SUPERSYMMETRY AND ACTIVATION RATES

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The supersymmetric connection between Fokker–Planck and Schrödinger equations is utilized to reduce the computation of the activation rate in one-dimensional bistable potentials to a variational calculation for the ground state level of a monostable quantum system. The results thus obtained are compared with the predictions of conventional approximate techniques for a class of weakly binding (soft) potentials.

Recently [1–3] it has been pointed out that the well-known [4] connection between the Fokker–Planck equation (FPE) and the imaginary-time Schrödinger equation (SE) can ease the numerical determination of the smallest non-vanishing eigenvalue λ_1 for the diffusion in bistable potentials. The crucial ingredient of the proposed procedure is provided by the supersymmetric quantum mechanics [5], which establishes the isospectrality of the eigenvalue problems associated with the two potentials

$$V_{\pm} = \frac{1}{4D}\left(\frac{\partial W}{\partial x}\right)^2 \pm \frac{1}{2}\frac{\partial^2 W}{\partial x^2}, \tag{1}$$

where the supersymmetric partners $V_-(x)$ (bosonic) and $V_+(x)$ (fermionic) are related to each other through the Fokker–Planck potential $W(x)$. The FPE for constant diffusion D,

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

is thus equivalent to the imaginary-time SE

$$\frac{\partial}{\partial t}\Psi(x,t) = -H_{\pm}\Psi(x,t)$$

$$= \left(D\frac{\partial^2}{\partial x^2} - V_{\pm}\right)\Psi(x,t) \tag{3}$$

after the transformation

$$\rho(x,t) = \exp[-W(x)/2D]\,\Psi(x,t)\,. \tag{4}$$

Solving eq. (2) for a bistable potential $W(x)$ exhibits the very same technical difficulties as integrating the SE for $V_-(x)$ in eq. (1): an exponentially small (and, therefore, hard to resolve) distance between the first two eigenvalues of the spectrum may occur due to the multistable nature of both $W(x)$ (thermal activation) and $V_-(x)$ (quantum mechanical tunneling). The problem simplifies when one passes to the SE for $V_+(x)$. The fermionic partner $V_+(x)$ is isospectral with $V_-(x)$ apart from the cancellation of the zero eigenvalue λ_0 [1–3]. λ_1 denotes then the fundamental state of $V_+(x)$ which is in general well separated from the higher eigenvalues. For our purpose $V_+(x)$ behaves as a monostable potential [1] and λ_1 can be well approximated by means of variational techniques [1,2]. In a few cases [3] $V_+(x)$ can be handled analytically to obtain an extremely accurate determination of λ_1, otherwise lying beyond the reach of our analytical tools.

In the present Letter we discuss the advantages (and limitations) of the procedure proposed by Bernstein and Brown [1] by comparing the variational estimates of λ_1 for the quantum mechanical problem (3) with some approximate predictions for the relevant activation rates in the stochastic problem (2) [4,6].

Let $W(x)$ be a symmetric bistable potential with extremal points, $W'(x)=0$, in $x=\pm x_m$ (stable) and $x=0$ (unstable, or potential barrier) and flex points, $W''(x)=0$, in $x=\pm x_f$ (with $x_f<x_m$). In order to ob-

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tain a good variational estimate for the ground state level, λ_1, of the hamiltonian H_+, (3), we notice that $H_+ \exp[W(x)/2D] = 0$. As the operator H_+ is positive definite [5], a natural choice for the trial function is

$$\Psi(x) = \exp[\phi(x)/2D] , \tag{5}$$

with

$$\begin{aligned} \phi(x) &= \phi(-x) \\ &= W(x) , \qquad 0 \leqslant x \leqslant c , \\ &= W(c) + W'(c)(x-c) , \quad x \geqslant c , \end{aligned} \tag{6}$$

where c is the only variational parameter in our scheme. The condition that $\Psi(x)$ is normalizable requires that $0 < c < x_m$ so that $W'(c)$ is negative definite. The variational method yields an upper bound for λ_1, i.e.

