Nonmonotonic behavior of mobility in a multidimensional overdamped periodic system

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The mobility motion of an overdamped particle subjected to a thermal white noise in a multidimensional coupled periodic potential tilted by a constant force is studied. An approximate expression for the mean velocity of the particle is obtained on the assumption that nontransport variables play the roles of parameters, and the theoretical prediction is compared with a Langevin simulation. It is observed that the two-dimensional mean velocity can be a nonmonotonic function of the temperature when the curvature of the potential at the barriers is less than that at local minima. Moreover, the peak of mean velocity drifts toward low temperatures and becomes sharper if a third degree of freedom is introduced.

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I. INTRODUCTION

The problem of Brownian motion in periodic potentials arises in several fields of science. Restricted to one-dimensional cases, one deals with particles that are subject to a thermal white noise and move in a washboard potential [1]. In a broad sense, the nonmonotonic behavior of the output signal as a function of some characteristics of the noise is a theoretical problem of considerable interest [2]. Recently, some authors have focused attention on the behaviors of the output signal in a symmetrical periodic potential [3–10], which might be the mobility velocity of the particle along the direction of external force, as a function of the noise intensity, namely, the temperature of the heat bath. It has been concluded that nonmonotonic behavior of the mobility with noise intensity cannot be observed in one-dimensional overdamped cases if the particle is subject to a time-independent external force [5,6]. Because the particles must climb over a periodic array of potential barriers, the steady velocity of the particles saturates for large noise intensity. However, Marchesoni [6] argued that the constant driving force can induce resonantlike mobility in the underdamped case. Dan *et al.* [9] claimed that this phenomenon occurred in a washboard potential in an inhomogeneous overdamped medium. For the above two cases, the inertia of the particle or the coordinate-dependent friction could act as a surrogate for an external oscillating field. On the other hand, the net current of a particle in a rocking ratchet becomes a peaked function of the noise intensity [11], in which the local symmetry of the periodic potential is broken and the driving force is a periodic function of time.

In the present paper, we observe and show the nonmonotonic dependence of the mean velocity of an overdamped Brownian particle with respect to the noise intensity, where the particle is moving in a multidimensional coupled symmetric periodic potential biased by a uniform constant force. This resonancelike phenomenon could be very useful in understanding the nature of completely symmetric periodic structures and in construction of devices, as well as for applications such as noisy Josephson junctions, mobility and diffusion of atoms in crystals, and supersonic conductivity.

II. MODEL

The mobility motion of an overdamped Brownian particle is described by a set of Langevin equations (in rescaled units)

$$\dot{q}_i(t) = -\frac{\partial U(q_1, q_2, \ldots, q_N)}{\partial q_i} + F\delta_{i1} + \sqrt{2T}\,\eta_i(t), \tag{1}$$

with

$$\langle \eta_i(t)\rangle = 0, \quad \langle \eta_i(t)\eta_j(t')\rangle = \delta_{ij}\delta(t-t'), \tag{2}$$

and $i,j = 1,2,\ldots,N$. Here F is a constant force along the q_1 direction and the temperature T is the intensity of the white noise η_i.

The potential $U(q_1,q_2,\ldots,q_N)$ is a periodic function of q_1 with period L, i.e., $U(q_1+L,q_2,\ldots,q_N) = U(q_1,q_2,\ldots,q_N)$, and, because the drift velocity of the particles must be bound, we require that $U(q_1,q_2,\ldots,q_N) \to \infty$ when $q_i \to \pm\infty$ $(i \geqslant 2)$. Here the potential is taken to have the form

$$U(q_1,q_2,\ldots,q_N) = U_1(q_1) + \frac{1}{2}\sum_{i=2}^{N} C_i(q_1)q_i^2. \tag{3}$$

The energetic activation potential $U_1(q_1)$ and the curvature functions $C_i(q_1)$ have the same period L [12], and the latter are positive everywhere. For any given q_1, a slice of the potential along each q_i direction $(i \geqslant 2)$ is a parabola, and this parabola becomes wider and narrower periodically.

