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Supersymmetry and Bistable Soft Potentials

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The diffusion of a Brownian particle is investigated for a class of potentials (soft bistable) which resist conventional techniques. A new method of solution based on supersymmetric quantum mechanics is shown to provide, with minimal effort, an accurate determination of the small eigenvalue of the relevant Fokker-Planck equation. The reciprocal of the small eigenvalue compares very closely with a refined definition of mean first-passage time.

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The diffusion of a Brownian particle in a one-dimensional bistable (double well) potential provides a useful model to understand the role of external fluctuations in driving an unstable system towards equilibrium.[1] Because of its significance in many areas of condensed-matter physics, this problem has received much attention over the past decades.[2] In a recent work,[3] the correspondence between the one-dimensional Fokker-Planck (FP) equation and the supersymmetric Schrödinger equation[4] was exploited to provide an elegant method for computing the smallest nonvanishing eigenvalue λ_1, i.e., the eigenvalue which characterizes the relaxation rate of a stochastic system. Later, a variational approach based on supersymmetry was applied to the computation of the quantum tunneling rate for a class of confining bistable potentials.[5]

Very refined analytical approximations to λ_1 are available in the current literature[1] of nonequilibrium statistical mechanics. Most stochastic techniques[2] were devised for treating the case of bistable systems with a discrete eigenvalue spectrum and λ_1 confined away from the higher eigenvalues. The extension of such techniques beyond the above-described situation becomes rather involved, whereas methods based on supersymmetry are expected to provide a systematic computational framework.

The use of supersymmetric quantum mechanics for solving a bistable FP equation has, indeed, two major advantages over other computational methods. First of all, in the relevant Schrödinger equation the bistable potential is replaced[3] with an essentially monostable (single well) supersymmetric partner. Moreover, the zero eigenvalue appearing in the spectrum of the FP equation is deleted and the determination of λ_1 does not require any difficult tunneling calculation[3]—we recall that in the low-temperature limit λ_1 is exceedingly small. Secondly, supersymmetry provides a way to construct[6] a family of Schrödinger equations, the eigenvalue spectrum of which differs only for the number of discrete states; as a consequence, diffusion problems with a different number of

time scales might be related to each other.

In the present Letter we address a new class of bistable potentials which, in spite of their potential application to modeling a number of relaxation processes in a condensed phase,[1] have resisted a conventional analysis. Contrary to the nonlinear potentials commonly studied in the literature, where the anharmonic behavior at infinity provides the confining mechanism of the Brownian particle (hard potentials), we focus here on potentials associated with asymptotically constant binding forces. We will call such potentials soft potentials. The eigenvalue spectrum of the related FP equation exhibits a continuum branch and, for noise intensity below a certain threshold, a finite number of discrete positive eigenvalues.[1]

This class of potentials poses a novel and interesting problem: It is well known that the mean first-passage time (MFPT) over the high barrier of hard bistable potentials equals the reciprocal of λ_1. The analytical determinations of λ_1 (and its connection with the MFPT) available in the literature[1,2] are based on the approximation[7] that the local relaxation inside a potential well occurs in a time interval negligible compared to the MFPT. Such an assumption does not work for soft potentials, where the Brownian particle takes an infinite time to approach a stable point from infinity.

In the Letter we show how supersymmetric quantum mechanics provides a systematic and simple method for determining λ_1 also in the case of soft bistable potentials. We shall compute, in fact, the smallest eigenvalue for a particular family of soft potentials, the shape of which may be varied by means of a tunable parameter R. Increasing R above a certain value changes the potential shape from monostable to bistable. Our choice of the potential enables us also to study the way by which local changes of the potential shape affect the approach to equilibrium of a Brownian particle. The results of our computation are compared with the exact numerical integration[8] of the Schrödinger problem associated with the FP equation and with two improved definitions of the MFPT.

