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Exact Solution for the Diffusion in Bistable Potentials

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We solve analytically the Fokker–Planck equation for a one-parameter family of symmetric, attractive, nonharmonic potentials which include double-well situations. The exact knowledge of the eigenfunctions and eigenvalues allows us to fully discuss the transient behavior of the probability density. In particular, for the bistable potentials, we can give analytical expressions for the probability current over the working barrier and for the onset time which characterizes the transition from uni- to bimodal probability densities.

KEY WORDS: bistable potentials, Fokker–Planck equation, exactly solved models.

1. INTRODUCTION

Owing to its wealth of applications, the $1D$ diffusion problem in nonharmonic potentials and more particularly bistable potentials remains the subject of many recent studies. The intrinsic nonlinearity present in this problem stimulates research both in the development of approximation schemes[(1-3)] and in the discussion of exactly soluble models.[(4-11)] This paper is devoted to the last approach, and we suggest a class of models for which the Fokker–Planck equation (F.P.E.) admits exact solutions. The potential $U_a(Z)$ from which the drift of the F.P.E. derives depends on a parameter a which, chosen at different values, leads to single- or double-well situations. For the class of models studied here the spectrum and the

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eigenfunctions are exactly known. Moreover, the potential $U_a(Z)$ and the effective potential $V_a(Z) = -(1/4)[U_a'(Z)]^2 + (1/2)U_a''(Z)$ are both differentiable (by opposition to the piecewise potential models). For special values of the parameter a, the diffusion process reduces to already known cases such as the Ornstein–Uhlenbeck process[12] or the Wong process.[7] For infinite probability densities delta-peaked on the axis of symmetry of $U_a(Z)$, the solution of the F.P.E. can be represented in a compact form already discussed in Ref. 16. This compact form permits us to calculate the branching time t_c which, for double-well potentials, characterizes the transition from a uni- to bimodal probability density. For very shallow wells, we find that t_c depends logarithmically on the bifurcation parameter a which controls the shape of $U_a(Z)$. Finally, we calculate the probability current over the working barrier, which is a crucial physical quantity in the double-well problem.

Our paper is organized as follows. In Section 2 we propose the model and construct the exact solution of the F.P.E. Section 3 is concerned with the discussion of a few special situations for which the probability density takes more compact forms. Finally, in Section 4 we calculate the branching time t_c and the probability current over the working barrier.

2. THE MODEL AND ITS SOLUTION

The diffusion problem we are able to solve reads

$$\frac{\partial P(Z,t\,|\,Z_0,0)}{\partial t} = \frac{\partial}{\partial Z}\left\{\left[\frac{d}{dZ}U_a(Z)\right]P(Z,t\,|\,Z_0,0) + \frac{\partial}{\partial Z}P(Z,t\,|\,Z_0,0)\right\},$$
$$Z \in \mathbb{R},\ t \in \mathbb{R}^+ \qquad (1)$$

with

$$U_a(Z) = 2\ln\{y_1(a,Z)\}$$
$$= 2\ln\left[e^{-Z^2/4}\,{}_1F_1\left(\frac{a}{2}+\frac{1}{4},\frac{1}{2},\frac{Z^2}{2}\right)\right] \qquad (1a)$$
$$a \geqslant -1/2 \qquad (1b)$$

and

$$P(Z,t=0\,|\,Z_0,0) = \delta(Z-Z_0) \qquad (1c)$$

The function $y_1(a,Z)$ is, for $a \geqslant -1/2$, a positive definite solution of the Weber equation[13]:

