Multidimensional and memory effects on diffusion of a particle

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The diffusion of an overdamped Brownian particle in the two-dimensional (2D) channel bounded periodically by a parabola is studied, where the particle is subject to an additive white or colored noise. The diffusion rate constant D^* of the particle is evaluated by the quasi-2D approximation and the effective potential approach, and the theoretical result is compared with the Langevin simulation. The properties of the diffusion rate constant are stressed for weak and strong noise cases. It is shown that, in an entropy channel, the value of D^* in units of Q decreases with increasing intensity of the colored noise. In the presence of energetic barriers, a nonmonotonic behavior of the reduced diffusion rate constant D^*Q^{-1} as a function of the noise intensity is shown.

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I. INTRODUCTION AND MODEL

The study of dynamical systems perturbed by various noise sources is of wide-ranging significance to the detailed understanding of transport processes and the characterization of nonlinear phenomena. In this context, the diffusion motion of a particle in a periodic potential is especially a long-standing theoretical problem of considerable interest. Restricting to the one-dimensional (1D) cases, one deals with an overdamped Brownian particle that is driven by a thermal white noise and moves in a sinuous potential [1], where the particle must climb over a periodic array of potential barriers, its diffusion rate constant D^*, measured by long time increase of the mean squared displacement, can be exactly expressed as an analytical formula [1] and is exponentially smaller than the free Brownian diffusion [2–4]. The most intensively studied phenomenon of noisy dynamics is that the coherent response of the system to an input signal can be enhanced by a noise, tending to be the maximal output at an optimal noise strength [5]. An enhancement of the diffusion coefficient has been recently observed in 1D rocked periodic potentials [6–8], where the particle is subject to both a thermal white noise and a time-periodic bias with an amplitude large with respect to the potential barriers.

In the absence of energy barriers, the white-noise-induced diffusion in a 2D periodic channel was considered in Ref. [9], where the particle should wander in before it is able to change its position, thus it takes long time to move in the unbounded direction. It has been demonstrated that the value of D^*Q^{-1} is independent of the noise intensity, and is determined by geometric structure of the potential. This 2D result is different from the 1D result of Refs. [10] and [11], the latter shows a monotonic behavior of the diffusion rate constant with the noise strength and reaches asymptotically saturation in the limit of $Q\to\infty$. Clearly, when a particle diffuses on a smooth surface, it is often the case that at least two degrees of freedom are strongly coupled. However, a systematic and theoretical understanding of the multidimensional effects is still not available.

Moreover, for more realistic physical systems, the consideration of the noise source with a finite correlation time has become a subject of current study [12,13]. Very recently there has been intense activity in the analysis of stochastically driven ratchets. These ratchets are spatially periodic systems where a spatial asymmetry in the potential imposes a directionality, and the memory effects may be from a temporarily correlated stochastic force (i.e., colored noise), thereby rectifying microscopic fluctuations to generate a directed particle drift. The applications of these concepts have been proposed as a possible explanation for the long-range cellular transport of the motor proteins [14]. So in a general way, the noise in the problem studied is nonwhite.

In this paper, we consider the diffusion process of an overdamped Brownian particle subjected to a white or colored noise, which moves in a two-dimensional coupled periodic potential $U(x,y)$ that is periodic in the x direction and parabolic in the y direction. The model is described by the following 2D Langevin equation written in a dimensionless form

$$\dot{x}(t)=-\frac{\partial U(x,y)}{\partial x}+\sqrt{2Q}\,\eta_x(t),$$

$$\dot{y}(t)=-\frac{\partial U(x,y)}{\partial y}+\sqrt{2Q}\,\eta_y(t), \tag{1}$$

where $\langle \eta_x(t)\rangle=\langle \eta_y(t)\rangle=0$, $\langle \eta_x(t)\eta_y(t')\rangle=\delta_{xy}k(|t-t'|)$, Q and $k(t)$ are the intensity and the correlation function of the noise, respectively. The potential is taken to be a coupled periodic channel,

$$U(x,y)=U_1(x)+\frac{1}{2}C(x)y^2, \tag{2}$$

with

$$U_1(x)=-U_{10}\sin(x),\quad C(x)=C_0[1-\lambda\sin(x+\phi)], \tag{3}$$

and $0\leqslant\lambda<1$, the periodic length of both $U_1(x)$ and $C(x)$ is equal to 2π. More nontrivially, in our potential the channel width is changed periodically.