$$\begin{aligned} \lambda_1 \leqslant \lambda_1^{\mathrm{V}} &= \min_{\{c\}} \frac{\langle \Psi(x) | H_+ | \Psi(x) \rangle}{\langle \Psi(x) | \Psi(x) \rangle} \\ &= \int_0^{\infty} \mathrm{d}x \exp\left(\frac{W'(c_m)}{D} \right) \\ &\times \left(\frac{W'(c_m + x)^2 - W'(c_m)^2}{4D} + \frac{W''(c_m + x)}{2} \right) \\ &\times \left[\int_0^{c_m} \mathrm{d}x \exp\left(\frac{W(x) - W(c_m)}{D} \right) - \frac{D}{W'(c_m)} \right]^{-1} . \end{aligned} \tag{7}$$

The minimization of λ_1^{V} with respect to the variational parameter c, amounts to determining (numerically) a function $c_m(D)$ which clearly admits of two analytical limits,

$$\lim_{D \to 0} c_m(D) = x_m , \qquad \lim_{D \to \infty} c_m(D) = x_f . \tag{8}$$

We shall discuss these limits and their implications at the end.

In the following we specialize our result (7) for a family of potentials $W(x; R)$ whose stability depends on the tunable parameter R ($R > 0$):

$$W(x; R) = 2 \ln\left(\frac{\cosh x}{\cosh^2 x + \sinh^2 R} \right) . \tag{9}$$

As shown in fig. 1 the shape of $W(x; R)$ changes from a single-well structure for $R = 0$ to a symmetric double-well structure for $R > R^* \approx 0.88$ ($\sinh R^* = 1$). Note that $W(x; 0) = -W(x; \infty)$. This potential is related to the stability of the static soliton of the double sine-Gordon theory [3,7].

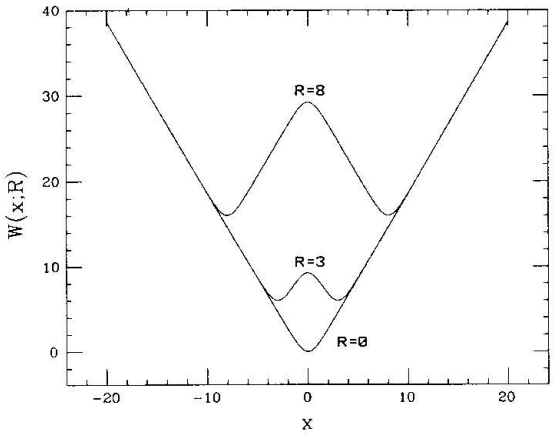

Fig. 1. The potential $W(x; R)$ for some values of the tunable parameter R.

The reason for our choice is that $W(x; R)$, due to its very peculiar shape, proved to resist a straightforward application of the conventional Fokker–Planck techniques for determining λ_1. The mean first-passage time, usually assumed to coincide with the reciprocal of λ_1 [4], results here to be ill-defined because of the linear behaviour of $W(x; R)$ at infinity, $W(x; R) \sim 2|x|$. (In ref. [3] $W(x; R)$ is termed soft potential.) The computation of λ_1 through Kramers' formula [6,8] is to hold good only for $D \ll 1$ [3]. The assumptions implicit in Kramers' approach are often summarized by the sole requirement that

$$\begin{aligned} D \ll \Delta W &\equiv W(0; R) - W(x_m; R) \\ &= 2 \ln\left(\frac{\cosh^2 R}{2 \sinh R} \right) \quad \text{for } R > R^* . \end{aligned}$$

Such a condition is meant to guarantee by 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 suitable parabolic curves in the vicinity of the extremal points $x = \pm x_m$ and $x = 0$. This is not the case of our soft potentials where the second condition corresponds to the further inequality [9] $D \ll W''(0; R)^2 / W^{(\mathrm{iv})}(0; R) \sim O(1)$. For this reason Kramers' formula

$$\lambda_1^{\mathrm{K}} = \frac{\sqrt{|W''(0;R)|\,|W''(x_{\mathrm{m}};R)|}}{\pi} \exp\left(-\frac{\Delta W}{D}\right) \tag{10}$$

is certainly inadequate for $D \sim 1$ even in the limit $R \to \infty$, where $\Delta W \approx 2R$ becomes infinitely large.

