

Kramers problem for overdamped systems driven by correlated noise: Results for vanishing diffusion coefficients

R. Mannella

Dipartimento di Fisica, Università degli Studi di Pisa, Piazza Torricelli 2, 56100 Pisa, Italy

V. Palleschi and P. Grigolini

Istituto di Fisica Atomica e Molecolare, via del Giardino 7, 56127 Pisa, Italy

(Received 20 November 1989; revised manuscript received 9 July 1990)

We have obtained results for the activation energy in bistable overdamped systems driven by colored noise. Our results cover the region of small diffusion coefficients and small to large correlation times. A scaling relation between the escape rate from one attractor to the other and the diffusion coefficient allows us to obtain results for the activation energy in the limit of vanishingly small diffusion coefficients. Numerical results for both the activation energy and the mean first-passage time are compared with theoretical predictions.

I. INTRODUCTION

In the recent past, one of the most debated problems within the community of stochastic physics has been the calculation of the activation rate in overdamped bistable systems in the presence of correlated fluctuations.¹ Quite a few conflicting theories have been presented, and in many cases the comparison with experiments (where with the experiment we mean the result of a Monte Carlo simulation, either digital² or analog,³ or the numerical solution of some eigenstate and eigenvalue problem,⁴ via, amongst others, the continued-matrix procedure⁵) has added to confusion, instead of helping in understanding the underlying physics. As already pointed out⁶ (see also Ref. 7), a source of difficulty is the fact that all (Monte Carlo) simulations are performed at finite and relatively large values of the diffusion coefficient, where the various theories proposed are not completely reliable. A most notable attempt to extrapolate results in the limit of vanishing diffusion coefficients can be found in Ref. 4(b), but unfortunately the scaling relations introduced there cannot be used in the most interesting regime, intermediate to large correlation times of the colored noise driving the system of interest. It is the purpose of this paper to prove that it is possible to find a relation between activation energies at finite values of the diffusion coefficient and the corresponding value for vanishing diffusion coefficients, even for intermediate to large correlation times of the external noise. Incidentally, our results allow the calculation of a meaningful (at logarithmic accuracy) escape rate virtually for any value of the diffusion coefficient (though we should say that for diffusion coefficients which are order of the barrier height probably the whole idea of escape rate should be revised), for small-to-large values of the noise correlation time. The activation energies and the escape rates that we have computed will then be compared to the predictions of some theoretical approaches. Finally, some conclusions will be drawn on the possibility of alternative derivations of Fokker-Planck like effective

operators for systems driven by colored noise via a path-integral approach.

II. THEORETICAL BACKGROUND

This section is not a full and comprehensive review of the topic, but simply a brief outline of the problems involved and a basis to understand the general background. We refer the reader to a recent review^{1(b)} for a more comprehensive approach and for a full bibliographic list. Another slightly more dated review,^{1(a)} devoted to "classical" problems, is worth mentioning. Here we will then limit our discussion to some recent theoretical developments which are of direct relevance to our work, and which have not been tested previously. We would like to add that other important approaches (like the ones based on the fluctuating potential ideas⁸⁻¹⁰), though very interesting on their own, will not be discussed here because of minor relevance to the present work.

Herein we will be interested in studying the system described by the Langevin equations

$$\begin{aligned}\dot{x} &= F(x) + y, \\ \dot{y} &= -\frac{1}{\tau}y + \frac{\sqrt{2D}}{\tau}f(t),\end{aligned}\tag{2.1}$$

where $f(t)$ is a Gaussian variable with average 0 and standard deviation 1. The particular form of the equation describing the evolution of y will guarantee that we have

$$\begin{aligned}\langle y(s) \rangle &= 0, \\ \langle y(s)y(t) \rangle &= \frac{D}{\tau} \exp\left[-\frac{|t-s|}{\tau}\right],\end{aligned}\tag{2.2}$$

i.e., that $y(t)$ is a colored noise. The "force" $F(x)$ is generally chosen to yield a bistable potential, and here we will consider the form

$$F(x) = x - x^3.\tag{2.3}$$

Very generally, it is possible to write the mean first-passage time (MFPT) in the form