The N-dimensional Fokker-Planck equation (FPE) corresponding to the Langevin equation (1) can be written as the continuity equation

$$\frac{\partial \rho(q_1,q_2,\ldots,q_N)}{\partial t} + \sum_{i=1}^{N}\frac{\partial J_i}{\partial q_i} = 0, \tag{4}$$

where the probability current J_i is defined by

$$J_i = -\left(\frac{\partial U}{\partial q_i} - F\delta_{i1}\right)\rho - T\frac{\partial}{\partial q_i}\rho. \tag{5}$$

Unfortunately, there does not exist an exact solution of the probability current for coupled cases. Now we use the ''quasimultidimensional approximation'' [13] to provide a prediction for the mean velocity of the particle in the stationary state, i.e., one first keeps q_i ($i \geqslant 2$) fixed and then integrates over these variables. Assuming that at fixed q_i ($i \geqslant 2$) the mobility motion of the particle in the q_1 direction can be treated as one dimensionasl (1D), J_1 must be q_1 independent as in the 1D case, that is, $J_1 = J_1(q_2, q_3, \ldots, q_N)$. Letting the variables q_i ($i = 2,3, \ldots, N$) play the roles of ($N-1$) parameters, we obtain the stationary solution of the FPE as if it is one dimensional and construct the probability current J_1 along the q_1 direction from Eq. (5) [1,13,14],

$$J_1(q_2,q_3,\ldots,q_N) = \frac{T[1-\exp(-FL/T)]}{\int_0^L dq_1 \exp[-\Psi(q_1,q_2,\ldots,q_N)/T] \int_{q_1}^{q_1+L} dq_1' \exp[\Psi(q_1',q_2,\ldots,q_N)/T]}, \tag{6}$$

with

$$\Psi(q_1,q_2,\ldots,q_N) = U(q_1,q_2,\ldots,q_N) - Fq_1. \tag{7}$$

The total current equals the integration of J_1 over all q_i ($i \geqslant 2$) within one spatial period of q_1 because $\overline{J_i} = 0$ ($i \neq 1$). So

$$\overline{J} = L^{-1}\langle \dot{q}_1 \rangle = \overline{J_1} = \int_0^L dq_1 \left(\prod_{i=2}^{N} \int_{-\infty}^{\infty} dq_i \right) J_1(q_2,q_3,\ldots,q_N)\rho(q_1,q_2,\ldots,q_N). \tag{8}$$

Here the distribution function ρ is given approximately by $\rho^{(0)}$ in the equilibrium state [13], i.e.,

$$\rho(q_1,q_2,\ldots,q_N) = \rho^{(0)}(q_1,q_2,\ldots,q_N) = \frac{\exp[-\Psi(q_1,q_2,\ldots,q_N)/T]}{\int_0^L dq_1 \left(\prod_{i=2}^{N} \int_{-\infty}^{\infty} dq_i \right) \exp[-\Psi(q_1,q_2,\ldots,q_N)/T]}. \tag{9}$$

Clearly, the total particle current determined by Eq. (8) can be reduced to one dimension when all curvature functions of the potential along nontransport degrees of freedom are equal to constants. In general, one needs to evaluate the multi-integrals in Eq. (8) numerically. I should like to remark that the above quasimultidimensional approximation is expected to give good results when the minima and the saddle points lie on straight lines as for the potential (3).