$$\frac{d^2}{dZ^2}y_1(a,Z) = \left(\frac{Z^2}{4}+a\right)y_1(a,Z) \qquad (2)$$

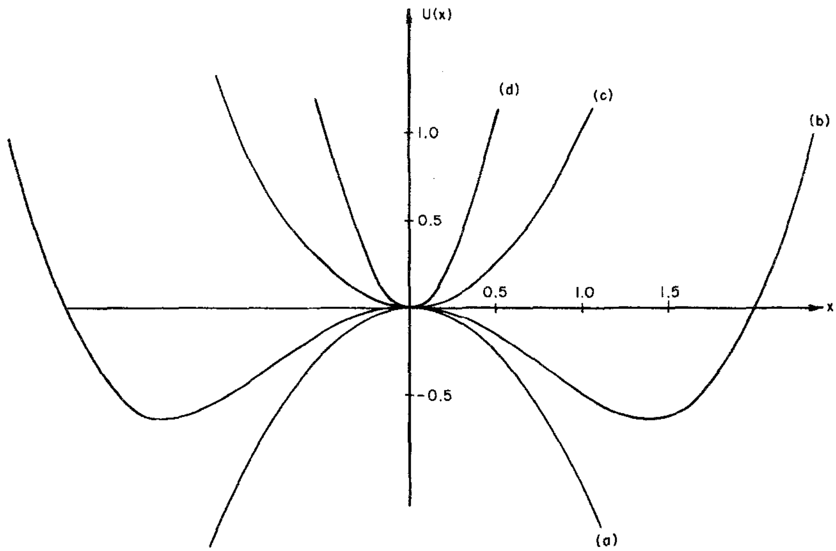

Fig. 1. Shape of $U(x)$ for (a) $a = -1/2$, (b) $a = -0.3$, (c) $a = 1/2$, (d) $a = 5/2$.

and the ${}_1F_1(a/2 + 1/4, 1/2, Z^2/2)$ stands for a Kummer's function.[13] The potential $U_a(Z)$ may exhibit the following behaviors[14] (Fig. 1):

$$\begin{aligned} &\text{(i)}\quad U_a(Z) = -\frac{Z^2}{4} && \text{when } a = -1/2 \\ &\text{(ii)}\quad U_a(Z) \text{ is an attractive double well} && \text{when } a \in]-1/2, 0[\\ &\text{(iii)}\quad U_a(Z) \text{ is an attractive single well} && \text{when } a > 0 \end{aligned} \tag{3}$$

To solve Eq. (1), we shall follow van Kampen's procedure,[4] and we first introduce the effective potential $V_a(Z)$ (Fig. 2):

$$V_a(Z) = \frac{1}{4}\left[\frac{d}{dZ} U_a(Z)\right]^2 - \frac{1}{2}\frac{d^2}{dZ^2} U_a(Z) \tag{4}$$

which, according to (1a), takes the form

$$V_a(Z) = -\frac{Z^2}{4} - a + 2\phi^2(Z) \tag{5}$$

with

$$\phi(Z) = \frac{d}{dZ} \ln\{y_1(a, Z)\} \tag{6}$$

The Schrödinger equation (S.E.) associated with our diffusion problem (1) then reads[4]

$$\frac{d^2}{dZ^2}\psi(Z) + [E - V(Z)]\psi(Z) = 0 \tag{7}$$

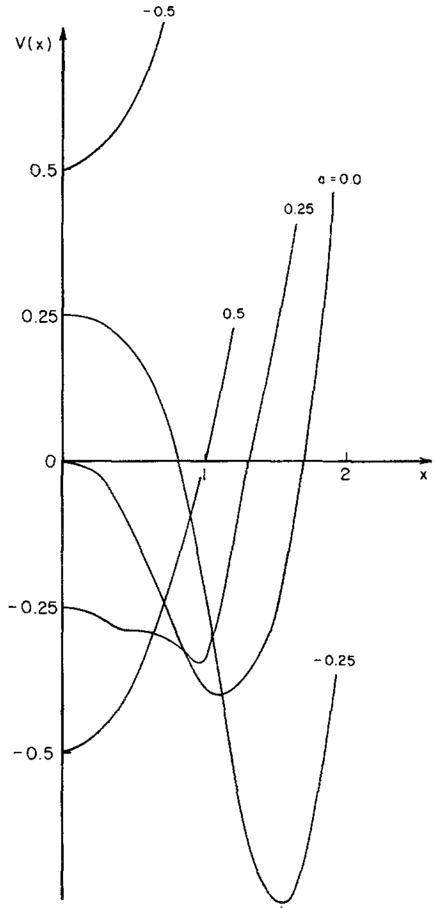

Fig. 2. Shape of $V(x)$.

