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Numerical Simulations of Stochastic Differential Equations

Ronald F. Fox[1]

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A simple, very accurate algorithm for numerical simulation of stochastic differential equations is described. Its relationship to colored noise is elucidated and exhibited by explicit results. The especially delicate problem of mean first passage times is highlighted and highly accurate agreement between the numerical simulations and analytic results are shown.

KEY WORDS: Numerical simulation; stochastic differential equations; colored noise; mean first passage times; bistability.

1. INTRODUCTION

My interest in numerical simulation of stochastic differential equations arose during a collaboration with R. Roy which concerned the noise properties of dye lasers.[1-4] These studies simultaneously involved the theory of multiplicative colored noise, measurements of noise characteristics in dye lasers, and numerical simulations of stochastic differential equations. By fitting certain noise parameters in the simulations, good agreement with the measurements could be obtained. However, this method was only as good as the simulations, and so we embarked on a study[5] of the accuracy of the then acceptable simulation algorithms.[6,7] This study resulted in the simple, improved algorithm to which I will return later in this paper.

Concurrently with the dye laser studies, I was also pursuing the study of the effects of colored noise on mean first passage times in bistability problems.[8] This problem was brought to my attention by Peter Hanggi,[9,10] with whom I have had a continuing dialogue on the subject.

[1] School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332.

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The literature on this subject has become diverse, confused, and contentious. Recently, I called for accurate numerical work[11] in order to help bring clarity to the problem. Since no such accurate numerical study was forthcoming, I was compelled to engage in such studies myself. The preliminary results of these studies are reported below.

2. COLORED NOISE AND BISTABILITY

The prolem of bistability and colored noise may be given the mathematical formulation

$$\dot{x} = W(x) + f \tag{1}$$

where $W(x) = ax - bx^3$ and f is "exponentially correlated" colored noise which is Gaussian, has zero mean, and satisfies

$$\langle f(t) f(s) \rangle = D_0 \lambda \exp(-\lambda |t-s|) \tag{2}$$

in which D_0 is the noise strength and λ^{-1} is the colored noise correlation time. In the limit of a short correlation time, f goes over to white noise, f_w, with correlation

$$\langle f_w(t) f_w(s) \rangle = 2D_0 \delta(t-s) \tag{3}$$

The colored noise problem is non-Markovian, but for weakly colored noise an effective Fokker–Planck description is possible[8] which provides one with a theory for all the statistical properties of the system. This effective theory is one dimensional, the x dimension, and several approximate theories have been proposed for it. Three versions are briefly described below.

All versions yield an effective Fokker–Planck equation of the form

$$\frac{\partial}{\partial t} P = -\frac{\partial}{\partial x} [W(x) P] + \frac{\partial^2}{\partial x^2} [D(x) P] \tag{4}$$

in which $D(x)$ is the effective diffusion "constant" for weakly colored noise. In one version,[12] often called the "best Fokker–Planck equation," a perturbation expansion in λ^{-1} is used to yield

$$D(x) = D_0 [1 + \lambda^{-1} W'(x)] \tag{5}$$

in which $W'(x)$ denotes the x derivative of $W(x)$. Van Kampen has analyzed this procedure and has observed that it is asymptotic in λ^{-1} because $D(x)$ becomes negative for sufficiently large $|x|$ and fixed λ^{-1}.

Only as λ^{-1} goes to zero does $D(x)$ remain positive for the whole domain of x, which is $(-\infty, \infty)$. Another version,[10] called the "Hanggi ansatz," yields

$$D(x) = D_0[1 + \lambda^{-1}(3b\langle x^2\rangle - a)]^{-1} \tag{6}$$

in which $\langle x^2\rangle$ denotes the mean square value of x. This is a "mean-field" type of approximation. For it, $D(x)$ is always positive. Using functional calculus, I found an essentially nonperturbative approach[8] to weakly colored noise which produced

$$D(x) = D_0[1 - \lambda^{-1}W'(x)]^{-1} \tag{7}$$

which shows a clear relationship to both (5) and (6). However, it is *not* asymptotic in λ^{-1} and remains positive for fixed, but sufficiently small λ^{-1}, throughout the entire x domain. Consequently, I called this a "uniform" approximation (for uniform positivity in x).