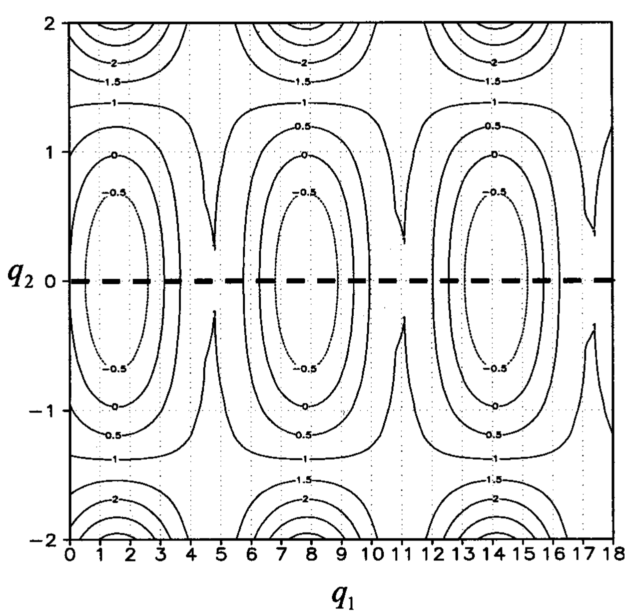

FIG. 1. The equipotentials of $U(q_1,q_2)$. The dashed line is the most likely path of the particle.

In this study, the energetic activation potential U_1 and the curvature functions C_i are taken to have the forms

$$U_1(q_1) = -\sin(q_1), \quad C_i(q_1) = 1.1 - \sin(q_1 + \phi_i), \tag{10}$$

and the period $L = 2\pi$. Here the phase angles ϕ_i ($i \geqslant 2$) play important roles; they determine particularly the curvature difference between local minima [$q_i^0 = (2n\pi + \pi/2)\delta_{i1}$, n integral] and maxima [$q_i^b = (2n\pi - \pi/2)\delta_{i1}$] of the potential. The 2D equipotentials of $U(q_1,q_2)$ with $\phi_2 = \pi$ are shown in Fig. 1. It is easy to prove that the most likely path of the particle is the solution of the deterministic equation (1) without noise [15], i.e., the bottom line of the potential surface.

In the high-temperature limit, the asymptotic expression of the flow for the potential (3) with Eq. (10) is given by

$$\overline{J} = \frac{F}{2\pi} N_0^{-1} \int_0^{2\pi} dq_1 \left(\prod_{i=2}^{N} \int_{-\infty}^{\infty} dq_i \right) \times \exp\left(-\sum_{i=2}^{N} [1.1 - \sin(q_1+\phi_i)] q_i^2 \right) I_0^{-2}(\sqrt{z}), \tag{11}$$

where I_0 is the modified Bessel function of zero order,

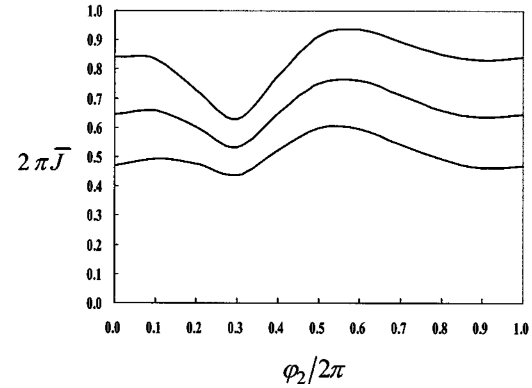

FIG. 2. The 2D mean velocity $2\pi\overline{J}$ predicted by Eq. (8) as a function of ϕ_2 when $T=1.5$ and for three values of $F=1.2$, 1.0, and 0.8 from top to bottom.

$$z=\sum_{i,j=2}^{N}\cos(\phi_i-\phi_j)(q_iq_j)^2, \tag{12}$$

and the normalization constant N_0 reads

$$N_0=\pi^{(N-1)/2}\int_0^{2\pi}\prod_{i=2}^{N}[1.1-\sin(q_1+\phi_i)]^{-1/2}dq_1. \tag{13}$$

The asymptotic behavior of the mobility, $\lim_{T\to\infty}2\pi\overline{J}/F<1$ because of $I_0>1$, should be noted; however, this quantity is equal to 1 in one dimension, and the 2D asymptotic current is independent of the phase angle ϕ_2. Moreover, in the absence of energy barriers U_1, the potential (3) is called the periodic channel. The mobility of the particle in a tilted multidimensional periodic channel is always smaller than the free mobility. For a 2D channel with q_1-independent curvature on the potential surface, the mean velocity of the particle along the q_1 direction is independent of the width of the channel. But any departure from the rectangular shape provides extra regions that the mobilized particle can wander in before it is able to increase its displacement along q_1 under a finite external force.

