Underdamped diffusion in the egg-carton potential

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It is shown by numerical solution of the Fokker-Planck equation in a coupled two-dimensional potential of square symmetry (egg-carton potential) that an ''anomalous'' dependence of the diffusion coefficient on the friction ($D\propto\eta^{-\sigma}$, with $\sigma<1$) holds in a rather wide friction range in the underdamped regime. The exponent σ is not universal, but depends on the parameters of the potential. [S1063-651X(97)11704-4]

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Very recently, a Langevin simulation of diffusion in a coupled two-dimensional (2D) potential of centered-rectangular symmetry, performed by Chen, Baldan, and Ying [1] has shown that an ''anomalous'' dependence of the diffusion coefficient D on the friction η holds in the underdamped regime. Precisely, Chen, Baldan and Ying found that $D\propto\eta^{-\sigma}$ with $\sigma=0.5$, as opposed to the η^{-1} dependence found in the case of one-dimensional (or separable) systems [2]. They explained their result in terms of the reduced probability of long jumps, due to the fact that, in their potential, the path connecting adjoining sites does not coincide with the direction of the easy crossing of the saddle points. Moreover, by some considerations about the enhanced deactivation behavior at low friction, they conjectured that the exponent should not be universal.

Here we solve numerically the Fokker-Planck equation (FPE) in a 2D potential of square symmetry and we will show the following results. First, we show that an anomalous dependence of D is found (in a wide friction range, see below) also in the case of a potential where the equilibrium sites lie always on the same line which connects the saddle points, i.e., in the easy-crossing direction; in particular, we focus on the limiting case where the barrier between minima is lowered to zero. Second, we will demonstrate explicitly that the exponent σ is not universal, as it depends on the details of the potential.

Let us consider a particle moving in a periodic square two-dimensional potential $V(\mathbf{r})$ of lattice constant a; the particle is in contact with a heat bath at temperature T which furnishes both fluctuation (modeled by a white noise) and dissipation (due to a friction η). In these conditions, the phase-space probability density f satisfies a four-variable FPE,

$$\frac{\partial f}{\partial t}=-\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}-\frac{\mathbf{F}(\mathbf{r})}{m}\cdot\frac{\partial f}{\partial \mathbf{v}}+\eta\frac{\partial}{\partial \mathbf{v}}\left(\mathbf{v}f+\frac{k_BT}{m}\frac{\partial f}{\partial \mathbf{v}}\right), \qquad (1)$$

where $\mathbf{r}=(x,y)$, $\mathbf{v}=(v_x,v_y)$, and m are the position, the velocity and the mass, $\mathbf{F}=-\nabla V$ is the periodic force.

The following dimensionless variables are introduced: $\bar{\mathbf{r}}=(2\pi/a)\mathbf{r}$; $\bar{t}=(2\pi/a)(k_BT/m)^{1/2}t$; $\bar{\mathbf{v}}=(m/k_BT)^{1/2}\mathbf{v}$; $\gamma=(a/2\pi)(m/k_BT)^{1/2}\eta$; $\bar{V}(\bar{\mathbf{r}})=V(\mathbf{r})/k_BT$. With this choice for $\mathbf{r}$, the unit cell goes from $-\pi$ to π. In the following the dimensionless variables will be rewritten without the overbar. In these variables, the dependence of D on the friction γ in the case of $\mathbf{F}(\mathbf{r})=\mathbf{0}$ is simply $D=\gamma^{-1}$. The quantities plotted in Figs. 1 and 2 are dimensionless. As a potential, we choose the so-called ''egg-carton'' form:

$$V(x,y)=-2g_0[\cos(x)+\cos(y)]+2g_1\cos(x)\cos(y). \qquad (2)$$

This model potential is often introduced in the study of nonlinear dynamics of a classical particle moving conservatively in a periodic field of force [3,4]. If g_0 and g_1 are positive and $g_1\leqslant g_0$ there are four minima at the corners of the cell, one central maximum, and saddle points at the midpoints of the edges, with energy barriers $E_b=4(g_0-g_1)$. Therefore, in the case $g_0=g_1$, the energy barriers vanish and the minima are connected by a network of flat channels, as can be seen in

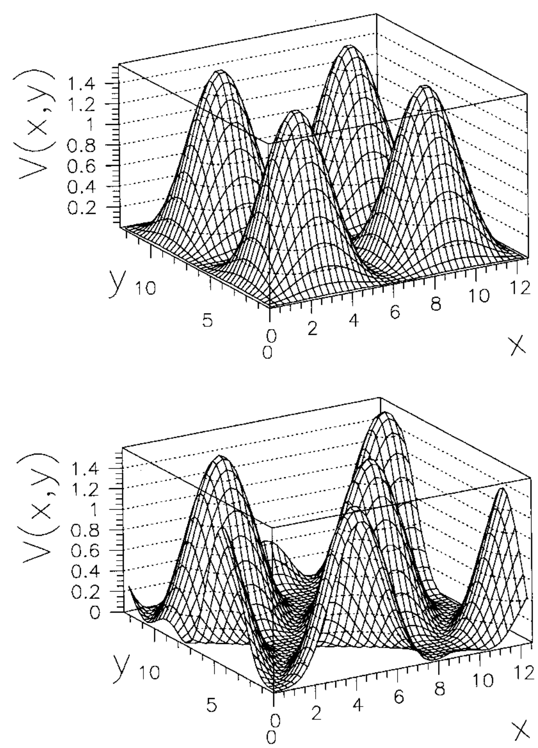

FIG. 1. The egg-carton potential in the flat-channel case $g_0=g_1$. In the lower panel the potential has been rotated in order to show the flat channel in perspective.

