CHIN. PHYS. LETT. Vol. 33, No. 2 (2016) 020202

Giant Enhancement of Diffusion in a Tilted Egg-Carton Potential *

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(Received 20 October 2015)

Diffusion of a particle on a tilted periodic surface such as the egg-carton potential is investigated using Langevin Monte Carlo simulations. It is found that the effective diffusion coefficient of the particle related to the one-dimensional case can be greatly enhanced, when the local minima of such potential along the x and y directions are close to vanishing. A relation between the group diffusion and the phase diffusion is used to analyze the enhancement mechanism of the diffusion.

PACS: 02.50.Ey, 05.40.Fb DOI: 10.1088/0256-307X/33/2/020202

Diffusion processes of atoms, molecules, and clusters of molecules on surfaces have become subjects of research for many decades due to their intrinsic interest and technological importance. For instance, diffusion of a particle subjected to a white noise in a tilted periodic potential plays a prominent role in Josephson junctions,[1,2] rotating dipoles in an external field,[3] superionic conductor,[4] charge density waves,[5] diffusion on crystal surfaces,[6] particle separation by electrophoresis,[7] and biophysical processes such as intracellular transport,[8] and the Brownian motor and ratchet system.[9,10] The two-dimensional (2D) periodic case is also of particular relevance, where the adatom mobility in the surface plane controls the dynamics of many processes involving mass transport. A particular common way to manipulate diffusion of a particle is by means of a spatially periodic potential with a nonvanishing systematic component. This device is called the biased washboard potential or the corrugated plane.[11] Solid state surfaces frequently present such periodic potential marred by some disorders.[12]

The quantity of foremost interest in a periodic configuration is the effective diffusion coefficient ($D_{\rm eff}$) of the particle. In the one-dimensional (1D) case, which is determined by $D_{\rm eff} = \lim_{t\to\infty}\sigma^2(t)/(2\,t)$, where $\sigma^2(t) = \langle x^2(t)\rangle - \langle x(t)\rangle^2$ is the coordinate variance and the bracket denotes the average over trajectories. As one knows, the diffusion of this kind is weaker than that of the force-free case, due to the fact that the particle needs to surmount the potential barriers. However, if a constant external force is introduced into the periodic potential and approaches the critical value, which leads to the local minima of potential being close to vanishing, $D_{\rm eff}$ can be enhanced for several orders of magnitude larger than that of the force-free case.[12–15] An approximate expression of diffusion coefficient was preformed by Reimann[12] in the one-dimensional tilted periodic potential. There is an intuitive explanation for the phenomenon of diffusion enhancement.[13,15] The optimal matching between an external force and a noise-driven distribution occurs, that is, the peaks of spatial distribution scatter at the potential hills and are disintegrated into small pieces. Then the effective diffusion coefficient of the particle is subsequently measured by the envelope width of its spatial distribution. In a two-dimensional (2D) periodic surface such as a tilted egg-carton potential, can the effective diffusion coefficient of the particle be enhanced? What are new features and alternative understanding for the diffusion?

In this Letter, we use the Langevin Monte Carlo simulation to calculate the effective diffusion coefficient of a particle in a two-dimensional tilted periodic potential. The enhancement mechanism of diffusion is analyzed by using the relation between the group and phase diffusions.

We consider the diffusion of a particle subjected to a white noise in a tilted 2D periodic potential $V(x,y)$. The motion of the particle is described by the following Langevin equation

$$m\ddot{x} = -\gamma\dot{x} - \frac{\partial V(x,y)}{\partial x} + \xi_x(t), \tag{1}$$

$$m\ddot{y} = -\gamma\dot{y} - \frac{\partial V(x,y)}{\partial y} + \xi_y(t), \tag{2}$$

where m is the mass of the particle, γ is the friction coefficient, and $\xi_i(t)$ obeys $\langle\xi_i(t)\rangle$=0 and $\langle\xi_i(t)\xi_j(t')\rangle = 2\gamma k_{\rm B}T\delta_{ij}\delta(t-t')$ $(i = x,y)$, in which $k_{\rm B}$ is the Boltzmann constant and T is the temperature. The potential $V(x,y)$ is chosen as the tilted egg-carton potential[16,17]

$$V(x,y) = V_0(x,y) - F_x x - F_y y, \tag{3}$$

$$V_0(x,y) = -g_0\left[\cos\left(\frac{2\pi}{L}x\right) + \cos\left(\frac{2\pi}{L}y\right)\right] + g_1\cos\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}y\right), \tag{4}$$

where L is the characteristic length scale, F_x and F_y are the two projections of external force along the x and y directions, g_0 and g_1 are the amplitudes of the decoupled and coupled potential, respectively. In