The point of all this is that for weakly colored noise, the existence of an effective Fokker–Planck equation makes it possible to apply well-understood procedures for Markov processes to a weakly non-Markov process.

On the other hand, it is also possible to reformulate the problem as a two-dimensional problem which is Markov for arbitrary noise coloring. This is done as follows:

$$\dot{x} = W(x) + \varepsilon \tag{8}$$

$$\dot{\varepsilon} = -\lambda\varepsilon + \lambda g_w \tag{9}$$

in which g_w is Gaussian, white noise with zero mean and correlation

$$\langle g_w(t)\, g_w(s)\rangle = 2D_0\delta(t-s) \tag{10}$$

The driven process ε has correlation

$$\{\langle \varepsilon(t)\, \varepsilon(s)\rangle\} = D_0\lambda \exp(-\lambda\,|t-s|) \tag{11}$$

just like in (2), except that here $\langle\cdots\rangle$ refers to averaging over g_w and $\{\cdots\}$ refers to averaging the initial value of ε, i.e., $\varepsilon(0)$, over the stationary distribution for $\varepsilon(0)$, i.e.,

$$P(\varepsilon(0)) = \frac{1}{(2\pi D_0\lambda)^{1/2}} \exp\left[-\frac{1}{2}\frac{\varepsilon^2(0)}{D_0\lambda}\right] \tag{12}$$

It is important to emphasize the necessity for this second averaging in (11) in order to get a stationary correlation. This feature is especially important

in the numerical simulations, where it has often been overlooked in the past.

While Eqs. (8) and (9) describe a bona fide Markov process in two dimensions, the corresponding Fokker–Planck equation

$$\frac{\partial}{\partial t} P = -\partial_x \{[W(x)+\varepsilon]P\} + \frac{\partial}{\partial \varepsilon}\left[\left(\lambda\varepsilon + D_0\lambda^2 \frac{\partial}{\partial \varepsilon}\right) P\right] \tag{13}$$

is very difficult to analyze because of its dependence on two variables, x and ε. This is the main reason so much effort went into finding effective Fokker–Planck equations in just one variable, x, even though these equations were still tough to analyze.

One quantity is very sensitive to whether a one-dimensional or a two-dimensional approach is used. This quantity is the mean first passage time. Its sensitivity on dimension results from the necessity of introducing absorbing boundaries in the calculation of the first passage time distribution. The boundary conditions in the two-dimensional formulation do not necessarily devolve into appropriate boundary conditions in the one-dimensional formulation. When they do not, the one-dimensional formulation is simply impotent when it comes to computing the mean first passage time.

The rest of this paper is divided as follows. Section 3 reviews earlier work which resulted in a simple, accurate algorithm for numerical simulation of stochastic differential equations. Section 4 presents a mean first passage time problem which is simpler than that for the bistability case and which allows comparison of analytic expressions and numerical results. In Section 5, a brief account of the current situation with respect to the bistability problem is given as a guide to future efforts.

3. NUMERICAL SIMULATIONS

To test the accuracy of numerical simulation algorithms for colored noise, it is necessary to find a problem which can be solved analytically in closed form so that a comparison of theory with simulation can be quantitative. The Kubo oscillator provides such a problem and we studied it in detail recently.[5]

Let ω_0 be a constant frequency and ω be a stochastic, real frequency with a Gaussian distribution, zero mean, and correlation

$$\{\langle \omega(t)\,\omega(s)\rangle\} = \tfrac{1}{2}Q\lambda \exp(-\lambda\,|t-s|) \tag{14}$$

The Kubo oscillator equation can be written in terms of the time evolution for a complex variable $a(t)$ which satisfies

$$\dot{a} = i(\omega_0 + \omega)a \tag{15}$$

where

$$\dot{\omega} = -\lambda\omega + \lambda g_w \tag{16}$$

in which g_w is Gaussian, white noise with zero mean and correlation

$$\langle g_w(t)\, g_w(s)\rangle = Q\delta(t-s) \tag{17}$$

$\langle\cdots\rangle$ denotes averaging with respect to g_w, whereas $\{\cdots\}$ denotes averaging with respect to the initial values for ω, $\omega(0)$, in accord with the stationary distribution

$$P(\omega(0)) = \frac{1}{(\pi Q\lambda)^{1/2}} \exp\left[-\frac{\omega(0)^2}{Q\lambda}\right] \tag{18}$$

Note the difference in factors of 2 between Eqs. (2) and (3) and Eqs. (14) and (17). This apparent inconsistency only represents a difference in convention, which is represented in the literature by roughly equal usages of each choice. By using both choices in one paper, I hope the reader will watch "like a hawk" the appearance of factors of 2, and thereby learn to avoid one of the simpler sources of error.

