes four regimes when bias force approaches but is less than its critical value and noises intensities are small. These behaviors can be attributed to the locked-to-running transition of particles.

1. Introduction

Much attention has been paid to the motion and diffusion of particles in a spatial periodic potential. The most common application of Brownian motion in a periodic potential is the diffusive dynamics of atoms and molecules on a crystal surface [1]. Surface diffusion in white noise and colored noise processes has been widely investigated [2–10]. The dynamics of Brownian particles in a tilted periodic potential is a basic nonequilibrium model of statistical physics that can be used to describes many physical systems, including a damped pendulum with torque [2], Josephson junctions [11], superionic conduction [12], charge-density wave [13], rotation of dipoles in an external field [14], phase-locking loop [15], diffusion on surface [16], and separation of particles by electrophoresis [17]. Various phenomena have been found in such a nonlinear stochastic system.

The diffusion of Brownian particles in a tilted periodic potential has been extensively studied. Successful analytical methods have been developed in over-damped case [18]. The giant enhancement of diffusion coefficient is found if the force is close to a critical value. This enhancement of diffusion becomes particularly pronounced under low temperatures, and the diffusion coefficient will diverge for $T \to 0$ if the bias force is exactly equal to its critical value. Numerical simulation has shown that when a Brownian particle driven by an internal white noise diffuses in a tilted periodic potential, an unusually large diffusion coefficient is exhibited in the underdamped regime [19], which is analyzed in terms of multiple jump statistics. Excess diffusion indicates the locked-to-running transition of Brwonian particles in the underdamped regime. Numerical simulations have shown that the diffusion coefficient exponentially increases with a drop in temperature in a certain interval of F [20]. This abnormal behavior is attributed to the exponential increase in velocity correlation time with inverse temperature when the temperature tends to zero. The underdamped motion of Brownian particles in tilted periodic potentials can be considered as overdamped motion in the velocity space in the effective double-well potential [21]. Simple analytical expressions for the mobility and diffusion coefficient have been derived and are in good agreement with numerical simulation results. Through numerical simulations with Langevin equations, the parameters regions for which the diffusion coefficient exponentially grows with inverse temperature have been identified in Ref. [22]. In addition, in the case of small bias forces close to the critical range, the diffusion coefficient presents a pronounced maximum as a function of temperature. These findings can be explained by means of the two-state theory of velocity. The anomalous diffusion behaviors of Brownian particles in a tilted periodic potential were investigated in Refs. [23–25]. Numerical simulations of a Brownian particle subjected to a thermal harmonic velocity noise show that the diffusion coefficient is enhanced and diffusive behavior is

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changed. Given that the curve of velocity distribution presents two peaks that corresponding to oscillating and moving particles, anomalous power is enhanced twice near the critical value of tilted force [23]. For a thermal non-Ohmic damping case, the locking state and the running state can coexist in the case of sup-Ohmic damping for moderate tilted force. The effective power index can be enhanced and is a nonmonotonic function of the temperature and the tilted force [24]. For Lévy noise and nonlinear friction case, the nonmonotonic behavior of the effective diffusion index and the superballistic diffusion are observed when the noise intensity is weak and the tilted force is close to its critical value [25]. Particles exist in either a running state or a long-tailed behind state in the spatial coordinate, the latter disintegrates into small pieces of the probability peaks. The distance between the above two-state centers increases with time and has a definitive role in superballistic group diffusion.

The diffusion of Brownian particles in a tilted periodic potential possesses rich phenomenology and should thus be further explored. In the present work, we study the diffusion of Brownian particles in a tilted periodic potential driven by an internal white noise and an external Ornstein-Uhlenbenck noise. The internal white noise model is commonly used in studies on this topic, and the external noise allows us to control the diffusion behavior through external means. Some features are identified through numerical simulations and their corresponding physical mechanisms are explored.

2. Definiteness and randomness

We consider a particle moving in a tilted periodic potential and subjected to an internal white noise and an external Ornstein–Uhlenbeck noise, which is governed by the following Langevin equation:

$$\dot{v} = -\gamma v - \frac{1}{m}\frac{\partial U}{\partial x} + \frac{1}{m}\xi(t) + \frac{1}{m}\varepsilon(t), \tag{1}$$

where the Ornstein–Uhlenbeck noise $\varepsilon(t)$ is the solution of the following equation

$$\dot{\varepsilon}(t) + \frac{1}{\tau}\varepsilon(t) = \zeta(t), \tag{2}$$

in which $\zeta(t)$ is a Gaussian white noise and τ is the correlation time of the Ornstein–Uhlenbeck noise. The correlation function of $\varepsilon(t)$ is given by