*Supported by the National Natural Science Foundation of China under Grant Nos 11575024 and 11175021, and the Plan of Beijing College Students' Scientific Research and EntrePrenurial Action under Grant No 105820.
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the calculation, the dimensionless units ($k_B = 1$ and $m = 1$) as well as $L = 1$ and $\gamma = 1$ are used. The three varying parameters are g_0, g_1, and F_x or F_y.

When g_0 and g_1 are positive and $g_1 < g_0$, there are four minima at the corners of the cell, one central maximum, and the saddle points are at the midpoints of the edges. The difference between the potentials at minima and saddle points is equal to $E_b = 2(g_0 - g_1)$. When $g_1 = 0$, the potential is trivially decoupled and the 2D problem is reduced into the 1D one; when $g_0 = 0$ the potential is again decoupled but rotated by $\pi/4$ related to the x direction. Considering the symmetry of egg-carton potential for the two variables x and y, we choose $F_x/F_y = 1$ to produce the maximal diffusion.

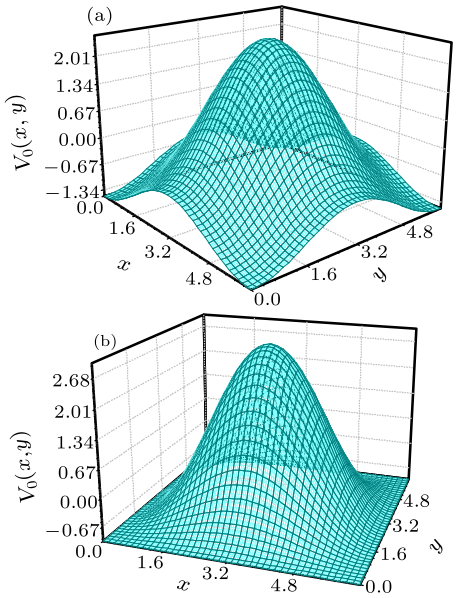

Fig. 1. The egg-carton potential within one period for various values of g_0 and g_1: (a) $g_0 = 1.0$ and $g_1 = 0.5$; and (b) $g_0 = 1.0$ and $g_1 = 1.0$.

In Fig. 1, we plot the potential $V_0(x, y)$, which looks like an egg carton and has a square symmetry. Notice that in the extreme case of very strong coupling, i.e., $g_1 = g_0$, as shown in Fig. 1(b), there exist flat passing channels around the center of egg-carton potential, thus there are potential energy differences between the saddle point and the potential minima along the channel vanish. The flat channel is propitious to mobility of the particle, while diffusion should not benefit from the configuration of this kind, due to the fact that the spatial distribution of the particle cannot be scattered into a series of small pieces without energy hills.

Similar to the 1D case, we define the effective diffusion coefficient of the particle in the 2D periodic potential as

$$D_{\text{eff}} = \lim_{t\to\infty} \frac{\langle x^2(t)\rangle - \langle x(t)\rangle^2 + \langle y^2(t)\rangle - \langle y(t)\rangle^2}{4t}. \quad (5)$$

The above quantity is the key quantity studied in the present work.

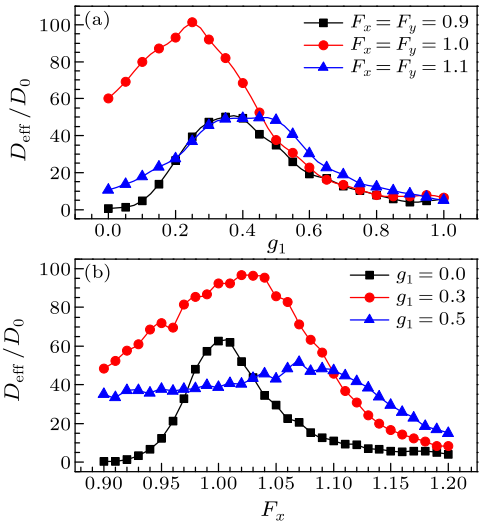

Fig. 2. The effective diffusion coefficient D_{eff}/D_0 as a function of g_1 (a) for various F_x or F_y; (b) for various g_1 at the fixed $g_0 = 1.0$.