For comparison, the stochastic Runge-Kutta algorithm is applied to simulate the Langevin equations (1), which is a rather simple and effective approach for smooth nonlinear potentials. However, it is very difficult to solve the N-dimensional FPE numerically when $N\geqslant 3$. The mean steady velocity of the overdamped particle is determined by

$$\langle\dot{q}_1\rangle=2\pi\overline{J}=\frac{1}{t}[\langle q_1(t)\rangle-q_1(0)],\quad \langle\dot{q}_i\rangle=0\quad (i\geqslant 2). \tag{14}$$

This averaging over the stochastic realization is repeated 1000 times starting from the same initial conditions $q_1(0)=\pi/2$ and $q_i(0)=0$ $(i\geqslant 2)$. For each set of parameters of the model the mobility process will be integrated over 10^5 time steps 5×10^{-3} to obtain the mean velocity of the particle with sufficiently high accuracy.

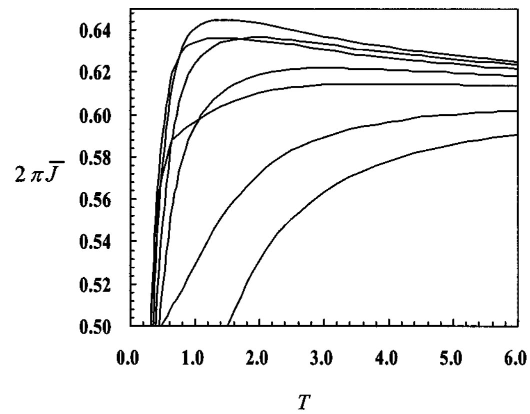

FIG. 3. The 2D mean velocity $2\pi\overline{J}$ predicted by Eq. (8) as a function of T for fixed $F=0.85$. The values of ϕ_2/π corresponding to the asymptotic mean velocities from top to bottom are 1.1, 1.2, 1.0, 1.3, 0.9, 0.8, and 0.7, respectively.

III. RESULTS AND DISCUSSION

All of the results are expressed in dimensionless units. Figure 2 shows the two-dimensional mean velocity of the particle $(N=2)$ as a function of ϕ_2 for different driving forces F in terms of Eq. (8). It is seen that the mean velocity has a maximum value in the region of $\pi<\phi_2<1.4\pi$ where $C_2(q_1^b)<C_2(q_1^0)$. Those kinds of potential shapes are conducive to mobility motion of the particles along the direction of external force. The 2D mean velocity obtained by using Eq. (8) as a function of T for different phase angles ϕ_2 is plotted in Fig. 3. It is observed that the mean velocity increases as the value of the ratio $C_2(q_1^b)/C_2(q_1^0)$ decreases for fixed F at finite temperatures. An important finding is that the 2D mean velocity of the particle in the stationary state can be a nonmonotonic function of the noise intensity when the value of ϕ_2 is taken near π. It has found that the 2D mean velocity is larger than the 1D values at low temperatures; however, the former is less than the latter in the limit of high temperature as predicted by Eq. (11). Thus the 2D mean velocity becomes a nonmonotonic function of the noise intensity. This feature results from the oscillating effect of the particles along the q_2 direction.

Figure 4 shows the temperature-dependent 2D mean ve-

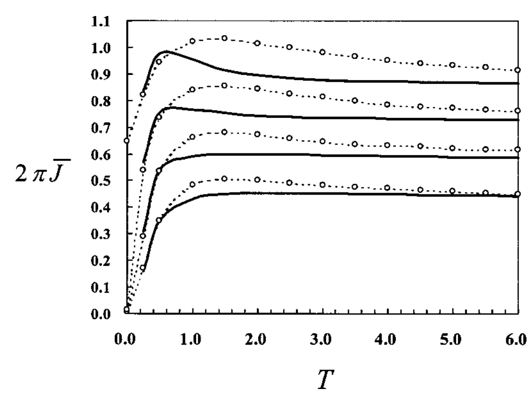

FIG. 4. The 2D mean velocity $2\pi\overline{J}$ as a function of T when $\phi_2=\pi$ and for four values of $F=1.2$, 1.0, 0.8 and 0.6 from top to bottom. The theoretical prediction (solid line) is compared with the Langevin simulation (dashed line with circles).