where $\psi(Z)$ is an eigenfunction of $P(Z, t \mid Z_0, 0)[P(Z, \infty \mid Z_0, 0)]^{-1/2}$. To solve the (S.E.) (7), we introduce the transformation $\mathcal{W}$ defined by[19]

$$\mathcal{W}\psi(Z) = \chi(Z) = [y_1(a, Z)]^{-1} \frac{d}{dZ} \{y_1(a, Z)\psi(Z)\} \tag{8}$$

and therefore

$$\mathcal{W}^{-1}\varphi(Z) = [y_1(a, Z)]^{-1} \int y_1(a, Z)\varphi(Z)\, dZ \tag{9}$$[6]

[6] To guarantee that $\mathcal{W}^{-1}\mathcal{W}\psi Z) = \psi(Z)$, the constant of integration K, up to which the primitive function in (9) is defined, has to be chosen $K = 0$.

From Eqs. (8) and (2), we obtain

$$\frac{d}{dZ}\chi(Z) = \chi(Z)\phi(Z) - E\psi(Z) \tag{10}$$

$$\begin{aligned}\frac{d^2}{dZ^2}\chi(Z) &= \left\{\phi^2(Z) + \frac{d}{dZ}\phi(Z) - E\right\}\chi(Z)\\ &= \left[\frac{Z^2}{4} + a - E\right]\chi(Z)\end{aligned} \tag{11}$$

Imposing natural boundary conditions for $\psi(Z)$ in Eq. (7), the eigenfunctions of the Schrödinger problem (11) are

$$\chi_n(Z) = \exp\left\{-\frac{Z^2}{4}\right\}H_n\left(\frac{Z}{\sqrt{2}}\right) \tag{12}$$

and the spectrum reads

$$E_n = n + a + 1/2 \tag{13}$$

According to Eqs. (12) and (13), the solution of the diffusion problem (1) can be written in the form[4]

$$\begin{aligned}P(Z,t \mid Z_0,0) = N^{-1}\left[y_1(a,Z)\right]^{-2}\\ + \frac{y_1(a,Z_0)}{y_1(a,Z)}\sum_{n=0}^{\infty}\exp\left\{-\left(n + a + \frac{1}{2}\right)t\right\}\varphi_n(Z)\varphi_n(Z_0)\end{aligned} \tag{14}$$

where

$$\begin{aligned}\varphi_n(Z) &= C_n \mathcal{W}^{-1}\chi(Z)\\ &= C_n\left[y_1(a,Z)\right]^{-1}\int \chi_n(Z)y_1(a,Z)\,dZ\\ &= C_n\left[y_1(a,Z)\right]^{-1}\int {}_1F_1\left(\frac{1}{4} - \frac{a}{2}, \frac{1}{2}, -\frac{Z^2}{2}\right)H_n\left(\frac{Z}{\sqrt{2}}\right)dZ\end{aligned} \tag{15}$$

and

$$\int_{\mathbb{R}} \varphi_n(Z)\varphi_m(Z)\,dZ = \delta_{mn} \tag{16}$$

The normalization constant N occurring in Eq. (14) is calculated in Refs. 15 and 19, and reads

$$N = \sqrt{2}\,\Gamma\left(\frac{a}{2} + \frac{1}{4}\right)\Big/\Gamma\left(\frac{a}{2} + \frac{3}{4}\right) \tag{17}$$

The normalization coefficients C_n are calculated in Ref. 19.

3. SOME SPECIAL CASES

In this section, we shall consider special cases for which the expansion (14) can be summed up.

Case (i): First, we consider the case for which $Z_0 = 0$. In this case Eq. (14) reduces to the form

$$P(Z,t\,|\,0,0) = \left[y_1(a,Z)\right]^{-2} \int \left[\frac{\partial}{\partial Z} G(Z,t)\right] y_1(a,Z)\,dZ \tag{18}$$

where

$$G(Z,t) = N(t)\exp\left\{-\tfrac{1}{2}\alpha(t)Z^2\right\} \tag{18a}$$

$$\alpha(t) = \tfrac{1}{2}\coth t \tag{18b}$$

$$N(t) = \pi^{-1/2}\exp\{-at\}\left[\alpha(t)\right]^{-1}\left[\sinh t\right]^{-3/2} \tag{18c}$$

By direct substitution, it is easy to verify that Eq. (18) is a solution of Eq. (1).