$$T = A(D, \tau) \exp[S(\tau)/D], \quad (2.4)$$

where D and τ are defined via Eq. (2.2). This expression becomes more exact the smaller D is made; there is also the assumption that $A(D, \tau)$ will stay finite or diverge less than exponentially when D goes to zero. We also want to stress that for the moment by MFPT we mean the time taken to go from one attractor to the other (the so-called T_{bot}): other possible definitions are the time taken to reach the separatrix of the deterministic flow (T_{sep}) or the time taken to reach the boundary $\{x=0, y \text{ anything}\}$ (T_{top}). Different definitions have been studied, amongst others, in Ref. 11.

Some of the most recent theoretical work has been based on a *path-integral* approach to the problem,¹²⁻¹⁴ where attention is devoted to computing, via an Onsager-Machlup functional,¹⁵ the contribution to some stationary probability distribution from which a conditional probability distribution (probability of being on one attractor at time 0 and on the other attractor at time t) is derived. Basically, for general potentials, this method allows the calculation of some kind of action [really an activation energy, in Kramers language, i.e., the quantity $S(\tau)$ appearing in Eq. (2.4)] via the most dominant path in the limit of the vanishing diffusion coefficient. We would like to stress that this calculation of the activation energy is far from trivial, and in the general case can only be done numerically; the only completely analytical result has been obtained in Ref. 13(b) approximating $F(x)$ with a piecewise linear potential (PWL). The result obtained there for $S(\tau)$ is

$$S_{\text{PWL}}(\tau) = \frac{1}{4} \frac{1 + \frac{27}{16}\tau + \frac{1}{2}\tau^2}{1 + \frac{27}{16}\tau}. \quad (2.5)$$

Of course, for a complete characterization of the escape mechanism, the calculation of the prefactor [the term $A(D, \tau)$ in Eq. (2.4)] should be carried out. Unfortunately this is possible only for particular potentials, like the connected parabolas introduced in Ref. 13(a) or around the white-noise limit ($\tau=0$).^{12(d)}

Given the force of Eq. (2.3), it is in any case possible to derive an analytical expression for the quantity $S(\tau)$ in the limit of large correlation times or in the opposite limit of white noise (τ going to zero). One obtains

$$S(\tau=0) = \frac{1}{4} \quad (2.6a)$$

and

$$S(\tau \rightarrow \infty) = \frac{2}{27}\tau, \quad (2.6b)$$

results one would also obtain taking the appropriate limits in Eq. (2.5).

Before the path-integral treatment became fashionable, the problem had been extensively studied within the standard approach introduced by Kramers¹⁶ in the case of white noise, i.e., via some sort of Fokker-Planck operator with suitable boundary conditions and more or less justified approximations. For the region of intermediate

to large noise correlation time, essentially we have two different theoretical approaches based on Fokker-Planck-like operators: the time-dependent Fokker-Planck operator of Ref. 8 and the unified colored-noise approximation (UCNA) of Ref. 17.

The approach based on the time-dependent Fokker-Planck operator⁸ is a kind of linear response theory applied to the bidimensional Fokker-Planck operator associated to Eqs. (2.1) and (2.2), where the interaction term is dealt with up to second order in perturbation and using an adiabatic elimination procedure (this approach will be referred to as local linearization theory or LLT). The final equation one has to solve is

$$\frac{\partial P(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[-F(x) + \frac{D}{\tau} \frac{\partial}{\partial x} \frac{1 - e^{(\tau F'(x) - 1)t}}{1 - \tau F'(x)} \right] P(x, t), \quad (2.7)$$

where the solution $P(x, t)$ must be derived numerically. From the decay of $P(x, t)$ starting, say, from a δ function centered in $x = -1$, one can derive a MFPT [we would like to say that for the noise intensities and correlations herein considered we have always observed an exponential decay for $P(x, t)$]. It has been noticed¹⁸ that for small enough values of τ such that over the whole x support the quantity $\tau F'(x) - 1$, appearing in the exponent in Eq. (2.7), is negative, the numerical solution for the MFPT from Eq. (2.7) coincides with the mean first-passage time computed via the Fox theory.¹⁹ Equation (2.7) thus allows a simple and direct extension of the Fox result in the region where a standard Fokker-Planck approach would break down due to the appearance of negative diffusion coefficients.