We consider a one-particle system with time evolution defined by the stochastic differential equation of the Langevin type

$$dx/dt = -\partial W/\partial x + \eta(t), \tag{1a}$$

where

$$W(x;R) = -2\beta \ln\left[\frac{\cosh\gamma x}{\cosh^2\gamma x + \sinh^2 R}\right], \tag{1b}$$

and $\eta(t)$ is a Gaussian stochastic noise with correlation functions $\langle\eta(t)\rangle = 0$ and $\langle\eta(t)\eta(t')\rangle = 2D\delta(t-t')$. For $\gamma \to 0$ the free-particle potential is obtained, while for $\gamma \to 0$ with $\gamma\beta = \text{const}$, (1b) produces the exactly solvable wedge potential.[9] In this Letter we set $\gamma = \beta = 1$. As the tunable parameter R varies, the potential shape changes from a single-well structure for $R < R^* \approx 0.88$ [$\sinh(R^*) = 1$] to a double-well structure (Fig. 1). Note that $W(x;0) = -W(x;\infty)$.

We shall now evaluate λ_1 for all values of the parameter R. The FP equation associated with Eq. (1),

$$\frac{\partial\rho(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\partial W}{\partial x} + D\frac{\partial}{\partial x}\right]\rho(x,t), \tag{2}$$

is transformed[10] into the imaginary-time Schrödinger equation

$$-\frac{\partial\psi(x,t)}{\partial t} = \left[-D\frac{\partial^2}{\partial x^2} + V\right]\psi(x,t), \tag{3}$$

after the transformation $\rho(x;t) = e^{-W/2D}\psi(x;t)$. In Eq. (3) the potential V is given by

$$V = \frac{1}{4D}\left[\frac{\partial W}{\partial x}\right]^2 - \frac{1}{2}\left[\frac{\partial^2 W}{\partial x^2}\right], \tag{4}$$

and, like $W(x;R)$, has a double-well structure for $R > R^*$.

Because of the form (4) of the potential, the Hamiltonian H_- is factorized as $H_- \equiv A^+A$ with $A = D^{1/2}\partial/\partial x + (4D)^{-1/2}\partial W/\partial x$. The supersymmetric partner $H_+ = AA^+$ has a single-well potential and for $D = 1$ accurate analytical expressions for its eigenfunctions ψ^+ have been derived by our replacing H_+ with a suitable Poeschl-Teller (PT) Hamiltonian H_+^{PT}.[11] In the remainder of our calculations we set D equal to one.[12]

The eigenfunctions of the two supersymmetric partner Hamiltonians corresponding to the same eigenvalue are related by $\psi^- = A\psi^+$. To compute the eigenvalue spec-

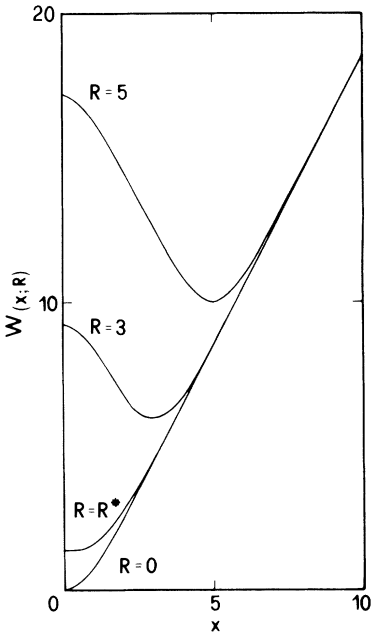

FIG. 1. Plot of the potential $W(x;R)$.

