

Multidimensional Effects on Diffusion of a Particle in Tilted Periodic Potentials

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Abstract

This study investigates the diffusive motion of a Brownian particle in a 2D tilted periodic potential, where bias force is exerted in the x direction. The dimension effect is revealed by simulating the Langevin equation. The diffusion coefficient in x and y directions is a nonmonotonic function of the bias force, and a massive enhancement is observed in x and y directions in comparison with the case without a tilt in x direction. The underlying physical mechanism is explored.

Keywords

Surface Diffusion, Tilted Periodic Potential, Dimensionality, Langevin Simulation

1. Introduction

Many physical situations can be described by the diffusion of a Brownian particle in a tilted periodic potential; such situations include Josephson junctions [1], rotating dipoles in external fields [2], rotation of molecules in solids [3], superionic conductors [4], charge density waves [5], mode locking in laser gyroscopes [6], diffusion of atoms and molecules on crystal surfaces [7], particle separation by electrophoresis [8]. For the diffusion of an overdamped Brownian particle in a tilted periodic potential, an exact analytical expression for the effective diffusion coefficient is derived for arbitrary potentials and arbitrary strengths of the thermal noise [9]. The effective diffusion coefficient in a critically tilted periodic potential may be, in principle, arbitrarily enhanced in comparison with the potential-free thermal diffusion. A study has shown that in the underdamped case the diffusion coefficient is increased exponentially by a decrease in temperature in a certain interval of bias force [10], which originates from the correlation time of velocity increases exponentially with an increase in the inverse tem-

perature. The nonmonotonic behavior of the effective diffusion index and superballistic diffusion are observed [11] when the noise intensity is weak and the external force is close to the critical value at which local minima of the potential just vanish. Lévy particles exist in either a running state or a long-tailed behind state, the distance at which the two-state centers increase with time plays a definitive role in superballistic diffusion. Langevin simulation has shown that for super-ohmic damping and certain parameters, the diffusive process of a particle in a tilted periodic potential sequentially undergoes four time regimes: thermalization, hyperdiffusion, collapse, and asymptotical restoration [12]. A reformational ballistic diffusive system is considered a marginal situation that does not exhibit the collapsed state of diffusion. The diffusion properties of a vibrational motor, in which an additional time-dependent driving brings the system out of equilibrium and the other time-periodic driving fills the role usually played by noise, are investigated in [13]. The diffusion coefficient exhibits a nonmonotonic function of bias force due to the coexisting attractors, and an enhancement of diffusion phenomenon was observed. The analytical form of the effective free energy function in the model of entropic resonance is changed with addition of a bias force in a periodic potential, as shown in [14].

For surface diffusion problem, at least two degrees of freedom are concerned. Several multidimensional effects have been investigated. Based on the previous research on one-dimensional periodic potential, this paper extends to two-dimensional, thus highlighting the innovation. Molecular dynamics simulations conducted based on the Bhatnagar-Gross-Krook model have shown that the x-y coupling suppresses a large proportion of long jumps causing a decrease in the diffusion coefficient for all values of damping [15]. This effect can be attributed to the narrowing of the saddles with respect to the well bottom. Two kinds of approximation schemes, namely quasi-2D approximation and effective potential approach, have been applied to predict the 2D diffusion rate of a particle [16]; the results of these schemes are qualitatively in agreement with the numerical results. The 2D diffusion rate constant over noise intensity shows a nonmonotonic behaviors function of noise intensity, in contrast to the monotonic behavior in 1D case [17] [18]. In the present work, the dimensional effect in a tilted periodic potential is investigated.

2. Model

We consider a Brownian particle diffusing in a 2D coupled periodic potential under the influence of Gaussian white noise; the particle is contact with a heat bath at temperature T which provides fluctuation and dissipation. The dynamics of the process is governed by the following Langevin equations

$$\begin{aligned}\dot{x} &= v_x, m\dot{v}_x + m\gamma v_x + \frac{\partial U}{\partial x} = f_x + \xi, \\ \dot{y} &= v_y, m\dot{v}_y + m\gamma v_y + \frac{\partial U}{\partial y} = \xi,\end{aligned}\tag{1}$$

where U is a 2D coupled periodic potential, given by

$$U = U(x, y) = u_0 [\cos x + \cos y] + u_1 \cos x \cos y, \quad (2)$$

and ξ is a zero mean Gaussian white noise satisfying the fluctuation-dissipation theorem

$$\langle \xi(t) \xi(t') \rangle = 2m\gamma k_B T \delta(t - t'), \quad (3)$$

where f_x is a constant force exerted in the x direction, m is the mass of the Brownian particle, γ is the damping coefficient, and k_B is the Boltzmann constant. The profile of the 2D tilted periodic potential

$V(x, y) = u_0 [\cos x + \cos y] + u_1 \cos x \cos y - f_x x$ is plotted in **Figure 1**. What we wish to investigate is the difference between the above-mentioned model and the 1D tilted periodic potential, and how the bias force in x direction f_x influences the diffusion in y direction.