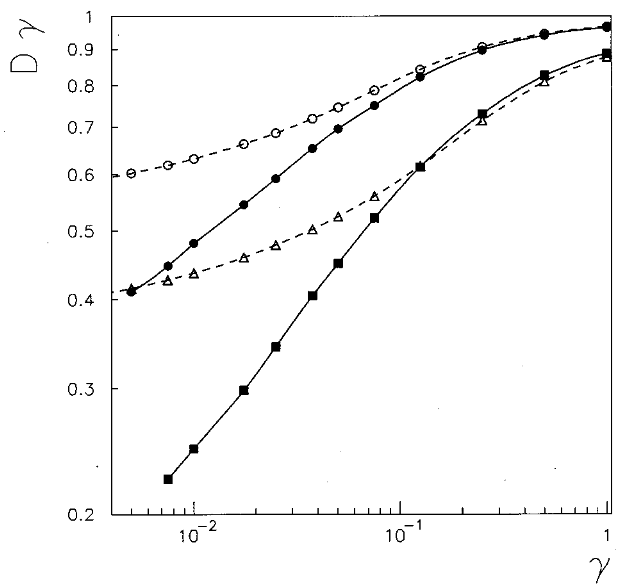

FIG. 2. Behavior of $D\gamma$ as a function of γ. The coupled cases $g_0=g_1=0.1$ (full circles), $g_0=g_1=0.2$ (full squares); and the decoupled cases $g_0=0.1$, $g_1=0$ (open circles), and $g_0=0.2, g_1=0$ (triangles) are considered. The lines are only guides to the eyes.

Fig. 1. For comparison, the coupled potential of centered-rectangular symmetry used by Chen, Baldan, and Ying [1] can be written as $U_{\mathrm{CBY}}(x,y)=2g[1+\sin(x)\sin(y/\sqrt{2})]$.

The FPE is solved by the matrix-continued-fraction method [2]. The dynamic structure factor is calculated and D is obtained by the proper Kubo relation. A detailed description of the method is found in [5] for 2D systems and in [2,6] for 1D systems.

The results of our calculations are presented in Fig. 2, where the quantity $D\gamma$ is reported down to $\gamma=5\times10^{-3}$. In the decoupled case (which is equivalent to a 1D problem), $D\gamma$ tends to a constant as $\gamma\rightarrow0$ [2]. Four different couples (g_0,g_1) are considered. Precisely, we consider the flat-channel cases $g_0=g_1=0.1$ (full circles) and $g_0=g_1=0.2$ (full squares), and compare the results to the decoupled cases $g_0=0.1, g_1=0$ (open circles) and $g_0=0.2, g_1=0$ (triangles). The behaviors are clearly different: the decoupled cases have an inflection point in the region near $\gamma=0.1$ and then accommodate slowly to a constant. The flat-channel cases show a linear behavior: $D\gamma\propto\gamma^{1-\sigma}$ from $\gamma=0.1$ and below, with $\sigma\simeq0.76$ at $g_0=g_1=0.1$ and $\sigma\simeq0.64$ at $g_0=g_1=0.2$. Of course, our calculations do not demonstrate that these behaviors would extend asymptotically to $\gamma\rightarrow0$; however, they show that there are significant differences between coupled and decoupled behaviors in a wide friction range, even in the case examined here, where the potential $V(\mathbf{r})$ is not large with respect to the temperature. We remark that, in the decoupled case, an energy barrier is present on the easiest diffusion path, while in the coupled case the barrier is absent. In spite of that, the diffusion coefficient is smaller. In the presence of coupling, the width of the channel is narrower at the saddle point positions than at the minima. This seems sufficient to cause an anomalous behavior. In the conservative case [3,4], the coupling may cause the localization during the particle motion and the appearance of anomalous diffusion (in conservative systems, the anomaly is not related to the behavior of D with friction, but to the behavior of the mean-square displacement as a function of time). The coupling allows the energy transfer between the x and y degrees of freedom; because of that, it may be difficult for the diffusing particle to perform long and straight inertial trajectories.

A coupled diffusion problem (at high friction), with some similarity with our flat-channel case was studied by Zwanzig [7], who considered the motion of a Brownian particle in a 2D channel with periodically varying width. No potential is present in the channel and the particle is subjected only to the geometrical constraint of a nonconstant channel width. Solving exactly the problem by means of a conformal transformation, Zwanzig showed that the diffusion coefficient is always smaller than γ^{-1}, i.e., of the result given by Einstein's relationship, except for a rectangular channel (decoupled case).

In conclusion, we have shown that an anomalous behavior of the diffusion coefficient is present, in a wide friction range in the underdamped regime, even for a potential in which no energy barrier is present along the straight line adjoining the minima. That behavior is characterized by the relation $D\propto\eta^{-\sigma}$, with $\sigma<1$; σ is not universal, even for a given symmetry or form of the potential, but depends on the parameters of the potential itself.

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