The UCNA (Ref. 17) is again based on an adiabatic elimination, but carried out at the Langevin equation level. One derives the Fokker-Planck operator

$$\frac{\partial P(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[-\frac{F(x)}{1 - \tau F'(x)} + D \frac{1}{1 - \tau F'(x)} \frac{\partial}{\partial x} \frac{1}{1 - \tau F'(x)} \right] P(x, t), \quad (2.8)$$

from which standard techniques allow us to derive a MFPT. This calculation is not completely straightforward: the final result, valid for large correlation times (τ) of the noise and small diffusion coefficients is

$$T = \left[\frac{27\pi}{2} D \left[\tau + \frac{1}{2} \right] \right]^{1/2} \exp \left[\frac{1}{4D} \left[\frac{4}{9} + \frac{8}{27}\tau \right] \right], \quad (2.9)$$

which yields the expression

$$S_{\text{UCNA}}(\tau) = \frac{1}{4} \left(\frac{4}{9} + \frac{8}{27}\tau^2 \right) \quad (2.10)$$

for $S(\tau)$. Note that this expression gives the right limit for large τ , but is incorrect in the opposite limit of white noise, as one would suppose, given the hypothesis assumed by the theory.

We will be comparing $S(\tau)$ predicted via the different

theories with the result of simulations. For the theoretical approach based on a path-integral formulation of the full (nonlinear) problem we will use the result of numerical integration.^{12(c)} For the LLT, the other approach for which no analytical expression is available, we will solve Eq. (2.7) numerically for D finite, and prove that the same scaling holding for the experimental MFPT holds true also for the MFPT calculated via the LLT, thus allowing us to derive a meaningful $S(\tau)$ for the comparison.

Also, given that all the theories give the same value for $S(\tau)$ when τ is large and all but the UCNA give the same value in the opposite limit of white noise, we will normalize $S(\tau)$ obtained from the different theories with the help of Eq. (2.6), i.e., we introduce the quantity $\delta S(\tau)$ defined as

$$\delta S(\tau) = \frac{S(\tau) - S(0)}{S(\infty)}. \quad (2.11)$$

It is straightforward to write $\delta S(\tau)$ for the different theories considered here.

Note that all theories presented here are supposedly exact in the limit of vanishing D . Of course, in this limit the dominant contribution to the MFPT comes from the exponent of Eq. (2.4) [the value $S(\tau)$, which is finite, is divided by a quantity D going to zero].

After considering the activation energy, we will turn to the comparison of the actual MFPT values from the simulations and the corresponding MFPT from the theoretical treatments. The problem of the activation rate has received considerable attention, particularly for small τ values. A very detailed discussion of the most important results can be found in Ref. 1(a). It should be noted, however, that at the best of our knowledge no comparison has ever been carried out between numerical simulations and the theoretical results for T_{sep} of Ref. 19 based on a two-dimensional Fokker-Planck operator, or the theoretical predictions on T_{bot} from Ref. 12(d).

The main result of Ref. 19 has been to derive expressions or T_{sep} via suitable expansions of a two-dimensional Fokker-Planck operator with appropriate boundary conditions. The authors there derived two different expressions for T_{sep} , depending on the relative value of τ and D . For $\tau \ll D$ the result found is

$$T = \frac{\pi}{\sqrt{2}} (1 + \frac{3}{2}\tau + \dots) e^{1/4D} \quad (2.12)$$

and in the opposite limit $\tau \gg D$,

$$T = \frac{\pi}{\sqrt{2}} \frac{\sqrt{1-4\tau}}{\sqrt{1+2\tau}} \frac{1+3\tau}{1-\frac{3}{2}\tau} \exp \left[\frac{1}{4D} \left(1 + \frac{\tau^2}{2} \right) \right]. \quad (2.13)$$