3. Langevin Simulation Results and the Underlying Physical Mechanisms

Langevin and the Fokker-Planck equations are most popular approaches for investigating surface diffusion. Although several analytical methods for the solution of 1D Langevin and Fokker-Planck equations are available [19], making any analytical progress is usually difficult on a set of multidimensional coupled equations. We simulate the Langevin Equation (1) by the second-order Runge-Kutta algorithm. In the calculation, the natural unit ($m = 1$, $k_B = 1$), the dimensionless parameter $V_0 = 1$, and the time step $\Delta t = 10^{-3}$ are used. The results are stable for time steps in the vicinity of the one we used. The test particles start from the a potential well and have zero velocity. The number of test particles $N = 2 \times 10^5$ is used to describe the surface diffusion motion of a Brownian particle. A quantity of fundamental interest in surface diffusion is the diffusion coefficient, which is defined as

$$D = \lim_{t \rightarrow \infty} \langle (\Delta \bar{r}(t))^2 \rangle / 2dt = \lim_{t \rightarrow \infty} \left[\langle (\Delta x(t))^2 \rangle + \langle (\Delta y(t))^2 \rangle \right] / 2dt, \quad (4)$$

where d is the spatial dimension. The mean square displacement $\langle (\Delta \bar{r}(t))^2 \rangle$ reveals a good linear relation at long times.

Figure 2 shows the influence of the tilt in x direction on the diffusion in y direction. The purpose of this figure is twofold. First, it presents a comparison of cases with and without tilt. Second, it displays a nonmonotonic relation of the diffusion coefficient with the tilt. The diffusion coefficient increases when the bias force is exerted. The physical mechanism is as follows: the particle with a high velocity in y direction accelerates in x direction, leading to a much larger resultant velocity; consequently, the particle can across the potential barrier in y direction along a direction between x and y axes, and the running state in y direction is formed. The coexistence of the locked state and running state results in rapid diffusion. Such a physical picture is confirmed by the velocity distribution in y direction (**Figure 3**). We can see that the number of particles with high

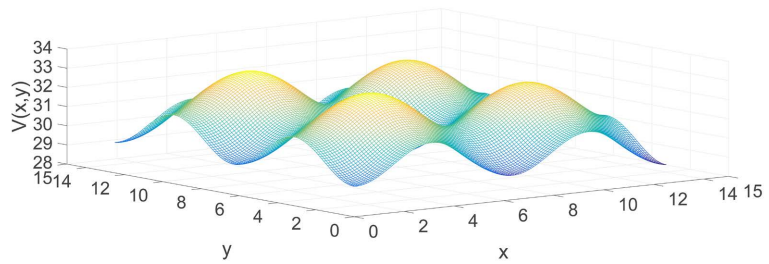


Figure 1. The profile of the 2D tilted periodic potential.

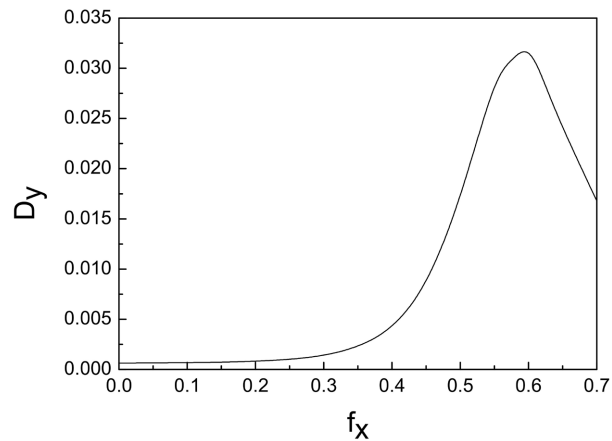


Figure 2. Diffusion coefficient in y direction versus the bias force in x direction. Where $T = 0.3$, $V_b = 1$, $\gamma = 0.2$.