The variable a can be equally well represented by two real variables, r and ϕ through

$$a = re^{i\phi} \tag{19}$$

When this is done, ϕ satisfies an "additive" stochastic differential equation instead of the "multiplicative" equation (15), and r is a constant. The exact equation for the probability distribution for ϕ is

$$\frac{\partial}{\partial t} P = -\omega_0 \frac{\partial}{\partial\phi} P + D(t) \frac{\partial^2}{\partial\phi^2} P \tag{20}$$

where $P(\phi, 0) = \delta(\phi - \phi_0)$, and

$$D(t) = \tfrac{1}{2}Q(1 - e^{-\lambda t}) \tag{21}$$

This is *not* a Fokker–Planck equation, because ϕ is *not* a Markov process, and P does not satisfy the Chapman–Kolmogorov equation. Nevertheless, $P(\phi, 0)$ does provide a great deal of statistical information about ϕ. In fact, $P(\phi, t)$ can be obtained in closed form:

$$P(\phi, t) = \frac{1}{2\pi} \sum_{m=-\infty}^{\infty} \exp\left[im\phi - im\phi_0 - im\omega_0 t - m^2 \int_0^t ds\, D(s)\right] \tag{22}$$

With this solution, we were able to compute exact expressions[5] for $\langle\phi\rangle$, $\langle\Delta\phi^2\rangle \equiv \langle(\phi - \langle\phi\rangle)^2\rangle$, and $\langle\Delta\phi^3\rangle/\langle\Delta\phi^2\rangle^{3/2}$ as functions of time. The reader is referred to ref. 5 for figures which show these results for several choices of the parameters Q and λ. (In fact, in all of the figures, $\omega_0 = 1$, $\phi_0 = 45°$, and the time axis is given in units of real time/2π. This last fact was inadvertently unstated in ref. 5 and must be noted if one attempts to reproduce our results.) In addition to these exact results, which are plotted as smooth, continuous curves in the figures, there are numerous small boxes superimposed on the curves and exhibiting the results of numerical simulation. The agreement is clearly excellent.

The following points are worth emphasis:

1. We used the Box–Mueller algorithm[13] to generate Gaussian random variables from uniform random variables. That is, to get g_w, we wrote

$$\begin{aligned} a &= \mathrm{RND}(1) \\ b &= \mathrm{RND}(1) \\ g_w &= \mathrm{SQR}(-2{*}Q{*}t{*}\ \mathrm{LOG}(a)){*}\ \cos(2\pi{*}b) \end{aligned} \tag{23}$$

in which t denotes the integration step size, which was kept constant throughout the simulation. To get the distribution for initial values of ω, $\omega(0)$, we used

$$\begin{aligned} m &= \mathrm{RND}(1) \\ n &= \mathrm{RND}(1) \\ \omega(0) &= \mathrm{SQR}(-Q{*}\lambda{*}\ \mathrm{LOG}(m)){*}\ \cos(2\pi{*}n) \end{aligned} \tag{24}$$

This second use of Box–Mueller was essential for accurate results!

2. We treated the coupled pair of equations (15) and (16) as three coupled equations in three real variables, ω, x, and y, where $a = x + iy$. The simulation algorithm we have developed regards x, y, and ω as ordinary variables everywhere in the simulation program except for just one line, the line in which g_w influences ω. To be explicit, the essential features of such a program are given below for a Runge-Kutta-2 program:

$$\begin{aligned} m &= \mathrm{RND}(1) \\ n &= \mathrm{RND}(1) \\ \omega_0 &= \mathrm{SQR}(-Q{*}\lambda{*}\ \mathrm{LOG}(m)){*}\ \cos(2\pi{*}n) \end{aligned} \tag{25}$$

$$a = \mathrm{RND}(1)$$
$$b = \mathrm{RND}(1) \tag{26}$$
$$g_w = \mathrm{SQR}(-2{*}Q{*}t{*}\ \mathrm{LOG}(a)){*}\cos(2\pi{*}b)$$