It is understood that in both cases D and τ must be (much) smaller than 1. In Ref. 19 the authors have also carried out a uniform expansion which yields the expression, valid for $D \ll 1$ and $\tau \ll 1$:

$$T = \frac{\pi}{\sqrt{2}} \left[\frac{1-2\tau(1-3D)}{1+\tau(4-3D)} \right]^{1/2} \times \exp \left[\frac{1}{4D} + \frac{9}{2}\tau - \frac{\tau^2}{8D} + \frac{3}{2}\tau^2 \right] \quad (2.14)$$

For the path-integral calculation of the escape rates, one has to calculate the fluctuations around the dominant path. We refer the reader to Ref. 12(d) for the details of the calculation, and we simply quote the final result, valid for the force of Eq. (2.3). Assuming that we can write the MFPT as in Eq. (2.4), the expression derived for the prefactor, valid for small τ and in the weak-noise limit, i.e., small D , is

$$A(D, \tau) = \frac{\pi}{\sqrt{2}} \frac{1}{1 - \frac{3}{2}\tau + \frac{9}{8}\tau^2 + O(\tau^3)} \quad (2.15)$$

where we have specialized the rather general expression of Ref. 12(d) to the force of Eq. (2.4). Note that here with MFPT we mean T_{sep} , not T_{bot} . The expression for T_{sep} has been obtained dividing T_{bot} by 2, after Ref. 9.

Equations (2.11)–(2.15) will be checked against numerical simulations in the following sections.

III. SIMULATIONS

The numerical simulations have been executed using the algorithm described elsewhere,²⁰ with a minor modification which allows a better accuracy²¹ with no increase of the CPU time. The original corrector step (see Ref. 22), an Adams-Moulton of order zero, has been replaced by an Adams-Moulton of order 1. Also, the calculation of the stochastic term, for speed reasons, has been kept up to terms of order 1 in the integration time step. The number of trajectories considered has always been 1000 and all trajectories have been initialized from the point $\{x = -1, y \text{ random from the appropriate Gaussian distribution}\}$. We have obtained values for the time taken to go from one attractor to the other, to reach the boundary $\{x = 0, y \text{ anything}\}$, and to reach the separatrix of the deterministic flow in the two-dimensional space of Eq. (2.1). Other quantities like noise distributions at the different boundaries have also been computed. Some of our computed values for the time taken to go from one attractor to the other (T_{bot}) and to reach the boundary $\{x = 0, y \text{ anything}\}$ (T_{top}) are reported, respectively, in Tables I and II.

The basic problem is that if it were rather simple to compute a MFPT for finite values of the noise intensity, it would be impossible to perform the simulations for vanishing diffusion coefficients. But we should not forget that at this stage we really need (and want) to compute the activation energy, not the MFPT. It is then natural to consider the quantity

$$S(\tau, D) = D \log_e(T), \quad (3.1)$$

which coincides with $S(\tau)$ when D goes to zero. In Fig. 1 we have plotted $S(\tau, D)$ from our simulations as function of D . The linear dependence of $S(\tau, D)$ on D is striking for the values here considered. Corrections to the prefactor due to finite diffusion coefficients would not show on this scale for the values of D considered. Note also that the statistical uncertainty is smaller than the symbols used in the figure. It is clearly possible and reasonable to assume for $S(\tau, D)$ a functional dependence on D given by a constant plus a linear term, in the form

TABLE I. Values of T_{bot} (time taken to go from one attractor to the other) for different values of τ and D .

$\tau \backslash D$	0.1	1	2	3	4	5	7	10
0.06	392.6	1993.8						
0.07	215.7	1016.4						
0.08	133.8	538.0						
0.09	102.6	342.6						
0.10	75.35	264.1	840.4					
0.11	61.05	191.7	617.9					
0.12	51.65	163.4	434.8	1127.7	2775.5	6754.8		
0.15	33.13	90.09	221.8	493.8	1051.8	2081.6	8203.4	58242
0.20	22.01	55.56	120.5	228.3	393.0	737.1	2051.4	8742.7
0.30	13.96	32.94	59.44	98.36	151.2	238.0	505.8	1582.0

$$S(\tau, D) = D\alpha + S(\tau). \quad (3.2)$$

The constant term will of course yield the $S(\tau)$ values needed for the comparison with the theory.