Let us now discuss a few special values of the parameter a.

Case (ii):

$$a = 1/2 \Rightarrow y_1(1/2, Z) = \exp\{Z^2/4\} \tag{19}$$

From Eq. (15), the eigenfunctions take the form

$$\varphi_n(Z) = \frac{C_n e^{-Z^2/4} H_{n+1}(Z/\sqrt{2})}{(n+1)\sqrt{2}} \tag{20}$$

and (16) gives[13]

$$\int_{\mathbb{R}} \frac{e^{-Z^2/2}\left[H_{n+1}(Z/\sqrt{2})\right]^2}{2(n+1)^2}\,dZ = C_n^{-2} = \frac{2^n\sqrt{\pi}\,n!}{n+1} \tag{21}$$

Using (20) and (21), we have

$$P(Z,t\,|\,Z_0,0) = \frac{e^{-Z^2}}{(2\pi)^{1/2}}\left[1 + \sum \frac{e^{-(n+1)t}}{(n+1)!} H_{n+1}\left(\frac{Z}{\sqrt{2}}\right) H_{n+1}\left(\frac{Z_0}{\sqrt{2}}\right)\right] \tag{22}$$

which, by means of the Mehler's formula,[7] can be written in the form

$$P(Z,t\,|\,Z_0,0) = \left[2\pi(1-e^{-2t})\right]^{-1/2}\exp\left[-\frac{(Z - Z_0 e^{-t})^2}{2(1-e^{-2t})}\right] \tag{23}$$

Case (iii): $a = 2n + 1/2$, $n \in \mathbb{N} - \{0\}$, $Z_0 = 0$. In this case, the Weber function assumes a simpler form, namely,[13]

$$y_1(2n + 1/2, Z) = (-1)^n \frac{n!}{(2n)!} e^{Z^2/4} H_{2n}\left(\frac{iZ}{\sqrt{2}} \right) \tag{24}$$

In particular, for $n = 1$, Eq. (24) gives

$$U_{5/2}(Z) = \frac{Z^2}{2} + \ln(1 + Z^2) \tag{25}$$

The potential (25) leads to a drift which, besides its linear part, presents a saturation term of a similar form as the one occurring in the problems of lasers with saturable absorbers.[17] For $Z_0 = 0$, Eqs. (24) and (18) give

$$\begin{aligned} P(Z, t \mid 0, 0) = {} & \frac{e^{-3/2t}}{(2\pi \sinh t)^{1/2}} \exp\left[-\frac{Z^2}{2(1 - e^{-2t})} \right] (1 + Z^2)^{-1} \\ & + \frac{e^{-t/2} (\sinh t)^{1/2}}{2\sqrt{\pi}\,(1 + Z^2)^2} \exp\left[-\frac{Z^2}{2(1 - e^{-2t})} \right] \end{aligned} \tag{26}$$

From Eq. (26), we can calculate the variance $\langle Z^2(t) \rangle$. We obtain[13]

$$\begin{aligned} \langle Z^2(t) \rangle &= \int_{\mathbb{R}} Z^2 P(Z, t \mid 0, 0)\, dZ \\ &= \frac{1}{8} \left\{ \frac{e^{-(3/2)t}}{(\sinh t)^{1/2}} U\left(\frac{3}{2}, \frac{3}{2}, \left[2(1 - e^{-2t}) \right]^{-1} \right) \right. \\ &\quad \left. + 4e^{-t/2} (\sinh t)^{1/2} U\left(\frac{3}{2}, \frac{3}{2}, \left[2(1 - e^{-2t}) \right]^{-1} \right) \right\} \end{aligned} \tag{27}$$

where $U(a, b, Z)$ is a combination of Kummer's functions.[13] For $t \ll 1$, Eq. (27) can be expanded by use of the asymptotic expansions. We have[13]

$$U(a, b, Z) = Z^{-a}\left[1 + O(|Z|^{-1}) \right], \qquad \Re Z \to \infty$$

and therefore

$$\langle Z^2(t) \rangle_{t \ll 1} \approx \frac{t}{2} + t^2 \approx \frac{t}{2} \tag{28}$$