$$\langle \varepsilon(t)\varepsilon(s)\rangle = \frac{Q}{\tau}\exp\left(-\frac{|t-s|}{\tau}\right), \tag{3}$$

where Q denotes the external noise intensity. The internal Gaussian white noise $\xi(t)$ satisfies the following fluctuation–dissipation theorem

$$\langle \xi(t)\xi(s)\rangle = 2m\gamma k_B T\delta(t-s). \tag{4}$$

where γ denotes the damping coefficient, m is particle mass, k_B is the Boltzmann constant, and T is environmental temperature. The potential $U(x)$ is given by

$$U(x) = -U_0 cos(x) - Fx, \tag{5}$$

F is a constant bias force. The critical value F_c of the bias force is defined as the one at which the local potential minima just vanish, $F_c = U_0$.

We simulate the Langevin Eq. (1) with the second order Runge–Kutta algorithm, in which the accurate solution of $\varepsilon(t)$ is used. The natural units is taken, in which $k_B = 1, m = 1$. The number of test particles is taken as $N = 10^6$, and the time step is $dt = 10^{-2}$, or $dt = 10^{-3}$ for some cases, they locate in stationary region.

For usual parameter values (excluding the parameter scope discussed in the next section), the Brownian particles exhibit a normal diffusion for long times. The diffusion behavior of the Brownian particles can be described by diffusion coefficient, which is defined by

$$D = \lim_{t\to\infty}\frac{\langle [x(t) - \langle x(t)\rangle]^2\rangle}{2t}. \tag{6}$$

Figs. 1–4 illustrate the diffusion coefficient as functions of various parameters and the interplay of various parameters in the problem.

Brownian particle diffusion is continuous when the intensities of internal and external noises are larger. If bias force is absent, the periodic potential force can be regarded as locally linear as long as the noise intensities are not large, such that particle motion of the particle within a small time step can be viewed as local and the corresponding Langevin equation can be solved analytically. Substituting the correlation functions of the noises yields the approximate linear dependence of the diffusion coefficient on the noise intensities [26], as shown in Fig. 1. This is not the case, however, when a bias force is present. The larger noise component must be cut off asymmetrically to fulfill the local linearization condition, the noise correlation relations for all realizations are deviated, thus a deviation from linear dependence of the diffusion coefficient on noises intensities is observed.

When the bias force is larger, the diffusion coefficient exhibits a nonmonotonic dependence on the correlation time of the external noise τ (a nonmonotonic behavior of D on correlation time for thermal Ornstein–Uhlenbeck noise may be found in Ref. [27]). If we approximate the periodic potential barrier by a parabolic form, the asymptotic variances of position and velocity are given by [28]

$$\sigma_{xx}^2(t\to\infty) = \frac{Q(\gamma\tau+1)}{\gamma\omega_b^2(1+\gamma\tau-\omega_b^2\tau^2)} \tag{7}$$
$$\sigma_{vv}^2(t\to\infty) = \frac{Q}{\gamma(1+\gamma\tau-\omega_b^2\tau^2)}$$

they show a nonmonotonic dependence on the correlation time τ, which can qualitatively explain the nonmonotonicity of the diffusion coefficient as a function of τ. The asymptotic variances of position and velocity tend to infinite at some value τ_m, which can be used to estimate the position of the extremum of the diffusion coefficient in intermediate to large damping where the barrier crossing of particles is insensitive to the barrier shape. The estimated values are $\tau_m = 1.62$ and $\tau_m = 2.41$ ($\omega_b^2 = 1$) for the parameters used in Fig. 2, they close to the simulation results. The rapid extension of the probability wave packet indicates a rapid diffusion. When bias force is small or absent, the number of the particles in barrier region is small, and the increase of the diffusion coefficient in the barrier region for small τ can not compensate for the decreased diffusion in the potential well region given that the escape rate from a potential well is a decrease function of correlation time τ [29]. Thus the diffusion coefficient becomes a decrease function of τ, as shown in Fig. 2.

The diffusion coefficients remains as negative power functions of the damping coefficient in the presence of bias force and external noise (Fig. 3). The absolute values of the power index is less than 1 in the absence of bias force and external noise but is larger than 1 in the presence of bias force and external noise. Thus bias force and external noise can significantly promote diffusion in the underdamped region.

The diffusion coefficient exhibits a nonmonotonic dependence on the bias force F. The extremum becomes particularly pronounced as the damping coefficient γ decreases. For small γ, the diffusion enhancement by a bias force can be understood by the coexistence of a locked state and running state. The underdamped