A similar procedure must be followed to obtain $S(\tau)$ for the LLT. In Fig. 2 we have plotted the quantity $S(\tau, D)$ obtained integrating Eq. (2.7), and it is clear that a fit with a constant plus a linear term is again appropriate. The constant term will be taken as the $S(\tau)$ for the LLT. For the sake of completeness, we would like to add that a fairly extensive study of the prefactor for different D and τ has been carried out in Ref. 9(c).

IV. COMPARISON BETWEEN SIMULATIONS AND THEORY: ACTIVATION ENERGY

The results of fitting our data with a constant plus a linear term are reported in Table III, together with the theoretical predictions from Ref. 12(c). The agreement is extremely good over the whole range of τ values considered. To carry out a better comparison, though, it is better to normalize both theoretical predictions and numerical results with the help of the asymptotic results [Eqs. (2.6)], considering $\delta S(\tau)$ instead of $S(\tau)$. For the predictions from Ref. 12(c) and for the LLT,⁸ as already pointed out, we will normalize $S(\tau)$ numerically. Indeed in Ref. 12(c) some expansions are derived around the lim-

iting cases of very small τ or very large τ , but their agreement with the result of our simulations would not be particularly good and they are not considered here. For the other theoretical approaches considered here, we readily obtain

$$\delta S_{\text{UCNA}}(\tau) = 1 - \frac{15}{8\tau} \quad (4.1)$$

for the approach based on the UCNA (Ref. 17) [Eq. (2.10)], and

$$\delta S_{\text{PWLA}}(\tau) = \frac{1}{1 + 16/27\tau} \quad (4.2)$$

for the path-integral approach applied to a piecewise linear approximation of the anharmonic potential [Eq. (2.5)].^{13(b)}

The comparison between different theories and the numerical simulations is presented in Fig. 3. The simulation results are in brilliant agreement with the theoretical predictions of Ref. 12(c). We believe that this theory is able to accurately describe the escape process, at least in the limit of small D . We can also add that the apparently astonishing rise of $\delta S(\tau)$ above its limiting value at large τ , very clear at finite τ , is probably due to the interplay of color and nonlinearity: in fact, the theory of Ref. 13(b) which is based on a piecewise linearization, fails in reproducing the nonmonotonous behavior of $\delta S(\tau)$; it is fair to

TABLE II. Values of T_{top} (time to reach the boundary $\{x=0, y \text{ any}\}$ starting from the initial attractor) for different values of τ and D .

$\tau \backslash D$	0.1	1	2	3	4	5	7	10
0.06	267.2	1872.2						
0.07	141.5	923.3						
0.08	87.8	491.1						
0.09	64.94	313.6						
0.10	48.35	238.2	825.3					
0.11	38.88	169.7	599.5					
0.12	29.81	144.4	422.6	1109.4	2748.6	6744.3		
0.15	19.68	76.17	210.8	483.7	1047.2	2069.4	8191.4	58241
0.20	12.02	46.45	113.0	221.0	386.6	732.9	2049.5	8741.0
0.30	7.301	26.31	53.57	93.55	145.4	235.6	503.1	1580.3

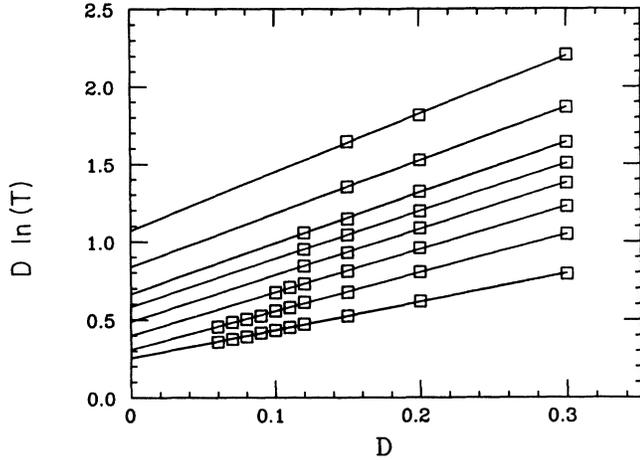


FIG. 1. Squares, natural logarithm of T_{bot} times D vs D for different values of τ from the digital simulations; straight lines, linear fits to the data. From bottom to top we have $\tau=0.1, 1, 2, 3, 4, 5, 7,$ and 10 .