$$j1 = t{*}(-(\omega_0 + \omega 0){*}\, y0)$$
$$k1 = t{*}((\omega_0 + \omega 0){*}\, x0) \tag{27}$$
$$h1 = t{*}(-\lambda{*}\omega 0)$$

$$j2 = t{*}(-(\omega_0 + \omega 0 + h1)){*}\ (y0 + k1)$$
$$k2 = t{*}((\omega_0 + \omega 0 + h1){*}\ (x0 + j2)) \tag{28}$$
$$h2 = t{*}(-\lambda{*}(\omega 0 + h1))$$

$$x1 = x0 + \tfrac{1}{2}(j1 + j2)$$
$$y1 = y0 + \tfrac{1}{2}(k1 + k2) \tag{29}$$
$$\omega 1 = \omega 0 + \tfrac{1}{2}(h1 + h2) + \lambda{*}g_w$$

$$x0 = x1$$
$$y0 = y1 \tag{30}$$
$$\omega 0 = \omega 1$$

At the end of this sequence, the program loops back to (25) and repeats. Note that in each line of (27) and (28) the step size t appears to the first power, whereas in the last line of (29) it also appears as a square root in g_w, as follows from the last line of (26).

3. One can also write down an Euler version of this program, which is of course shorter. However, a shorter step size is required in order to achieve comparable accuracy. One must always check that the exponential decay implicit in Eq. (16) is in fact accurately simulated, since it can already provide error. Thus, Runge-Kutta-2 or even Runge-Kutta-4 is preferable.

4. A very useful insight gained from these studies is that "weakly" colored noise is essentially white noise. This means that a simulation of colored noise with λ^{-1} sufficiently small is effectively a white noise simulation. This perspective is precisely the viewpoint of Stratonovich in his version of the so-called Ito stochastic calculus.[14] It is the reason why everything presented in this paper has been in the Stratonovich version. What constitutes "sufficiently small λ^{-1}" is determined by the secular time scales in the problem. For example, in the Kubo oscillator simulation, the

time scale is set by the period of oscillation, $2\pi/\omega_0$, which is just 2π for $\omega_0 = 1$. A look at the figures in ref. 5 shows that the figures for a directly white noise algorithm (Figs. 10–12) are indistinguishable from the figures for the weakly colored algorithm (Figs. 7–9), which were obtained for $\lambda = 10$, i.e., for $\lambda^{-1} = 0.1$. This means that when the colored noise correlation time is approximately 63 times smaller than the period of secular oscillation, we have effectively white noise. Now, as far as ϕ is concerned, these six figures show indistinguishable results, but this is not the case for r, as is discussed in the next point.

5. The quantity r is supposed to remain constant according to (15) and (19). Using initial conditions for which $r = 1$, Fig. 15 of ref. 5 shows that the weakly colored noise algorithm ($\lambda = 10$) satisfies this constraint. The figure shows the result of ten full periods of time evolution and no observable deviation from $r = 1$. On the other hand, the direct white noise algorithm, which does so well for ϕ, as exhibited in Figs. 10–12, does not preserve r for a time step identical with that used in Fig. 15. This is shown in Figs. 13 and 14 of ref. 5. How can this be? The answer has to do with dependence on step size in the respective algorithms. For the direct white noise algorithm, the program which replaces the colored noise algorithm given above in Eqs. (23)–(30) is

$$a = \mathrm{RND}(1)$$
$$b = \mathrm{RND}(1) \tag{31}$$
$$g_w = \mathrm{SQR}(-2{*}Q{*}t{*}\ \mathrm{LOG}(a)){*}\cos(2\pi{*}b)$$

$$j1 = t{*}(-\omega_0 + y0)$$
$$k1 = t{*}(\omega_0 + x0) \tag{32}$$

$$j2 = t{*}(-\omega_0{*}(y0 + k1))$$
$$k2 = t{*}(\omega_0{*}(x0 + j1)) \tag{33}$$

$$x1 = x0 + \tfrac{1}{2}(j1 + j2) + g_w$$
$$y1 = y0 + \tfrac{1}{2}(k1 + k2) + g_w \tag{34}$$

$$x0 = x1$$
$$y0 = y1 \tag{35}$$

The crucial difference is between lines (29) and lines (34). In lines (29), $x1$ and $y1$ contain terms of order t, whereas in lines (34) they *also* contain terms of order $t^{1/2} \gg t$, through g_w. Since these lines do not conserve $r =$