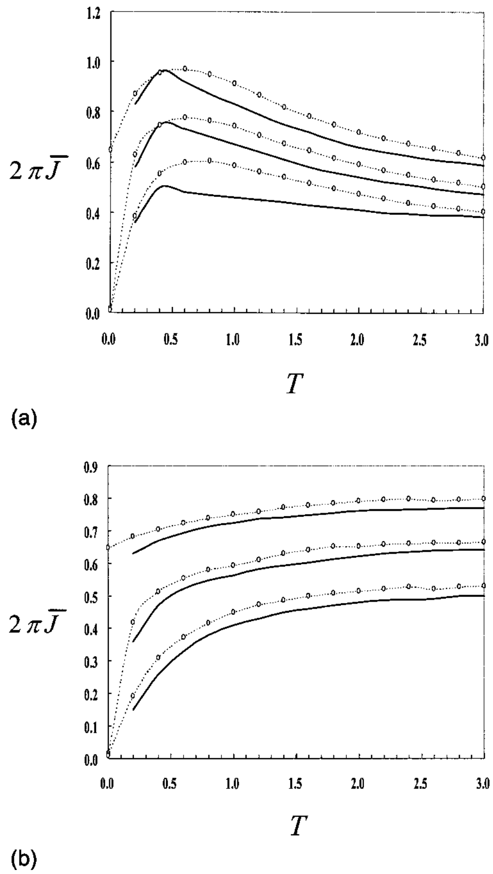

FIG. 5. The 3D mean velocity calculated by the theory (solid line) and the Langevin simulation (dashed line with circles) as a function of T for three values of $F=1.2$, 1.0, and 0.8 from top to bottom. Here (a) $\phi_2=\phi_3=\pi$; (b) $\phi_2=\pi$, $\phi_3=0$.

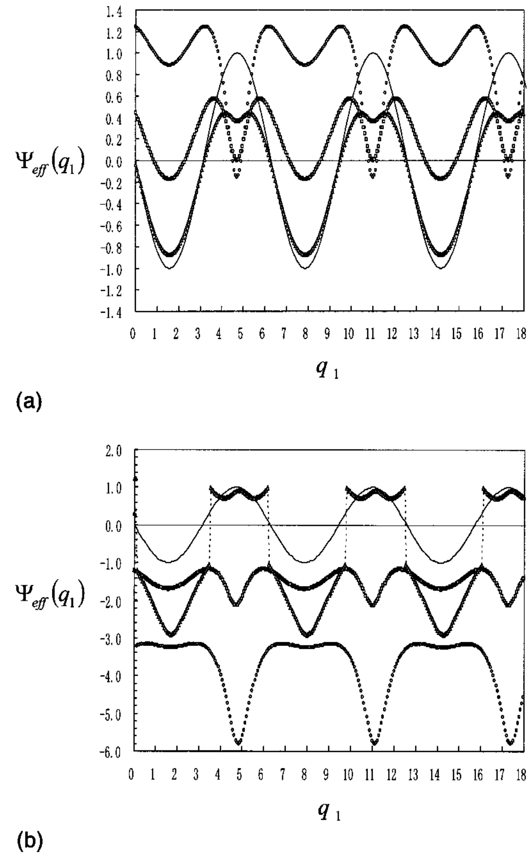

FIG. 6. The effective potential compared with the original 1D potential (solid line, $T=0.0$) for different temperatures when $F=0$ and $\phi_2=\pi$. (a) $N=2$ with $T=2.0$ (circles), $T=1.2$ (squares), $T=0.5$ (triangles); (b) $N=3$ with $T=1.5$ and $\phi_3=\pi$ (circles), $T=0.8$ and $\phi_3=\pi$ (squares), $\phi_3=0$ and various T (triangles).