say that nevertheless Eq. (4.2) is a remarkably good interpolation formula from small to large τ . As for the UCNA of Ref. 17, Fig. 3 shows that it reproduces the correct behavior of $\delta S(\tau)$ only in the limit of very large τ : we think that the UCNA, very useful when describing equilibrium situations, might have limitations in describing dynamic processes (though a Fokker-Planck operator of the UCNA type appears in the path-integral formalism when the dominant contribution to the action is evaluated, but see below). Also, we should bear in mind that the UCNA does not pretend to describe the escape mechanism in every detail for small to intermediate τ , but only to work in the limit of very large τ . It is arguable that probably amongst the theories considered here the UCNA is the easiest to derive but also the one with the

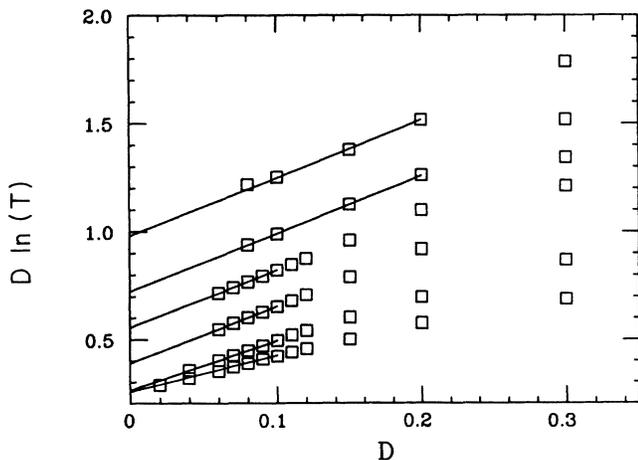


FIG. 2. Symbols, natural logarithm of T_{bot} times D vs D for different values of τ from the numerical solution of the Fokker-Planck operator of the LLT; straight lines, linear fits to the data. From bottom to top we have $\tau=0.1, 1, 3, 5, 7,$ and 10 .

TABLE III. Values of the fitting parameters of the $D \ln(T_{\text{bot}})$. The fitting formula used is $D \ln(T_{\text{bot}}) = \alpha + DS(\tau)$. For comparison, theoretical values of $S_{\text{theor}}(\tau)$ from Ref. 12(c) are reported.

τ	$S(\tau)$	α	$S_{\text{theor}}(\tau)$
0.1	0.2516	1.8115	0.2512
0.5	0.2721	2.1548	0.2727
1.0	0.3083	2.4689	0.3129
2.0	0.3996	2.7609	0.4008
3.0	0.4875	2.9691	0.4892
4.0	0.5814	3.0776	0.5765
5.0	0.6633	3.2641	0.6627
7.0	0.8368	3.4380	0.8323
10.0	1.0702	3.7849	1.0818

narrowest range of application. As for the LLT of Ref. 8, still based on a Fokker-Planck approach, the predicted escape rate gives a better agreement with the simulations than the UCNA over the whole τ range at the cost of some slightly involved calculations, though both are worse than the approaches based on the path integral formalism. It is an open question whether the corrections to the LLT carried out with the method of Der,²⁴ taking into account the interplay between color and anharmonicity, could lead to a better agreement with simulations.

In the inset of Fig. 3 we have plotted $\delta S(\tau)$ at $D=0.1$ (diamonds), together with $\delta S(\tau)$ at $D=0$ (squares) and the theory (solid line) of Ref. 12(c). It is striking how the behavior of $\delta S(\tau)$ is *qualitatively* different for $D=0.1$ and $D=0$, and also that, though we could still with some difficulty claim that the limit of $\delta S(\tau)$ for large τ is some-