$x^2 + y^2$ exactly, the error in (34) is larger than in (29) for identical step size. As shown in Fig. 13 of ref. 5, the step size which preserves $r = 1$ for ten periods with the colored noise algorithm (Fig. 15) almost completely destroys r after ten periods with the direct white noise algorithm. Thus, for fixed step size, the weakly colored noise algorithm is a more accurate method than the direct white noise algorithm. Various alternative algorithms which introduce g_w into lines (32) and (33) instead of into (34) do not change these results in any significant way.

We are now in a position to attempt accurate numerical simulations of mean first passage times.

4. FIRST PASSAGE TIMES

Because closed-form analytic results for the first passage time distribution in the bistability problem do not exist, we looked for a problem for which closed-form expressions did exist. The simplest possibility is a colored-noise Brownian motion, or random walk, described by the equations

$$\dot{x} = \varepsilon \tag{36}$$

$$\dot{\varepsilon} = -\lambda\varepsilon + \lambda g_w \tag{37}$$

in which g_w is Gaussian, white noise with zero mean and correlation

$$\langle g_w(t)\, g_w(s)\rangle = 2D\delta(t-s) \tag{38}$$

These equations imply that ε is also Gaussian with zero mean and correlation

$$\{\langle \varepsilon(t)\, \varepsilon(s)\rangle\} = D\lambda \exp(-\lambda\,|t-s|) \tag{39}$$

where $\{\cdots\}$ refers to averaging over the initial values of ε, $\varepsilon(0)$, which are distributed by the Gaussian, stationary distribution

$$P_{eq}(\varepsilon(0)) = \frac{1}{(2\pi D\lambda)^{1/2}} \exp\left[-\frac{\varepsilon(0)^2}{2D\lambda}\right] \tag{40}$$

The tractability of this problem has the virtue that we can look at both its two-dimensional representation and its reduced, one-dimensional representation. Using van Kampen's lemma,[15,16] we obtain directly from (36) and (39) the probability distribution evolution equation in one dimension:

$$\frac{\partial}{\partial t} P(x, t) = D(1 - e^{-\lambda t}) \frac{\partial^2}{\partial x^2} P(x, t) \tag{41}$$

This is *not* a Fokker–Planck equation, in parallel with the situation for Eq. (20). Using van Kampen's lemma again, Eqs. (36)–(38) imply the bona fide, two-dimensional Fokker–Planck equation

$$\frac{\partial}{\partial t}\bar{P}(x,\varepsilon,t)=-\frac{\partial}{\partial x}[\varepsilon\bar{P}(x,\varepsilon,t)]+\frac{\partial}{\partial\varepsilon}\left[\left(\lambda\varepsilon+D\lambda^2\frac{\partial}{\partial\varepsilon}\right)\bar{P}(x,\varepsilon,t)\right] \tag{42}$$

These two equations are related in another way as well. If the initial distribution $\bar{P}(x,\varepsilon,0)$ is written

$$\bar{P}(x,\varepsilon,0)=P(x,0)\,P_{\text{eq}}(\varepsilon) \tag{43}$$

and we introduce differential operators L and K defined by

$$L=-\frac{\partial}{\partial x}\varepsilon \tag{44}$$

$$K=\frac{\partial}{\partial\varepsilon}\left(\lambda\varepsilon+D\lambda^2\frac{\partial}{\partial\varepsilon}\right) \tag{45}$$

then we can prove that

$$P(x,t)=\int_{-\infty}^{\infty}d\varepsilon\,\exp[t(L+K)]\,P(x,0)\,P_{\text{eq}}(\varepsilon) \tag{46}$$

satisfies Eq. (41). That is, the contraction of $\bar{P}(x,\varepsilon,t)$ over ε yields $P(x,t)$. This identity follows from the commutator algebra for L and K, which may be summarized by

$$[K,\cdot]^{2n}L=(-\lambda)^{2n}L \tag{47}$$

$$[K,\cdot]^{2n-1}L=(-\lambda)^{2n-1}\frac{\partial}{\partial x}\left(\varepsilon+2D\lambda\frac{\partial}{\partial\varepsilon}\right) \tag{48}$$

These results suggest that Eq. (41) provides an exact reduction of Eq. (42) and that the statistics for x alone are completely accounted for by $P(x,t)$.