locity calculated by the theoretical prediction for $\phi_2=\pi$ and for different F; it is also compared with the Langevin simulations within the same graph. The mean velocity increases from zero with increasing T and is a peaked function of the temperature. However, the mean velocity does not equal zero at $T=0$ when $F>1$, because the energy barriers of the washboard potential vanish along the line $q_2=0$. The nonmonotonic behavior of the mean velocity with T for different F is observed also in the simulation results, although the theoretical values are systematically less than the numerical data for moderate to large temperatures, and the peak's position predicted by the theory occurs before the numerical one.

We fix $\phi_2=\pi$ and analytically and numerically evaluate the three-dimensional mean velocity ($N=3$) shown in Figs. 5(a) and 5(b). We now change ϕ_3 to match the condition for a nonmonotonic phenomenon. The occurrence of a maximal velocity is also observed in Fig. 5(a) when $\phi_3=\pi$, resulting in a shift of the flow's peak toward smaller T and in a corresponding reduction of the peak's height. The 3D peak is also sharper than the 2D peak. But this nonmonotonic effect cannot be observed when $\phi_3=0$ [see Fig. 5(b)].

In order to have a qualitative understanding of the dynamical influence of the nontransport variables on the mobility motion, we propose a one-dimensional effective potential $\Psi_{eff}(q_1)$ through eliminating the variables q_i ($i\geqslant 2$) [13,16,17]. By definition

$$\exp[-\Psi_{eff}(q_1)/T]=\prod_{i=2}^{N}\int_{-\infty}^{\infty}dq_i \times\exp[-\Psi(q_1,q_2,\ldots,q_N)/T]; \tag{15}$$

thus

$$\Psi_{eff}(q_1)=U_1(q_1)-Fq_1+\frac{1}{2}T\left(\sum_{i=2}^{N}\ln C_i(q_1)-(N-1)\ln(2\pi T)\right). \tag{16}$$

In the absence of an external force F, the effective potential is plotted in Figs. 6(a) ($N=2$) and 6(b) ($N=3$) for fixed $\phi_2=\pi$, and the original 1D potential $U_1(q_1)$ is also shown in the same figures. It is seen from the two figures that this effective potential depends on the noise intensity and has a complex shape; also, its barrier height $\Delta\Psi_{eff}$ becomes a nonmonotonic function of the temperature. That is, the barrier height of the effective potential shows a minimum at an optimal temperature. It can be shown that the 3D optimal temperature when $\phi_3=\pi$ is less than the 2D one. Therefore, both 2D and 3D mean velocities of the particle can achieve maxima at finite temperatures. Nevertheless, the barrier height of the 3D effective potential remains invariant for any T when $\phi_3=0$. In this case $C_2(q_1^0)>C_2(q_1^b)$, $C_3(q_1^0)<C_3(q_1^b)$, and $C_2(q_1^0)C_3(q_1^0)=C_2(q_1^b)C_3(q_1^b)$; thus a resonantlike velocity cannot be shown. This is because the dynamical influence of the two nontransport degrees of freedom on the mobility motion has been counteracted.

IV. SUMMARY

The overdamped Brownian particle moving in a one-dimensional periodic potential under a constant force cannot show resonantlike mobility, but this phenomenon is actually possible in a multidimensional coupled potential. As a consequence, the mean velocity of the particle increases with decreasing ratio of curvature between local maxima and minima of the potential at low temperatures. The asymptotic value of the multidimensional mobility is always less than that in the limit of high temperature. Thus it is observed that the 2D particle velocity in the stationary state can be a peaked function of the noise intensity for a more open parabola of the potential perpendicular to the barriers. Further, either the mean velocity peak is shifted toward smaller temperatures or the nonmonotonic behavior of mobility is counteracted, if a third nontransport degree of freedom is introduced. Finally, these effects can be understood well in terms of a temperature-dependent one-dimensional effective potential.

ACKNOWLEDGMENTS

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