For very large time the particle is distributed over many wells and its diffusion motion along the y direction is bounded, thus the diffusion rate constant of the particle is evaluated by

$$D=\frac{1}{2}\lim_{t\to\infty}\frac{1}{t}\langle[x(t)-x(0)]^2\rangle. \tag{4}$$

For the free Brownian motion, one can find that $D_{free}=Q$ is valid even in the colored noise cases as long as the gradient of the potential is position independent.

The coupled channel model may have a wide application [15–18], and one can represent the influence of the irrelevant degrees of freedom on the relevant part of the system. The present 2D problem also differs from the diffusion in the egg-carton potential [19] and the multiple hops of activated surface diffusion [20]. Here the dependence of the diffusion rate of a particle on the noise intensity will be nonmonotonic varying. Notice that the nonmonotonic phenomenon proposed in this work could be very useful in understanding the nature of completely symmetric periodic structures, as well as for applications such as noisy Josephson junction, mobility and diffusion of atoms in crystals, and supersonic conductivity.

II. MULTIDIMENSIONAL EFFECTS

For a 2D coupled periodic system, an exact expression for the overdamped diffusion is not available. However, it is possible to generalize the method leading to exact 1D results and to obtain an analytical 2D approximation. In a recent series of papers [21–23], the variational transition state theory for multidimensional activated rate processes have been developed intensively by Berezhovskii and co-workers, which will be the starting point of the present work. Indeed, the diffusion rate constant of a particle is connected to its mobility and the latter is determined by $\mu(F)=F^{-1}\langle\dot{x}\rangle=2\pi J/F$, in which F is an introduced constant force along the x axis and J is the probability current. In the absence of external driving force, the diffusion rate of the particle is thus given by the free diffusion constant multiplied by the mobility according to the linear response theory [1,8], i.e., $D^*=\mu(0)Q$. Notice that the value of $\mu(0)$ is finite because the current vanishes if $F=0$ for the symmetrical periodic potential (2) with Eq. (3).

Now, we consider the case of a white noise, thus $k(|t-t'|)=\delta(t-t')$. In the following, we treat two different approximate approaches. The first approach is called the "quasi-2D approximation." The variable y is assumed to play the role of a parameter, namely, the influence of y on the diffusion should be treated parametrically rather than oscillating. Assuming that at fixed y the diffusion of the particle along the x direction has been considered as being one dimensional, we carry out a y-dependent diffusion rate D_1^*,

$$D_1^*(y)=Q(2\pi)^2\left\{\int_0^{2\pi}\exp[-U(x,y)/Q]dx \times\int_0^{2\pi}\exp[U(x,y)/Q]dx\right\}^{-1}. \tag{5}$$

The mean diffusion rate of the particle equals the integration of y from $-\infty$ to ∞ for $D_1^*(y)$ within one spatial period,

$$D^*=\frac{\int_{-\infty}^{\infty}dy\int_0^{2\pi}dxD_1^*(y)P_{st}(x,y)}{\int_{-\infty}^{\infty}dy\int_0^{2\pi}dxP_{st}(x,y)}, \tag{6}$$

where the equilibrium distribution $P_{st}(x,y)$ reads [18,24–26],

$$P_{st}(x,y)=\exp[-U(x,y)/Q]. \tag{7}$$

Hence, the diffusion rate constant is finally predicted by

$$D^*=Q\frac{\int_{-\infty}^{\infty}dy\left\{\int_0^{2\pi}dx\exp[U(x,y)/Q]\right\}^{-1}}{\int_{-\infty}^{\infty}dy\int_0^{2\pi}dx\exp[-U(x,y)/Q]}. \tag{8}$$

If the potential shape is chosen to be the form of Eqs. (2) and (3), we can rewrite Eq. (8) as

$$D^*=Q\frac{\int_{-\infty}^{\infty}dy\exp(-\frac{1}{2}C_0y^2)I_0^{-1}(z)}{\int_{-\infty}^{\infty}dy\exp(-\frac{1}{2}C_0y^2)I_0(z)}, \tag{9}$$

with

$$z=z(y)=\left\{h^2+\left(\frac{1}{2}C_0\lambda y^2\right)^2+hC_0\lambda y^2\cos(\phi)\right\}^{1/2}, \tag{10}$$

where $h=U_{10}/Q$ and I_0 is the modified Bessel function of zeroth order.