A different analytical estimate of λ_1 can be obtained at large R, where $W(x; R)$ is closely approximated by a double-wedge potential

$$W(x;R) \approx W_{\mathrm{w}}(x;R) \equiv \Delta W |1 - |x|/R| \quad (R \to \infty)\,. \tag{11}$$

In fact, under the condition $\Delta W \gg D \gg 1$ the detailed shape of the potential about the extremal points becomes irrelevant to the activation process and no great inaccuracy is expected on replacing $W(x; R)$ with $W_{\mathrm{w}}(x, R)$ in eqs. (2) and (3). The relevant eigenvalue spectrum can be given analytically; in particular [10]

$$\lambda_1^{\mathrm{W}} = \frac{1}{4D}\frac{\Delta W^2}{R^2} - D\frac{a^2}{R^2}\,, \tag{12}$$

where a is the solution to the transcendent equation

$$\tanh a = \frac{a}{\Delta W/D - a}\,. \tag{13}$$

For $D \geqslant \Delta W$ the discrete eigenvalue λ_1^{W} is absorbed into the continuum at $\lambda \geqslant 1/D$.

In fig. 2 we compare our results for λ_1^{V}, λ_1^{K} and λ_1^{W} at several values of D and R. In order to appreciate the accuracy of the diverse approximations we display the ratios of the above quantities to the precise determination of λ_1 obtained by numerical integration of the SE for $V_-(x)$ [10]. One sees immediately that

(i) λ_1^{V} is well-defined only for $R > R^*$ as understood in our variational approach where the bistable structure of $W(x; R)$ is always assumed. For $R > 2$, λ_1^{V} approximates λ_1 within up to 40% for the whole range of D values considered; an excellent agreement (within 1%) is obtainable for both $D \ll \Delta W$ and $D \gg \Delta W$;

(ii) in the limit $D \ll \Delta W$ and $D \ll 1$, λ_1^{V} and λ_1^{K} come close to each other as expected;

(iii) in the limit $\Delta W \gg D > 1$, λ_1^{W} appears to provide the best approximation to λ_1 and would replace

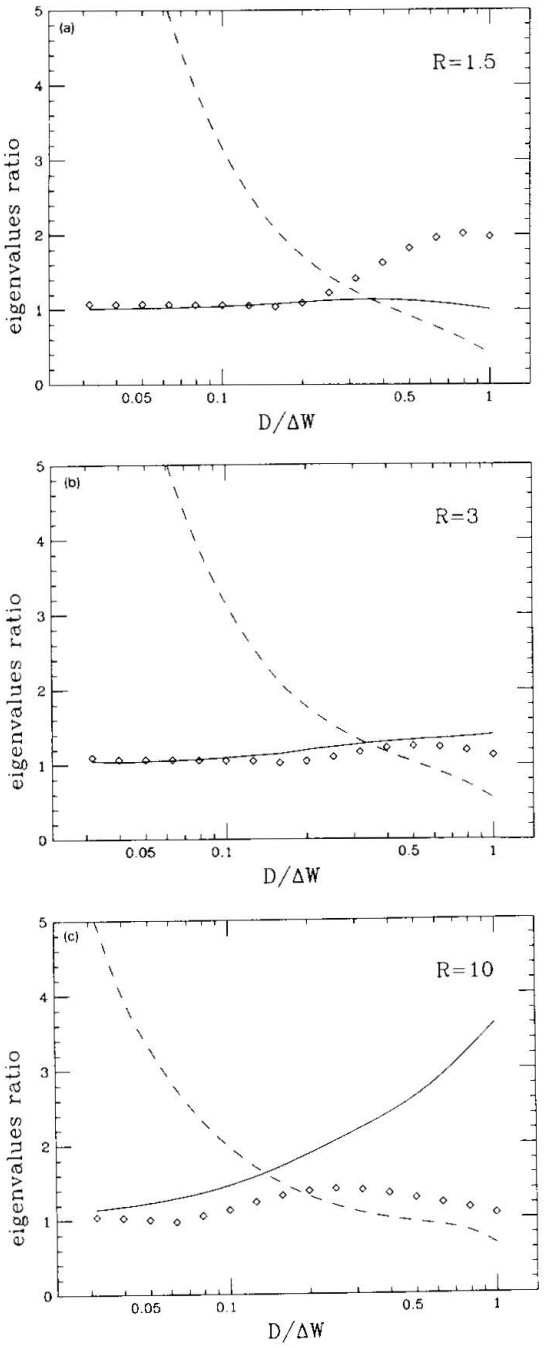

Fig. 2. Ratios $\lambda_1^{\mathrm{V}}/\lambda_1$ (lozenges), $\lambda_1^{\mathrm{K}}/\lambda_1$ (solid line) and $\lambda_1^{\mathrm{W}}/\lambda_1$ (dashed line) as a function of D at different values of R.