trum of the original FP equation, we utilize the exact Hamiltonian H_+. In particular, our best determination of λ_1 is given in terms of the bound state ψ_b^+ of H_+^{PT}, i.e.,

$$\lambda_1 = \langle \psi_b^+ | H_+ | \psi_b^+ \rangle / \langle \psi_b^+ | \psi_b^+ \rangle, \tag{5}$$

with[11]

$$\psi_b^+ = (\cosh \alpha x)^{-s}. \tag{6}$$

In (6) α and s are functions of the tunable parameter R (Ref. 11):

$$\alpha = \tanh^2 R \frac{\sinh 2R}{\sinh 2R - 2R},$$

$$2s = \left[-1 + \left(1 + \frac{8 \tanh^2 R}{\alpha^2} \right)^{1/2} \right].$$

From (5) we have $\lambda_1 = 1$ for $R = 0$ and $\lambda_1 \approx 8e^{-2R}$ for $R > 2$. The behavior of λ_1, Eq. (5), as a function of R is displayed in Fig. 2 and it is compared with the value of λ_1 obtained from numerical integration[8] of the Schrödinger equation (3). We see that the computation of λ_1 using the supersymmetric quantum mechanics gives an excellent agreement with the exact numerical computation for all values of R, including the range $R < 2$ where the usual semiclassical approximations are no longer tenable.[8]

To obtain the correct result for λ_1 with use of standard FP techniques is less straightforward. In fact, the computation of λ_1 through Kramers' formula turns out to hold only for $D \ll 1$. The assumptions implicit in Kramers' method are often summarized by the requirement

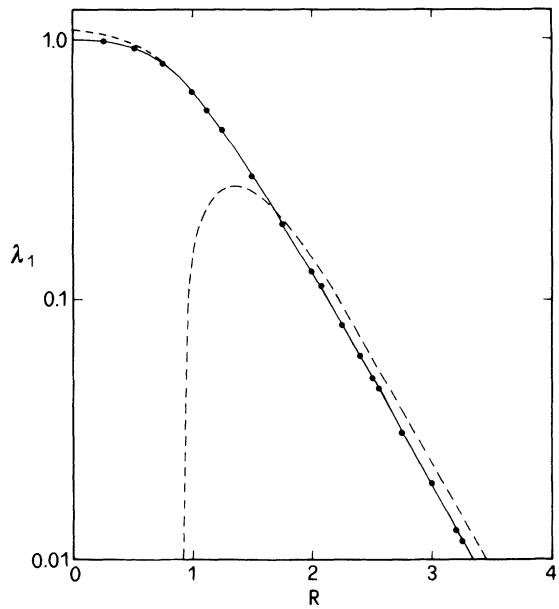

FIG. 2. λ_1 vs R. The analytic supersymmetric result (5) (solid line) is compared with the reciprocal of T_c, Eq. (10) (dashed line), the numerical integration of Ref. 8 (dots), and Kramers' approximation (7) (dotted-dashed line).

that

$$D \ll \Delta W \equiv W(0;R) - W(\pm x_m;R)$$
$$= 2 \ln(\cosh^2 R / 2 \sinh R),$$

where $\pm x_m$ denote the position of the potential minima (for $R > R^*$). Such a condition is meant to guarantee with one token that the potential barrier ΔW is much larger than the average energy fluctuation D and that the bistable potential can be approximated to parabolic curves in vicinity of the extremal points $x = 0$ and $\pm x_m$. This is not the case for soft potentials where the second condition corresponds to the further inequality[13] $D \ll W''(0;R)^2 / W^{iv}(0;R) \approx O(1)$. This explains why Kramers' formula[7] for λ_1,

$$\lambda_1^K = \frac{1}{\pi} [| W''(0;R) | W''(\pm x_m;R)]^{1/2} \exp(-\Delta W / D)$$
$$= \frac{8}{\pi} \frac{\sinh^2 R - 1}{\cosh^4 R} \tanh R, \tag{7}$$

is apparently inadequate at $D = 1$ even in the limit $R \to \infty$ (Fig. 2), where $\Delta W \approx 2R$ becomes infinitely large.