For the decoupling cases ($\lambda=0$), $D^*=QI_0^{-2}(h)$, leading to

$$\frac{\partial(D^*Q^{-1})}{\partial Q}=2hI_1(h)I_0^{-3}(h)\geqslant 0, \tag{11}$$

where I_1 is the modified Bessel function of the first order. So that the 1D diffusion rate in units of Q is an increasing function of the noise intensity and reaches asymptotically a constant $\lim_{Q\to\infty}D^*=Q$. Further, in the absence of energy barriers, the diffusion rate times the inverse of the noise intensity is reduced to

$$D^*Q^{-1}=\frac{\int_{-\infty}^{\infty}\exp(-\tfrac{1}{2}C_0y^2)dyI_0^{-1}(\tfrac{1}{2}C_0\lambda y^2)}{\int_{-\infty}^{\infty}\exp(-\tfrac{1}{2}C_0y^2)dyI_0(\tfrac{1}{2}C_0\lambda y^2)}, \quad (12)$$

which is a Q-independent constant.

The second approximation is the ''effective potential approach'' (EPA). In the EPA, the 2D problem is simplified to the 1D problem with a reduced potential $V_1(x)$ through eliminating the variable y [18,19,21]. We integrate over y from $-\infty$ to ∞ in the equilibrium distribution (7), thus the reduced potential is given by

$$V_1(x)=-Q\ln\left\{\int_{-\infty}^{\infty}dy\exp[-U(x,y)/Q]\right\}$$
$$=U_1(x)+\frac{1}{2}Q\ln\left[\frac{C(x)}{2\pi Q}\right]. \quad (13)$$

The diffusion rate constant can be written as

$$D^*=Q(2\pi)^2\left\{\int_0^{2\pi}\exp[-V_1(x)/Q]dx\right.$$
$$\left.\times\int_0^{2\pi}\exp[V_1(x)/Q]dx\right\}^{-1}$$
$$=Q(2\pi)^2\left\{\int_0^{2\pi}\frac{1}{\sqrt{C(x)}}\exp[-U_1(x)/Q]dx\right.$$
$$\left.\times\int_0^{2\pi}\sqrt{C(x)}\exp[U_1(x)/Q]dx\right\}^{-1}. \quad (14)$$

According to Schwarz's inequality, we have

$$\left(\frac{1}{2\pi}\int_0^{2\pi}\frac{dx}{\sqrt{C(x)}}\right)\left(\frac{1}{2\pi}\int_0^{2\pi}\sqrt{C(x)}dx\right)$$
$$\leqslant\left[\frac{1}{2\pi}\int_0^{2\pi}\frac{C^{1/4}(x)}{C^{1/4}(x)}dx\right]^2=1. \quad (15)$$

This means that the asymptotic value of the 2D diffusion rate constant is always not larger than that of the 1D one, since $\lim_{Q\to\infty}D^*=Q$ for the 1D case. Oppositely, when Q is much smaller than the barrier height E_b of the potential $U_1(x)$, the saddle point method approximates the formula (14) as

$$D^*=Q\sqrt{\frac{C(x_0)}{C(x_b)}}\exp(-E_b/Q), \quad (16)$$

here x_0 and x_b denote the coordinates of the minimum and maximum of the potential $U_1(x)$. It is noticed that the 2D diffusion rate should be larger than the 1D diffusion rate, if $C(x_b)<C(x_0)$. Namely, the presence of an x-y coupling can make the diffusion of the particle more rapid at low noise intensities.