Kramers' formula for $D \gg 1$ (see fig. 2).

More suggestive is the discussion of the variational formula (7). $c_m(D)$ in fig. 3 has been computed numerically. For $D \to 0$, $\lambda_1^V(D)$ reproduces the analytical form of $\lambda_1^K(D)$ provided that $c_m^K(D) = x_m - \alpha\sqrt{D} + O(D)$ with $\alpha \approx 1.3$. $c_m^K(D)$ is also plotted in fig. 3. At large D, instead, $c_m(D)$ approaches x_f. The abrupt change in the behaviour of $c_m(D)$ is related to the relative weight of the two terms in the integral at the numerator of eq. (7), whence the rather good estimate for the critical value D_c, $D_c = W'(x_f)^2/4$ at which the transition between the two regimes $c_m(D) \approx c_m^K(D)$ $(D < D_c)$ and $c_m(D) \approx x_f (D > D_c)$ takes place. For $\Delta W \gg D > D_c$ the activation rate is no longer reproduced by Kramers' formula; a good approximation is given by eq. (7) where c_m is set equal to x_f. For $D \to \infty$ (i.e. $D \gg \Delta W$)

$$\lambda_1^V \approx \frac{1}{2} \frac{W'(\infty; R) - W'(x_f; R)}{x_f - D/W'(x_f; R)} . \tag{14}$$

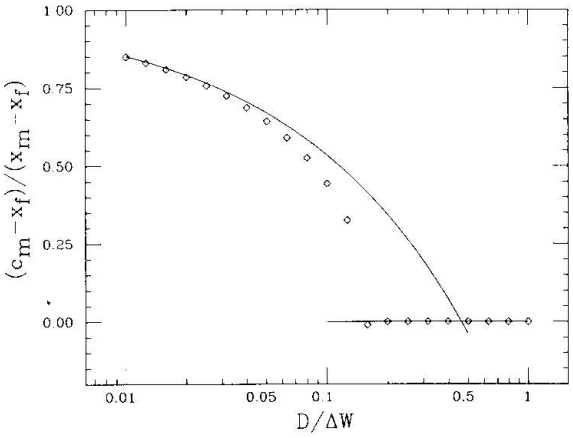

Fig. 3. Minimizing variational parameter $c_m(D)$ (lozenges) compared with the asymptotic expressions $c_m^K(D)$ and x_f (solid line).

At large values of R, $W'(\infty; R) \approx -W(x_f; R) \approx 2$ and $\lambda_1^V(D \to \infty) \approx 4/D$. In the same limit the continuum branch of the corresponding eigenvalue spectrum starts at $\lambda \approx 1/D$ so that the variational upper-bound $\lambda_1^V \geq \lambda_1$ is not of great use any more.

In conclusion, we have shown how supersymmetric quantum mechanics provides a useful complement to the variational techniques in resolving *fine eigenvalue structures* (namely, activation rates) of one-dimensional bistable potentials. The extension of the procedure presented herein to multi-dimensional bistable systems is matter of ongoing research work.

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References

[1] M. Bernstein and L.S. Brown, Phys. Rev. Lett. 52 (1984) 1933.
[2] P. Kumar, M. Ruitz-Altaba and B.S. Thomas, Phys. Rev. Lett. 57 (1986) 2749.
[3] F. Marchesoni, P. Sodano and M. Zannetti, Phys. Rev. Lett. 61 (1988), to be published.
[4] H. Risken, The Fokker–Planck equation (Springer, Berlin 1984) ch. 4.
[5] C.M. Bender, F. Cooper and B. Freedman, Nucl. Phys. B 129 (1983) 61.
[6] T. Fonseca, J.A.N.F. Gomes, P. Grigolini and F. Marchesoni, Adv. Chem. Phys. 62 (1985) 389;
P. Hanggi, J. Stat. Phys. 42 (1986) 105.
[7] D.K. Campbell, M. Peyrard and P. Sodano, Physica D 19 (1986) 165;
P. Sodano, C.R. Willis and M. El-Batanouny, Phys. Rev. B 34 (1986) 4936.
[8] H.A. Kramers, Physica 7 (1940) 284.
[9] W. Renz and F. Marchesoni, Phys. Lett. A 112 (1985) 124.
[10] H. Risken, private communication.