In order to take into account the effect of softness, one has to generalize Stratonovich's definition[14] of the MFPT. The mean time for a Brownian particle placed at $t = 0$ in x_1 to reach a point x_2 with $x_1 < x_2$ is denoted by $T(x_1, x_2)$. In the presence of a binding potential, the following boundary conditions may be imposed: $dT/dx_1 |_{x_1 = -\infty} = 0$ (reflecting wall at $-\infty$) and $T(x_2, x_2) = 0$ (absorbing wall in x_2). $T(x_1, x_2)$ is thus determined by[14]

$$T(x_1, x_2) = \int_{x_1}^{x_2} dy [D(y) \rho(y)]^{-1} \int_{-\infty}^{y} \rho(z)\, dx, \tag{8}$$

where $D(x)$ is the diffusion function of a generic one-dimensional FP equation and $\rho(x)$ is the relevant stationary solution normalized to one.

In the case of hard bistable potentials, $T(-\infty, 0)$ defines[1,2] the MFPT for a Brownian particle sitting about the bottom of the negative potential well at $-x_m$ to cross over the potential barrier located at the origin $x = 0$. For the class of soft potentials (1b) such a definition of MFPT is illegitimate for two types of reasons. Being the smallest eigenvalue λ_1 close to the continuum, the hopping phenomenon over the potential barrier may not be distinguishable from the relaxation inside a single potential well. Furthermore, as a consequence of the potential softness, $T(x_1, 0)$ diverges for $x_1 \to -\infty$.

A well-behaved definition of MFPT can be obtained on averaging $T(x_1, 0)$ with respect to the normalized distribution of the negative starting points $2\rho(x_1)$:

$$\langle T(0) \rangle = 2 \int_{-\infty}^{0} T(x_1, 0) \rho(x_1) dx_1$$
$$= 2 \int_{-\infty}^{0} dx \left[\int_{-\infty}^{x} \rho(y) dy \right]^2 [D(x) \rho(x)]^{-1}. \tag{9}$$

The connection to λ_1 is now assumed as for hard bistable potentials, i.e., $\lambda_1 = \langle T(0) \rangle^{-1}$. The relevant determination of λ_1 compares fairly closely with the results of numerical integration[8] for $R > 1.5$ only.

The absence of a clear-cut time-scale separation between the relaxation inside a potential well and the hopping phenomenon for smaller values of R requires an even more refined definition of the MFPT. We propose to substitute definition (9) with the autocorrelation time[15] of the variable $x(t)$,

$$T_c = \frac{2}{\langle x^2 \rangle} \int_{-\infty}^{0} dx \left[\int_{-\infty}^{x} y \rho(y) dy \right]^2 [D(x)\rho(x)]^{-1}, \quad (10)$$

where $\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 \rho(x) dx$. Such a substitution is expected to better account for the relaxation process of the *activated* Brownian particle.[15] T_c and $\langle T(0) \rangle$ are almost indistinguishable from λ_1^{-1} in the case of high potential barriers (e.g., $R > 2$), whereas the largest disagreement occurs at $R = 0$, namely, $\lambda_1^{-1} = 1$, $T_c \approx 0.9$, and $\langle T(0) \rangle = 0.5$. In Fig. 2 the reciprocal of the MFPT (10) is displayed for $D = 1$. A comfortable agreement with the results derived by means of supersymmetry is obtained over the *whole range of R*. The small discrepancy between λ_1 and T_c^{-1} in $R = 0$ (about 10%) should be ascribed to the presence of a continuum branch in the eigenvalue spectrum of Eq. (2).

In this Letter we have determined only the relaxation dynamics of the Brownian particle for long time scales. In order to analyze its behavior at shorter times, one should take into account the contribution coming from the continuum part of the spectrum. This is, in general, a very difficult problem. For the class of potentials treated here, however, one hopes to make some progress since a good approximate expression for the unnormalized continuum eigenfunctions—as well as for the density of states[16]—had been already obtained by means of supersymmetry. This is the subject of ongoing research and a future publication.[17]

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