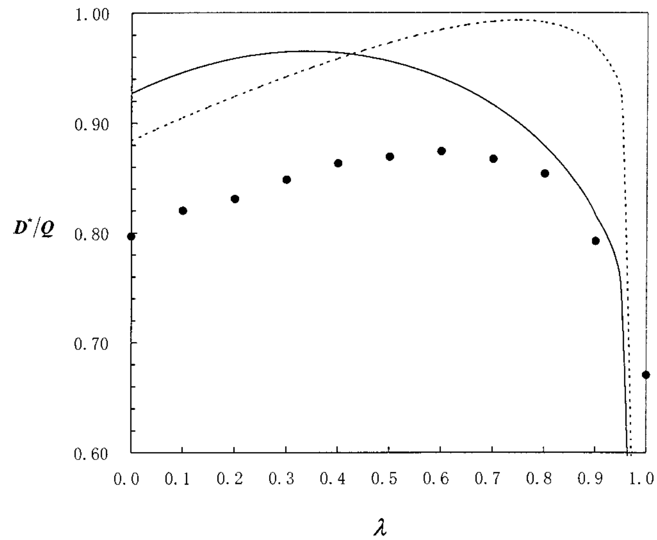

FIG. 1. Dependence of D^*Q^{-1} on the coupling λ at fixed $Q=2.0$, $\tau_c=0$, and $\phi=\pi$. The black dots correspond to the Langevin simulation, the dash-dotted line to the EPA and the solid line to the quasi-2D approximation.

It is straightforward to simulate numerically a set of Langevin equations in terms of the predictor-corrector algorithm [25,26]. If initially the particles are at $x(0)=\pi/2$ and $y(0)=0$ they will diffuse to adjacent wells. In the following calculations, the fixed parameters are $U_{10}=1$ or 0, $C_0=1$, and $\phi=\pi$ except in Figs. 2 and 3, as well as the time step of integrating Langevin equations, $\Delta t=10^{-2}$, the diffusion time takes $t=200$, and number of the test particles is $N=2000$.

Let us compare the approximations with the accurate numerical result. In Fig. 1, the quasi-2D approximation corresponds to the solid line, the EPA to the dash-dotted line and the points are the numerical data. It is seen that the EPA is simple and shows right behavior of the diffusion rate constant for weak coupling. The quasi-2D approximation should predict better result for strong coupling, this is due to the minima and the saddle points of the potential (2) with Eq. (3) lying on a straight line, i.e., $y=0$.

The value of $\ln(Q/D^*)$ as a function of Q^{-1} is plotted in Figs. 2(a) and 2(b) by means of the quasi-2D approximation and the EPA, and compared with the Langevin simulation at fixed coupling parameter $\lambda=0.8$. A linear behavior is expected in the case of small Q. It is seen that, if the Arrhenius limit is reached, the plot should be linear with a slope that represents the barrier height. For the $\sin(x)$ potential the barrier height is equal to 2, both Figs. 2(a) and 2(b) show a slope of 2. Also, it is observed that the above two kinds of theoretical predictions are good in agreement with the numerical result for the week noise case. In addition, in the Arrhenius limit, the formula (16) has described correct behavior of the reduced diffusion rate constant for different values of ϕ.

In the presence of energy barriers, the full 2D diffusion rate D^*Q^{-1} as a function of Q for different ϕ is shown in Fig. 3. As a consequence, a new nonmonotonic behavior is observed. At intermediate noise intensities, the value of