The last remark was checked by comparing the prediction of Eq. (41) for the mean square deviation in x, $\Delta x=x-x_0$, for a time interval t:

$$\langle\Delta x^2\rangle=2D[t+\lambda^{-1}(e^{-\lambda t}-1)] \tag{49}$$

with numerical simulations of Eqs. (36)–(38) done with a program of the type described in Eqs. (25)–(30). Using a step size of 10^{-6}, D values of 0.5, 1, and 10, and λ^{-1} values of 0.01 and 0.001 in various combinations,

accuracy of 0.1% is obtained! This clearly confirms both our theoretical perspective and our numerical algorithm.

The situation for the mean first passage time is much different. To analytically solve a mean first passage time problem, one must first find a solution for the first passage time distribution which satisfies the so-called backward equation[17,18] associated with the forward equation [either Eq. (41) or (42) in this case] with absorbing boundary conditions. Specifically, if x starts at $x=L$, and we seek the first passage time distribution for x arriving at either 0 or at $2L$ for the first time, and then the backward equation associated with Eq. (41) is

$$\frac{\partial}{\partial t} Q = D(1-e^{-\lambda t}) \frac{\partial^2}{\partial x^2} Q \tag{50}$$

with absorbing boundaries at 0 and $2L$. This problem can be solved in closed form[19] and we get

$$Q(x', t; x, 0) = \frac{1}{[4\pi D(t)]^{1/2}} \sum_{l=-\infty}^{\infty} \left\{ \exp\left[-\frac{(x'-x+4lL)^2}{4D(t)} \right] - \exp\left[-\frac{(x'+x+4lL)^2}{4D(t)} \right] \right\} \tag{51}$$

where $D(t) = D(t+\lambda^{-1}(e^{-\lambda t}-1))$ and $x \in [0, 2L]$. $Q=0$ for $x=0$ and $x=2L$ is manifest. The mean first passage time to reach these boundaries from any initial point $x \in [0, 2L]$ is denoted by $T(x)$ and is given by[17]

$$T(x) = \int_0^{\infty} dt \int_0^{2L} dx'\, Q(x', t; x, 0) \tag{52}$$

Starting from the middle of the interval, a lengthy calculation yields

$$T(L) = \frac{L^2}{2D} + \lambda^{-1} \sum_{m=1}^{\infty} \frac{m^{m-1} e^{-m}}{m!} \times \left\{ 1 - \frac{2}{\exp[(m/D\lambda^{-1})^{1/2} L] + \exp[-(m/D\lambda^{-1})^{1/2} L]} \right\} \tag{53}$$

This formula has a leading term, $L^2/2D$, which is the well-known white noise result, which can readily be confirmed by numerical simulation. In addition, there are two λ^{-1} corrections, one by itself and one involving an infinite summation. It is relatively easy to evaluate this formula numerically, although some care must be exercised in evaluating the summation over m. Having said all this, and using parameter values and step

sizes for which Eq. (49) was verified to better than 0.1%, repeated numerical simulations for colored noise failed to confirm (53)!! Only in the white noise limit of weakly colored noise did agreement occur. What has gone wrong?

The answer to this plea is a bit subtle. It requires looking at the first passage time problem in the two-dimensional context of Eq. (42). When formulated in two dimensions, approximate boundary conditions in two dimensions are required. If we work with the backward equation associated with Eq. (42), these boundary conditions are that there are absorbing boundaries in the x–ε plane. One boundary is at $x = 2L$ and extends along the ε axis from $\varepsilon = 0$ to $\varepsilon = \infty$. The negative half of this line, i.e., from $\varepsilon = 0$ to $\varepsilon = -\infty$ is *not* included. This is because the arrival of x at $x = 2L$ for the first time must have $\varepsilon \geqslant 0$ since $\dot{x} = \varepsilon$. Similarly, the other boundary is at $x = 0$ and extends along the ε axis from $\varepsilon = 0$ to $\varepsilon = -\infty$ because the first arrival at $x = 0$ requires that $\dot{x} = \varepsilon \leqslant 0$. These boundary conditions in the x–ε plane are *not* preserved by the boundary conditions imposed on Eq. (50) for the reduced, one-dimensional description because the reduced description involved integration over ε from $-\infty$ to ∞, as is explicitly seen in Eq. (46). Thus, the boundary conditions needed for a first passage time calculation do not contract along with the contraction of the forward equation for the probability distribution. One is obliged to stay in the higher-dimensional picture in order to get mean first passage times.