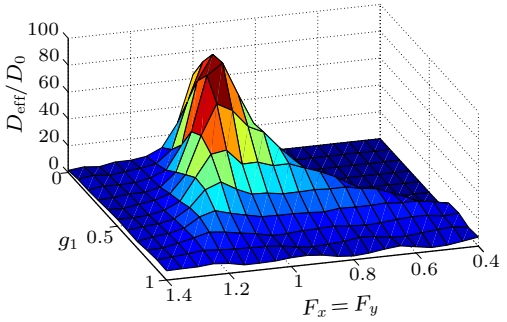

Fig. 3. A three-dimensional combining plot of Figs. 2(a) and 2(b).

In Figs. 2(a) and 2(b), we show the effective diffusion coefficient in units of D for various g_1 and F, respectively. For the present potential at a given g_0, its barrier height increases when g_1 decreases, which should expend the kinetic energy of the particle for diffusion, thus the particle diffuses with difficulty in the case of small g_1. This implies that the role of the parameter g_1 is to control the shape of the potential $V_0(x, y)$. When a constant external force is added, the particle surmounts easily the next barrier. In particular, the 2D periodic potential channel becomes flatter for large g_1, which is also detrimental to the fact that the peak of spatial distribution of the particle scats at the barrier and is disintegrated into a series of small pieces.

Upon inspection, we find a prominent result: there exists huge enhancement of diffusion of the particle on the tilted egg-carton surface, i.e., D_{eff} is increased to 1–2 orders of magnitude larger than that of the 1D case ($g_1 = 0$), when the parameters g_1 and F become optimum matching. This occurs under the condition that there are two critical channels with approximate vanishing potential barriers along the x and y direc-

tions. This is illuminated in Fig. 4.

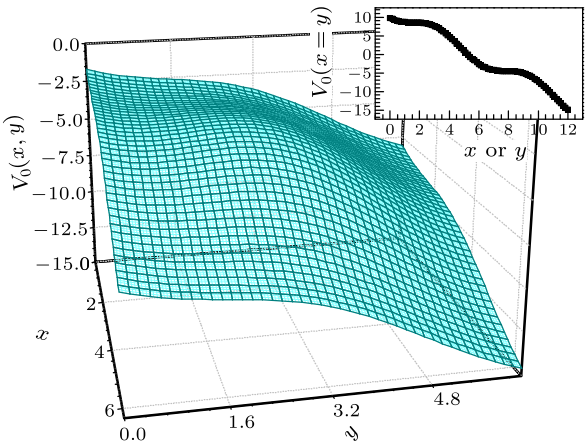

Fig. 4. The potential shape corresponding to the maximal diffusion. The parameters used are $g_0 = 1.0$, $g_1 = 0.3$, and $F_x = F_y = 1.02$.

In Fig. 3, we plot the effective diffusion coefficient of the particle as functions of both g_1 and F, simultaneously. We try to find the condition of maximal diffusion from this figure. It is seen that $D_{\rm eff}/D_0$ arrives at the maximal value for finite g_1 and F, where D_0 is the diffusion coefficient of the particle in the force-free case. This gives us a result that either the high potential barrier or the flat surface is worthless to the diffusion.

Figure 4 shows the corresponding potential shape when the effective diffusion coefficient of the particle becomes the maximal value, where the local minima of potential are close to vanishing along both the x and y directions. Due to the symmetry, the x direction has the same trend as the y direction as shown in Fig. 4.

To analyze the enhancement phenomenon of diffusion, we apply a relation between the group and phase diffusion coefficients in the one-dimensional case.[18] Assume that the spatial distribution of the particle along the x direction is composed of a number of sub-distributions $W_i(x,t)$, i.e.,

$$W(x,t) = C_1 W_1(x,t) + C_2 W_2(x,t) + \ldots + C_n W_n(x,t), \tag{6}$$

where $C_i > 0$ $(i = 1, 2, \ldots, n)$, $\sum_{i=1}^{n} C_i = 1$ and $\int_{-\infty}^{\infty} W_i(x,t)dx = 1$. The ith sub-distribution has the mean position $\langle x_i(t)\rangle$ and the variance $\sigma_i^2(t) = \langle x_i^2(t)\rangle - \langle x_i(t)\rangle^2$, thus the center position and the variance of the total distribution are given by

$$\langle x(t)\rangle = \sum_{i=1}^{b} C_i \langle x_i(t)\rangle, \tag{7}$$

$$\sigma^2(t) = \sum_{i=1}^{n} C_i \sigma_i^2(t) + \sum_{i\neq j}^{n} C_i C_j [\langle x_i(t)\rangle - \langle x_j(t)\rangle]^2. \tag{8}$$