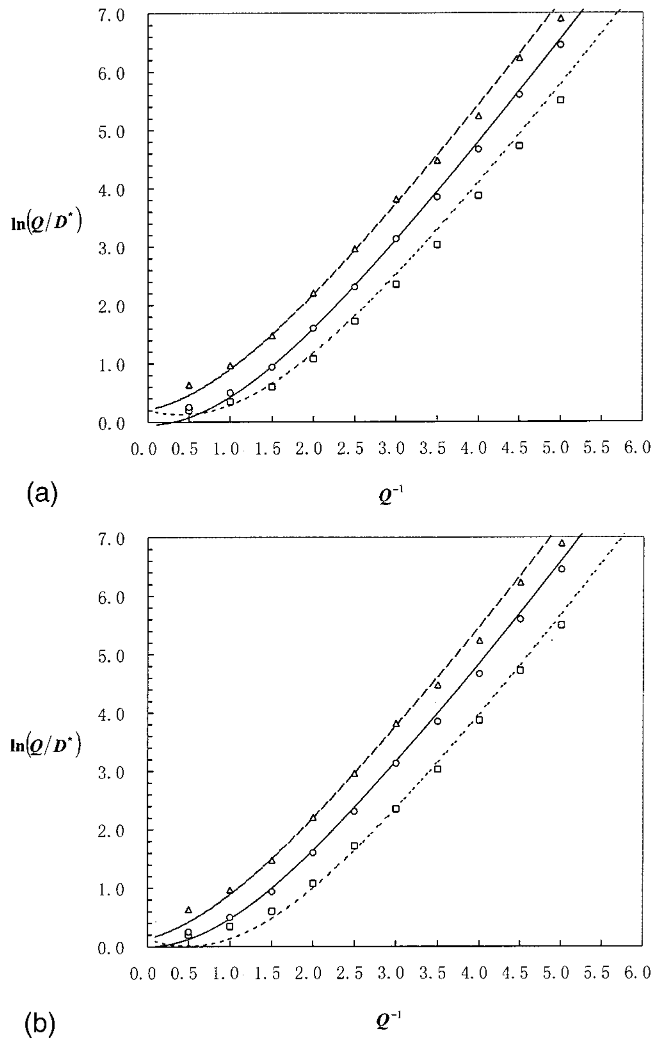

FIG. 2. Arrhenius plot of the reduced diffusion rate at fixed $\lambda=0.8$ and $\tau_c=0$. The dots correspond to the numerical results; the lines to the quasi-2D approximation [Eq. (9)] in (a) and the EPA in (b) [Eq. (14)]. The solid line and circles correspond to the 1D; the dashed line and triangles to the 2D with $\phi=\pi/4$; and the dotted-dashed line and squares to the 2D with $\phi=\pi$.

D^*Q^{-1} is larger than that of the limits of $Q\rightarrow 0$ and $Q\rightarrow\infty$. Thus the reduced diffusion rate constant has a local maximum for a value of the noise intensity of the order of the barrier height of the energetic potential. This phenomenon opens interesting perspectives, e.g., to manipulate reaction-diffusion system.

Moreover, the condition of the nonmonotonic behavior of D^*Q^{-1} can be observed in Fig. 3. We derive the following expressions from Eq. (12),

$$\frac{\partial(D^*Q^{-1})}{\partial Q}=\frac{1}{Z^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dy\,d\overline{y}\times\exp\left[-\frac{C_0}{2}(y^2+\overline{y}^2)\right]\cdot\left\{-\frac{I_1(u)}{I_0^2(u)}I_0(v)\frac{\partial u}{\partial Q}-\frac{I_1(v)}{I_0(u)}\frac{\partial v}{\partial Q}\right\}, \tag{17}$$

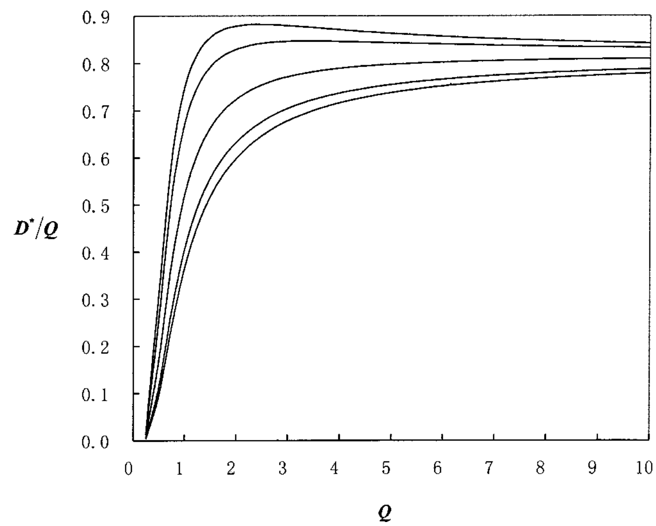

FIG. 3. The 2D reduced diffusion rate calculated by Eq. (9) as a function of Q at fixed $\lambda=0.8$, $\tau_c=0.0$, as well as for different $\phi=\pi$, $\pm\frac{3}{4}\pi$, $\pm\frac{1}{2}\pi$, $\pm\frac{1}{4}\pi$, and 0 from top to bottom.

where

$$Z=\int_{-\infty}^{\infty}dy\,\exp\left[-\frac{1}{2}C_0y^2\right]I_0(u), \tag{18}$$

$u=z(y)$, $v=z(\overline{y})$, and

$$\frac{\partial u}{\partial Q}=-\frac{1}{Qu}[h^2+hC_0\lambda y^2\cos(\phi)],$$

$$\frac{\partial v}{\partial Q}=-\frac{1}{Qv}[h^2+hC_0\lambda\overline{y}^2\cos(\phi)]. \tag{19}$$

The values of $\partial u/\partial Q$ and $\partial v/\partial Q$ could become zero and thus $\partial(D^*Q^{-1})/\partial Q=0$ at a finite noise strength Q_m, if $\cos(\phi)<0$, i.e., $\frac{1}{2}\pi<\phi<\frac{3}{2}\pi$.