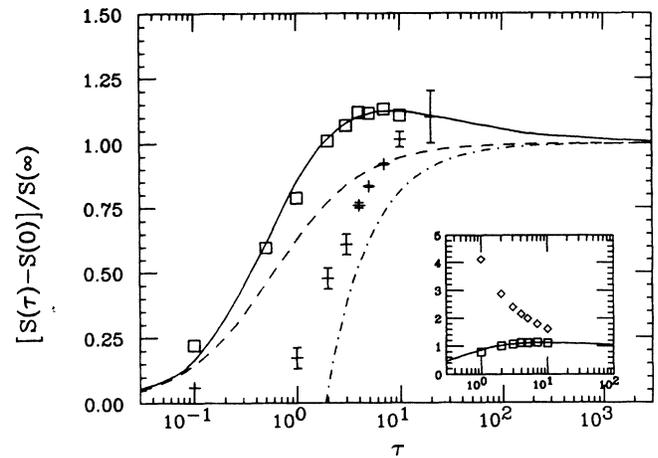


FIG. 3. Value of $\delta S(\tau)$ for different theories and for our simulations vs τ . Solid line, theory of Ref. 12(c); dashed line, Eq. (4.2); dash-dotted line, Eq. (4.1); crosses plus error bars, numerical solution of the LLT (from Ref. 8); squares, values for $\delta S(\tau)$ obtained from our simulations. Note the remarkably good agreement between simulations and the theory of Ref. 12(c). Inset: $\delta S(\tau)$ at $D=0.1$ (diamonds), $D=0$ (squares), and theory (solid line) of Ref. 12(c) vs τ . Note the qualitative different behavior of $\delta S(\tau)$ and the slower rate of convergency to a limiting value when D is changed from 0 to 0.1.

where around 1, the convergency is incredibly slower (see for a similar point Ref. 9).

V. COMPARISON BETWEEN SIMULATIONS AND THEORY: MEAN FIRST-PASSAGE TIMES

The comparison between the MFPT (T_{sep} , in this section) predicted from the theory and the numerical simulations should again be carried out for very small values of D . Of course, with the help of Eqs. (4.1) and (4.2), for the experimental MFPT's we have immediately

$$T = \frac{1}{2} \exp \left[\alpha(\tau) + \frac{S(\tau)}{D} \right], \quad (5.1)$$

where the factor $\frac{1}{2}$ is due to the fact that we are considering T_{sep} . It is then straightforward to derive values of the MFPT for a variety of D .

The comparison is presented in Fig. 4, where we have plotted the MFPT as function of D for different values of τ , and in Fig. 5 where we have plotted the MFPT as function of τ for different values of D . The symbols are always the result of the numerical simulations, normalized to the white-noise limit. The upper solid curve is Eq. (2.14), the lower solid curve is Eq. (2.13), the dash-dotted line is Eq. (2.12) and the dashed line is the prediction from the path-integral treatment. In Fig. 4(c) no curve corresponding to Eq. (2.13) is present due to breakdown of the expression for the values of τ considered. First of all, we note that the path-integral approach is in reasonable agreement with the result of the simulations, the agreement becoming not satisfactory only for large values of D , where probably not only the prefactor is not accurate enough but even the idea of using the extremizing path to compute the activation energy is not correct (in other words, paths which are fairly distant from the extremizing one are probably contributing with an appreciable weight to the escape rate). Note that Eq. (2.14) is also in reasonable agreement with the simulations over the range of τ and D values; one might expect it to work (small τ and D). Equation (2.13), on the other hand, seems to be of much narrower application (we remind the reader that it should work for $D \ll \tau$): only (see Fig. 4) at very small D the theory seems to agree well with the numerical simulations, and even in this region it does not do better than the path-integral formulation or the expression of Eq. (2.14). The amazing thing is however the very good agreement between Eq. (2.12) and the simulations. We would expect it to work in the region where $\tau \ll D$: this is indeed the case, as it is clear from Fig. 5. The most surprising thing, of course, is that, as one *a posteriori* would expect, the agreement theory and numerical simulations gets *worse* the smaller D is made (in fact, in this case the inequality $\tau \ll D$ is no longer satisfied). It should be appreciated that Eq. (2.12) was first suggested (for small τ and D , with no explicit mention to the relative magnitude) to describe the escape rate mechanism,²⁵ and for a long time, basing the proof on experimental simulations performed at finite D , it was assumed that it would work better the smaller the diffusion coefficient was made. We think that our results show clearly that

this is not the case, and as D is made smaller the range of validity of Eq. (2.12) narrows down to smaller and smaller values of τ . We would like to conclude this section saying that both the theoretical predictions of Ref. 19