Case (iv): $a \to \infty$. To discuss this limiting case, let us introduce the change of variables:

$$x = \frac{Z}{(2\sqrt{A})^{1/2}}, \qquad a = \frac{B}{2\sqrt{A}} \tag{29}$$

With Eq. 29, Eq. (2) reads

$$\frac{d^2}{dx^2} y_1\left[\frac{B}{2\sqrt{A}}, (2\sqrt{A})^{1/2} x \right] = (Ax^2 + B) y_1\left[\frac{B}{2\sqrt{A}}, (2\sqrt{A})^{1/2} x \right] \tag{30}$$

Hence, in the limit $A \to 0$, we have

$$\lim_{A \to 0} y_1\left[\frac{B}{2\sqrt{A}}, (2\sqrt{A})^{1/2} x\right] = \cosh(\sqrt{B}\, x) \tag{31}$$

and therefore $U_\infty(x) = 2\ln\{\cosh(\sqrt{B}\, x)\}$.

It is interesting to note that this case has been studied in Ref. 7. Indeed, Wong considered the F.P.E.[7]:

$$\frac{\partial}{\partial t} P(y,t \mid y_0, 0) = (2K-1)\frac{\partial}{\partial y}\left[yP(y,t \mid y_0,0)\right] + \frac{\partial^2}{\partial y^2}\left[(1+y^2)P(y,t \mid y_0,0)\right] \tag{32a}$$

For $K = 1$ and in terms of the new variable $x = \sinh y$, Eq. (32) takes the form

$$\frac{\partial}{\partial t} P(x,t \mid x_0,0) = -2\frac{\partial}{\partial x}\{\tanh x P(x,t \mid x_0,0)\} + \frac{\partial^2}{\partial x^2} P(x,t \mid x_0,0) \tag{32b}$$

Equation (32b) is precisely the F.P.E. obtained with the force field derived from $U_\infty(x) = 2\ln\{\cosh(\sqrt{B}\, x)\}$. When $Z_0 = 0$, Eq. (18) can be easily identified as the Wong solution.[7] Indeed, using Eq. (31) and Eq. (18) we obtain for $B = 1$:

$$P(Z,t \mid Z_0,0) = \frac{e^{-t}}{(4\pi t)^{1/2}} e^{-Z^2/4t}\cosh Z + \frac{1}{4}\{E_+(Z,t) - E_-(Z,t)\} \tag{33}$$

where the error functions $E_\pm(Z,t)$ read

$$E_\pm(Z,t) = \text{erf}\left[\frac{Z}{(4t)^{1/2}} \pm \sqrt{t}\right]$$

4. PROBABILITY CURRENT AND BRANCHING TIME

The solution (14) permits immediately to calculate the probability current at $Z = 0$. We have

$$\begin{aligned} J(Z_0,t) &= \left.\frac{\partial P(Z,t \mid Z_0,0)}{\partial Z}\right|_{Z=0} \\ &= \sum_{n=0}^{\infty} (C_n)^2 \exp\left\{-\left(n + a + \frac{1}{2}\right)t\right\} H_n(0) \\ &\quad \times \int^{Z_0} {}_1F_1\left(\frac{1}{4} - \frac{a}{2}, \frac{1}{2}, -\frac{Z^2}{2}\right) H_n\left(\frac{Z}{\sqrt{2}}\right) dZ \end{aligned} \tag{34}$$

For $t \gg 1$, only the first eigenvalue ($n = 0$) contributes to Eq. (34), and we can write

$$J(Z_0, t \gg 1) \approx 2C_0^2 Z_0\, {}_1F_1\left(\frac{1}{4} - \frac{a}{2}, \frac{3}{2}, -\frac{Z_0}{2}\right)\exp\left\{-\left(a + \frac{1}{2}\right)t\right\} \quad (35)$$

Equation (35) clearly indicates that for $a \approx -1/2$, namely, for very deep wells, the transfer of probability from one well to the other is very slow, and we are in a situation of metastability.