III. THE ROLE OF COLOR OF NOISE

Now we investigate the diffusion induced by an Ornstein-Uhlenkeck noise (OUN), i.e., $k(|t-t'|)=\tau_c^{-1}\exp[-|t-t'|/\tau_c]$, where τ_c is the correlation time of the colored noise. In the case of weak colored noise, namely, the correlation time τ_c is much smaller than the diffusion time, the current satisfies the Fokker-Planck equation [14],

$$J_i=\frac{\partial U}{\partial q_i}P-\frac{\partial}{\partial q_i}[\Theta_i P]\quad(q_i=x,y),$$

$$\Theta_i=D\left[1+\tau_c\mu_1^iM_{ii}-\frac{\tau_c^2}{2}\mu_2^i(R-M^2)_{ii}+O(\tau_c)^3\right], \tag{20}$$

where the matrix elements $M_{ij}=-\partial^2U(x,y)/\partial q_i\partial q_j$, $R_{ij}=\Sigma_k(\partial U/\partial q_k)(\partial^3U/\partial q_i\partial q_j\partial q_k)$, and μ_1^i and μ_2^i are the first and second moments, respectively, of the correlation function k. The role of color of the noise is thus to make the effective noise intensity position dependent. However, for any small correlation time there is a value of y such that Θ_i is negative. So the above treatment [Eq. (20)] should not apply to the present coupled periodic potential (2).

In order to predicate the diffusion rate constant of the particle induced by the OUN, we integrate over y from $-\infty$ to ∞ for the equilibrium distribution [Eq. (7)] if color of the noise is not considered, and then the colored effects [27,28] of the noise are introduced through an effective potential. Simpler to the 1D case, we solve the mobility $\mu(0)$ of the stationary solution for the 1D effective Fokker-Planck equation with a small τ_c [1,29–31]. The diffusion rate constant is written as

$$D^* = Q(2\pi)^2 \left\{ \int_0^{2\pi} g^{-1}(x,\tau_c)\exp[-\Phi_{eff}(x)/Q]dx \times \int_0^{2\pi} \exp[\Phi_{eff}(x)/Q]dx \right\}^{-1}, \tag{21}$$

where the effective potential Φ_{eff} is given by

$$\begin{aligned}\Phi_{eff}(x) &= \int^x V_1'(\bar{x})g^{-1}(\bar{x},\tau_c)d\bar{x} = V_1(x) + \frac{1}{2}\tau_c[V_1'(x)]^2 \\ &= U_1(x) + \frac{1}{2}Q\ln\left[\frac{C(x)}{2\pi Q}\right] \\ &\quad + \frac{1}{2}\tau_c\left\{U_1'(x) + \frac{1}{2}Q\frac{C'(x)}{C(x)}\right\}^2,\end{aligned} \tag{22}$$

and

$$g(x,\tau_c) = \frac{1}{1+\tau_c V_1''(x)}. \tag{23}$$

Here, $\Phi_{eff}(x)$ depends on the noise intensity Q. It is found from Eq. (22) that the barrier height of $\Phi_{eff}(x)$ increases with increasing noise intensity in the absence of energetic potential ($U_1=0$), thus this potential can be called an entropy channel. It is true that $D^*(\tau_c \neq 0) < D^*(\tau_c=0)$ according to Eqs. (21) and (22).