The relation between the group diffusion coefficient $D_{\rm g}$ and the phase diffusion coefficient $D_{\rm p}$ is given by

$$D_{\rm g} = \lim_{t\to\infty} \frac{\sigma^2(t)}{2t} = D_{\rm p} + \lim_{t\to\infty} \sum_{i\neq j}^{n} C_i C_j \frac{[\langle x_i(t)\rangle - \langle x_j(t)\rangle]^2}{2t}, \tag{9}$$

where the phase diffusion coefficient is determined by

$$D_{\rm p} = \lim_{t\to\infty} \sum_{i=1}^{n} C_i \frac{\sigma_i^2(t)}{2t}. \tag{10}$$

In Fig. 5(a), we plot the probability density distribution (PDF) of coordinates of the particle along the x or y direction. It is found that the spatial PDF of the particle has been split into several small probability waves. Let us define the central position of the ith wave pack to be l_i; the distance between the near neighbor wave has the same length L. The pack of each sub-distribution is assumed approximately to be a Gaussian function: $W_i(x,t) = (2\pi\sigma_0^2(t))^{-1/2} \exp[-(x(t) - l_i)^2/(2\sigma_0^2(t))]$. The velocity PDF of the particle along the x or y direction is also depicted in Fig. 5(b). Upon inspection, we find that the velocity distribution of the particle has a nonzero-center and a long tail. This leads to a result that the test particles can be distributed in a wide range on the potential surface.

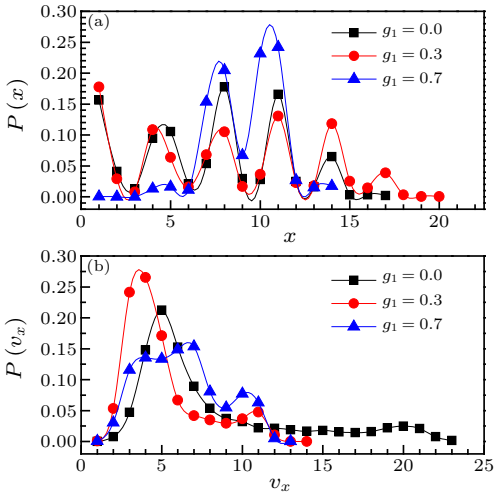

Fig. 5. The distribution density functions of the x-coordinate (a) and the v_x velocity (b) of the particle at time $t = 50$.

It is seen from Fig. 5(a) that the numbers of small sub-wave packs are 5, 6 and 2 for $g_1 = 0.0$, 0.3 and 0.7, which correspond to the maximal value of $D_{\rm eff}/D_0 = 63.12$, 93.84 and 13.22, respectively. According to Eq. (9), the larger the number of small sub-packs or the greater the distance between near neighbor packs is, the greater the effective diffusion coefficient is. Moreover, most test particles pass barriers through the first critical channel along the x or y direction for $g_1 = 0.3$, so as to form a wider envelope width of the whole distribution.

A large coupling coefficient g_1 results in the particle passing easily over potential barriers or arriving at a high velocity state. Comparing the results of $g_1 = 0.7$ and $g_1 = 0.0$, we find that even if there are only two sub-hills for the case of $g_1 = 0.7$, the two sub-hills are far away from the original point of the coordinate. In addition, the particle has a large velocity for $g_1 = 0.7$. When g_1 is taken to be a large value, the less the barrier is, the more the test particles pass over the potential barriers.

In summary, we have found a huge enhancement of diffusion of a particle in a tilted egg-carton potential, in which the effective diffusion coefficient of the particle can be enhanced into several orders of magnitude related to the one-dimensional case. This occurs under a condition that the local minima of potential are close to vanishing along the x and y directions. Thus the spatial distribution of the particle is easy to scatter into a number of small wave-packs at the potential hills. We have used a relation between the group diffusion and the phase diffusion to analyze the enhancement mechanism of diffusion, that is, the number of sub-wave packs and the distance between different probability peaks play a significant role to increase diffusion of the particle. The effects revealed in this work may be helpful for designing appropriate devices or adjusting the stochastic which can significantly enhance the diffusion.

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