Finally in the double-well cases ($a < 0$), we can, for $Z_0 = 0$, calculate the branching time t_c which characterizes the transition from a uni- to a bimodal probability density. According to the symmetry of the problem, t_c is defined by the equation

$$\left.\frac{\partial^2}{\partial Z^2} P(Z, t = t_c \mid 0, 0)\right|_{Z=0} = 0 \quad (36)$$

Using Eq. (18), Eq. (36) takes the form

$$\frac{\partial^2}{\partial Z^2} G(Z, t_c) - 2a \int \frac{\partial}{\partial Z} G(Z, t_c) y_1(a, Z)\, dZ = 0 \quad (37)$$

By substitution of (1a) into Eq. (18), we obtain

$$P(Z, t \mid 0, 0) = -\frac{N(t)\alpha(t)}{[y_1(a, Z)]^2} \times \int Z \exp\left\{-\left[\alpha(t) + \frac{1}{2}\right]\frac{Z^2}{2}\right\} {}_1F_1\left(\frac{a}{2} + \frac{1}{4}, \frac{1}{2}, \frac{Z^2}{2}\right) dZ \quad (38)$$

or equivalently

$$P(Z, t \mid 0, 0) = -\frac{N(t)\alpha(t)}{[y_1(a, Z)]^2} \sum_{n=0}^{\infty} \frac{(a/2 + 1/4)_n \cdot M_n(Z, t)}{(1/2)_n n! [\alpha(t) + 1/2]^n} \quad (39)^7$$

with

$$M_n(Z, t) = \int^{[\alpha(t) + 1/2](Z^2/2)} e^{-\omega} \omega^n\, d\omega \quad (39a)$$

By integration, Eq. (39) gives

$$P(Z, t \mid 0, 0) = \frac{N(t)\alpha(t) \exp\{-[\alpha(t) + 1/2](Z^2/2)\}}{[y_1(a, Z)]^2 [\alpha(t) + 1/2]} \times \sum_{n=0}^{\infty} \frac{(a/2 + 1/4)_n (1)_n}{n! (1/2)_n [\alpha(t) + 1/2]^n} l_n\left\{\left[\alpha(t) + \frac{1}{2}\right]\frac{Z^2}{2}\right\} \quad (40)$$

[7] $(\alpha)_n = \Gamma(\alpha + n)/\Gamma(\alpha)$ is a Pochhammer coefficient.

where

$$l_n(x) = \sum_{K=0}^{n} \frac{c^K}{K!} \tag{40a}$$

Using Eq. (40) and Eq. (37), we have

$$-2a\left[\alpha(t_c) + 1/2\right]^{-1/2} {}_2F_1\left[\begin{matrix} \frac{a}{2} + \frac{1}{4}, 1 \\ \\ \frac{1}{2}; \end{matrix} \quad \frac{1}{\alpha(t_c) + 1/2}\right] = 1 \tag{41}$$

Now, we introduce the linear transformation[13]

$$\begin{aligned} {}_2F_1\left(\begin{matrix} a, b \\ c; \end{matrix} \; Z\right) &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} {}_2F_1\left[\begin{matrix} a, b \\ a+b-c+1; \end{matrix} \; 1-Z\right] \\ &\quad + (1-Z)^{c-a-b} \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)} \\ &\quad \times {}_2F_1\left[\begin{matrix} c-a, c-b \\ c+1-a-b; \end{matrix} \; 1-Z\right] \end{aligned} \tag{42}$$

For very shallow wells (i.e., $a \sim 0^-$), $t_c \gg 1$. Hence, we obtain

$$t_c \approx \frac{2}{3} \ln\left\{ -\frac{3\Gamma(5/4)}{2\sqrt{\pi}\,\Gamma(7/4)} a^{-1} \right\} \tag{43}$$

Equation (46) indicates that t_c depends logarithmically on the bifurcation parameter a which controls the shape of the potential $U_a(Z)$. This point has recently been discussed by Horsthemke.[18] A generalization to include asymmetric double-well situations is presently under study.

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