In the absence of energy barriers, the reduced diffusion rate constant is expressed by

$$\begin{aligned}D^*Q^{-1} = (2\pi)^2 \Bigg\{ \int_0^{2\pi} &\left\{1+\frac{1}{2}\tau_c Q[C'(x)/C(x)]'\right\} C(x)^{-1/2} \\ &\times \exp\left\{-\frac{\tau_c}{8}Q[C'(x)/C(x)]^2\right\}dx \\ &\times \int_0^{2\pi} C(x)^{1/2}\exp\left\{\frac{\tau_c}{8}Q[C'(x)/C(x)]^2\right\}dx \Bigg\}^{-1}.\end{aligned} \tag{24}$$

Note that the value of D^*Q^{-1} decreases and then vanishes when $Q\to\infty$, because the height of the entropy barrier is proportional to the noise intensity Q, and the occurrence of the maximum of this quantity appears in the limit of zero Q, $\lim_{Q\to\infty}(D^*Q^{-1}) < (D^*Q^{-1})|_{Q=0}$. Further, it is easy to prove that $\partial(D^*Q^{-1})/\partial Q < 0$.

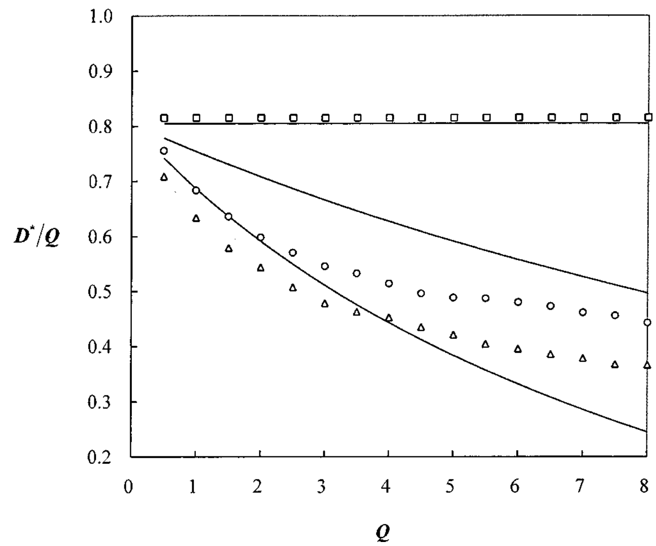

FIG. 4. Dependence of D^*Q^{-1} on Q in the absence of energy barriers ($U_{10}=0$) at fixed $\lambda=0.9$, $\phi=\pi$ and for three values of $\tau_c=0$, 0.2, and 0.5 from top to bottom. The dots are the Langevin simulations and the solid lines to the EPA [Eq. (21)].

We stress that, for our model, the stronger the colored noise, the higher is the entropy barrier. In the absence of energy barriers, the diffusion rate constant as a function of the noise intensity for different τ_c is plotted in Fig. 4. Of particular interest is the dependence of the reduced diffusion rate on the intensity of the colored noise, namely, the value of D^*Q^{-1} decreases with the increase of either Q or τ_c. This implies that the parameters Q and τ_c have the same influences on D^*Q^{-1}. However, the reduced diffusion rate of the particle is a constant and depends only on geometric structure of the periodic channel for the 2D white noise case [9]. Here, the existence of a vanishing asymptotic value of D^*Q^{-1} indicates the occurrence of a phenomenon of the inhibition diffusion.

The noise-intensity dependence of the full 2D reduced diffusion coefficient shown in Fig. 5 is nonmonotonic. Because all motion freezes as $Q\to 0$, while as $Q\to\infty$ the entropy channel exerts much influence on the diffusion of the particle, in particular, in the latter case a large energy is transferred to the y degree of freedom from the diffusion direction [20]. For the fixed coupling parameter λ and phase difference ϕ, the peak position changes slightly with the noise correlation time τ_c, and the value of the maximum D^*Q^{-1} decreases monotonically with the increase of τ_c.

Finally, the effective potential $\Phi_{eff}(x)$ is plotted in Fig. 6. The nonmonotonic property of the reduced diffusion rate in the 2D coupled periodic channel can be understood well through the notion of a Q-dependence barrier $E_{b,eff}$ for the 1D effective potential (22). Here, a minimum of $E_{b,eff}$ corresponding to a maximal value of D^*Q^{-1} is always a direct signature for the nonmonotonic behavior of the reduced diffusion coefficient with the noise intensity.