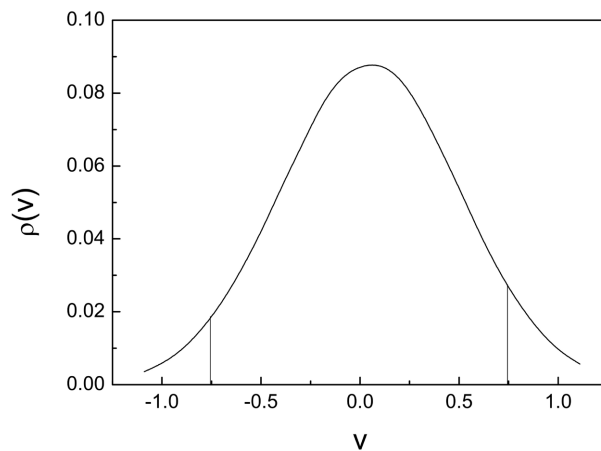


Figure 3. Velocity distribution in y direction. Where $T = 0.2$, $V_b = 1$, $\gamma = 0.2$, $f_x = 0.5$, and time $t = 300$.

positive velocities is obviously greater than that with negative values. The non-monotonic dependence on bias force can be explained as follows: as the bias force increases, the resultant velocities tend to x direction, and the number of particles in running state in y direction decreases gradually. These phenomena imply that the diffusion in one direction can be controlled by exerting a force in another direction. A comparison of the diffusion coefficient for x direction in two and one dimensions is shown in **Figure 4**. The dependence of the diffusion

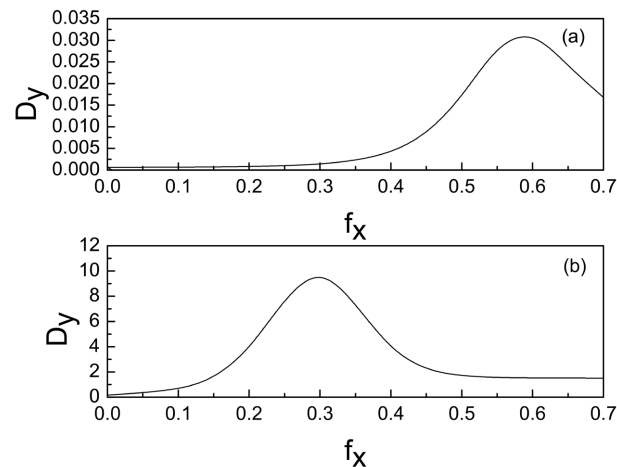


Figure 4. Diffusion coefficient in x direction versus the bias force in x direction. Where $T = 0.3$, $V_b = 1$, $\gamma = 0.2$, (a) for 2D case; (b) for 1D case.

coefficient on the bias force presents a nonmonotonic relation. In contrast to the diffusion coefficient arriving its maximum when $f_x < f_{xc}$ (f_{xc} is the critic tilt where the potential barrier vanishes, here $f_{xc} = 0.5$) in the 1D case, the maximum is achieved when $f_x > f_{xc}$ in two dimension case. The coexistence of the locked state and running state leads to a rapid diffusion, the locked state survives under $f_x > f_{xc}$ in the 2D case due to the diffusion in y direction and coexistence of the locked state and running state. The massive enhancement of the diffusion coefficient in x direction in the 2D case is attributed to the coexistence of the locked state and running state in y direction benefits the maintenance of locked state for x direction. For periodic potential without bias force, the particle wanders in various directions before it jumps along x direction, leading to a slower diffusion in the 2D case compared with that in the 1D case [15]. However, the rapid diffusion in tilted periodic potential in y direction that comes from the coexistence of locked state and running state benefits the maintenance of locked state for x direction. In addition, the coexistence of two states leads to rapid diffusion in medium to long periods.

4. Conclusion

We studied the diffusive motion of a particle moving in a 2D tilted periodic potential, where bias force is exerted in x direction. The diffusion coefficients were presented as nonmonotonic functions of bias force. The dimensionality is embodied in the interplay of the diffusion in x and y directions. Hence, it is possible to control the diffusion in one direction by applying force in the vertical direction. Bias force helps the particle form a running state in y direction, and leads to rapid diffusion, which benefits the maintenance of locked state in x direction, and leads to a rapid diffusion in this direction. The diffusion coefficient in x direction in the 2D tilted periodic potential exhibits massive enhancement compared with that in the 1D tilted periodic potential.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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