Obviously, we should now proceed to solve the backward equation obtained from Eq. (42) with the boundary conditions described above and then compute the mean first passage time for comparison with the numerical simulations. This is not an easy task! In fact, no one has been able to do this with full generality. However, certain asymptotic results have recently been reported[20] which yield a formula which I have been able to check *and* confirm. These results actually involve solving the forward equation, Eq. (42), with appropriate associated boundary conditions, rather than the backward equations. Under certain conditions, satisfied in this case, although not generally, it is possible to use the forward equation to obtain first passage time results. Hagan *et al.*[20] obtained

$$T = \frac{L^2}{2D} + \left|\zeta\left(\frac{1}{2}\right)\right| L\left(\frac{\lambda^{-1}}{D}\right)^{1/2} + \lambda^{-1}\left[\frac{1}{2}\zeta\left(\frac{1}{2}\right)^2 + \kappa - \frac{1}{2}\right] \tag{54}$$

to within a transcendentally small error of order $\exp[-L(D\lambda^{-1})^{-1/2}]$, i.e., provided $D\lambda^{-1} \ll L^2$. Here $\zeta(1/2)$ is the Riemann zeta function evaluated at 1/2 and has the value $-1.46035...$, and κ has the value 0.2274981.... I have confirmed this prediction with numerical simulations for eight sets of

Table I

L	D	λ^{-1}	Δt	T	$\exp[-L/(D\lambda^{-1})^{1/2}]$	Sim	Er	Its
0.05	1.0	10^{-5}	10^{-6}	1.489×10^{-3}	1.35×10^{-7}	1.480×10^{-3}	1.0046	4580
0.01	1.0	10^{-5}	10^{-6}	1.041×10^{-4}	4.2×10^{-2}	1.048×10^{-4}	1.023	5000
0.05	5.0	10^{-5}	10^{-6}	3.612×10^{-4}	8.49×10^{-4}	3.588×10^{-4}	1.010	5000
0.08	12.0	2×10^{-5}	10^{-6}	4.334×10^{-4}	5.7×10^{-3}	4.332×10^{-4}	1.0069	5000
0.05	10.0	10^{-5}	10^{-6}	2.060×10^{-4}	6.7×10^{-3}	2.099×10^{-4}	1.0143	5000
0.2	10.0	10^{-5}	10^{-6}	2.300×10^{-3}	2.0×10^{-9}	2.291×10^{-3}	1.0036	5000
0.1	10.0	10^{-4}	10^{-6}	1.041×10^{-3}	4.23×10^{-2}	1.037×10^{-3}	1.0023	5000
0.1	10.0	5×10^{-5}	10^{-6}	8.66×10^{-4}	1.14×10^{-2}	8.62×10^{-4}	1.0032	3136

parameter values, to better than 1% in each instance. The results are tabulated in Table I. In Table I, the symbols L, D and λ^{-1} are defined as in the text, and T denotes formula (54). Δt denotes the step size used in the numerical simulations, the results of which appear in the column labeled Sim. When these simulations are run, the position x always exceeds L by some small amounts which depend on L and D. This excess is measured by the quantity given in the column labeled Er, which records the average excess for the total number of iterations run, the number recorded in the last column.

5. BISTABILITY

We are now in a position to engage in numerical simulations for mean first passage times in a double-well potential, i.e., bistability. Several attempts[21–23] at analytic results have already been proposed for various parameter domains, within the two-dimensional context. One attempt[21] utilizes a matrix continued fraction approach to the solution of the two-dimensional Fokker–Planck equation and computes the smallest eigenvalue, the reciprocal of which is related to the mean first passage time. The value of this eigenvalue depends upon the boundary conditions in the two-dimensional representation space. Another approach[23] involves asymptotic methods and a direct solution of the two-dimensional mean first passage time equation, with appropriate boundary conditions. Numerical simulations can now bring clarity to these efforts.

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