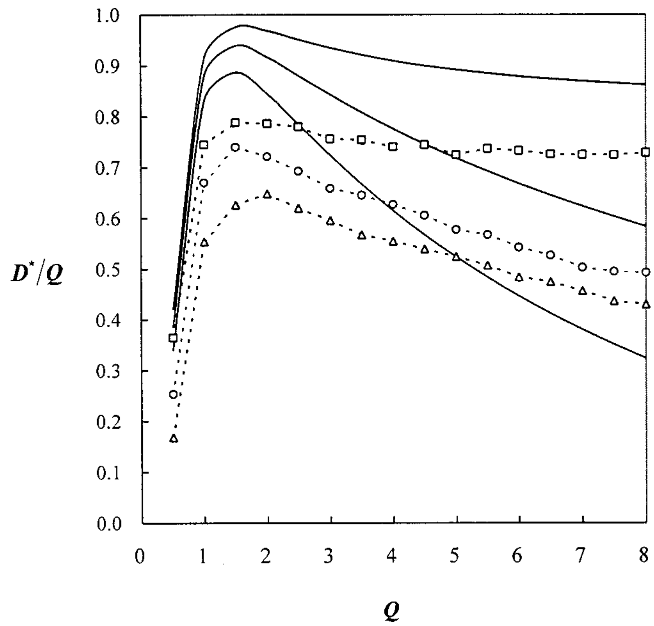

FIG. 5. The 2D reduced diffusion rate as a function of Q at fixed $\lambda=0.9$, $\phi=\pi$ and for different $\tau_c=0$, 0.2, and 0.5 from top to bottom. The dots correspond to the Langevin simulations and the solid lines to the EPA [Eq. (21)].

IV. CONCLUSIONS

The motivation of the present work was twofold. First, we apply two kinds of approximate schemes to predicate the two-dimensional diffusion rate of a particle driven by a white or colored noise, which is qualitatively in agreement with the numerical result. Second, the dependence of the reduced diffusion rate constant on the parameters of the model is discussed, thus we can perform from energy-controlled to external parameters-controlled diffusion.

Activated diffusion is restricted to low noise intensities or high energy potential barriers, however, unactivated diffusion can occur in a periodic entropy potential. The latter phenomenon is due to the fact that the energy is transferred to the irrelevant degree of freedom from the diffusion path of the system. Different from the previous studies, here in the absence of energy barriers, the 2D reduced diffusion rate constant is a decreasing function of the intensity Q of the colored noise and vanishes asymptotically in the limit of $Q \to \infty$. Moreover, the increase of either the correlation time of the colored noise or the coupling strength between the two degrees of freedom makes this effect observable.

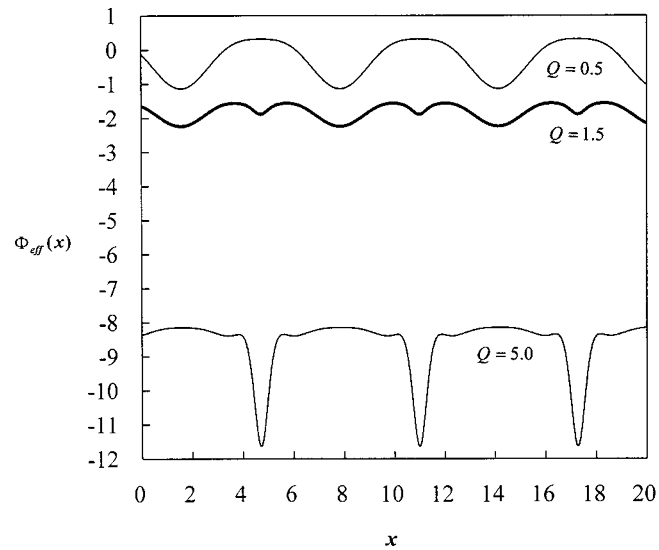

FIG. 6. Plot of the effective potential $\Phi_{eff}(x)$ [Eq. (22)] for different noise intensities. The parameters used are $\tau_c=0.5$ and $\lambda=0.8$.

In the presence of energy barriers, the 2D reduced diffusion rate constant as a function of the noise intensity shows a nonmonotonic behavior.This can be well understood from an idea of the effective potential. The barrier height $E_{b,eff}$ of this potential is a nonmonotonic function of the noise intensity, and a minimal value of $E_{b,eff}$ may exist at a finite noise intensity, which corresponds to a maximum of the reduced diffusion rate constant.

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