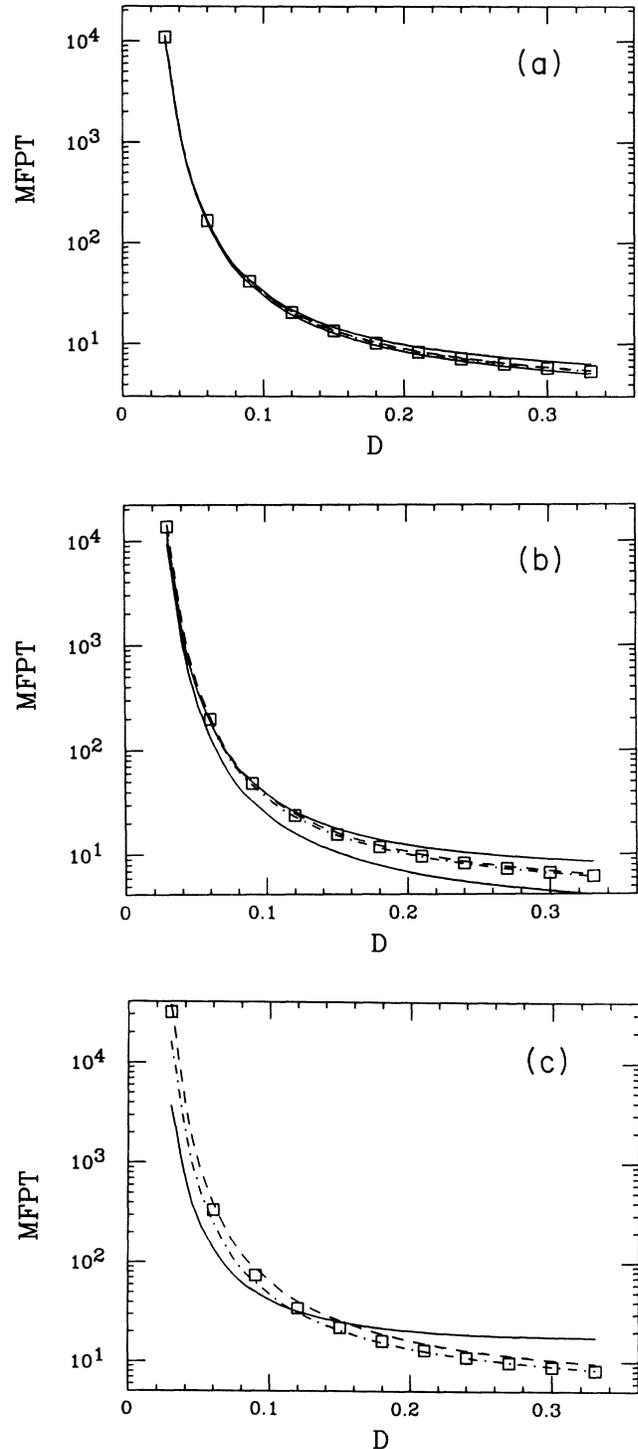


FIG. 4. T_{sep} (MFPT) vs D for (a) $\tau=0.1$, (b) $\tau=0.2$, and (c) $\tau=0.5$. The upper solid curve is Eq. (2.14), the lower solid curve (when present) is Eq. (2.13), the dash-dotted curve is Eq. (2.12), and the dashed line is the path-integral approach prediction. The symbols are obtained from the numerical simulations.

and the path integral formulation of the escape problem¹² seem to be fully vindicated by our numerical simulations.

VI. COMMENT ON THE RELATION BETWEEN DOMINANT PATHS IN THE ACTION AND MOST PROBABLE PATHS IN THE PHASE SPACE

In the previous sections we have noted the very good agreement between numerical simulations and the

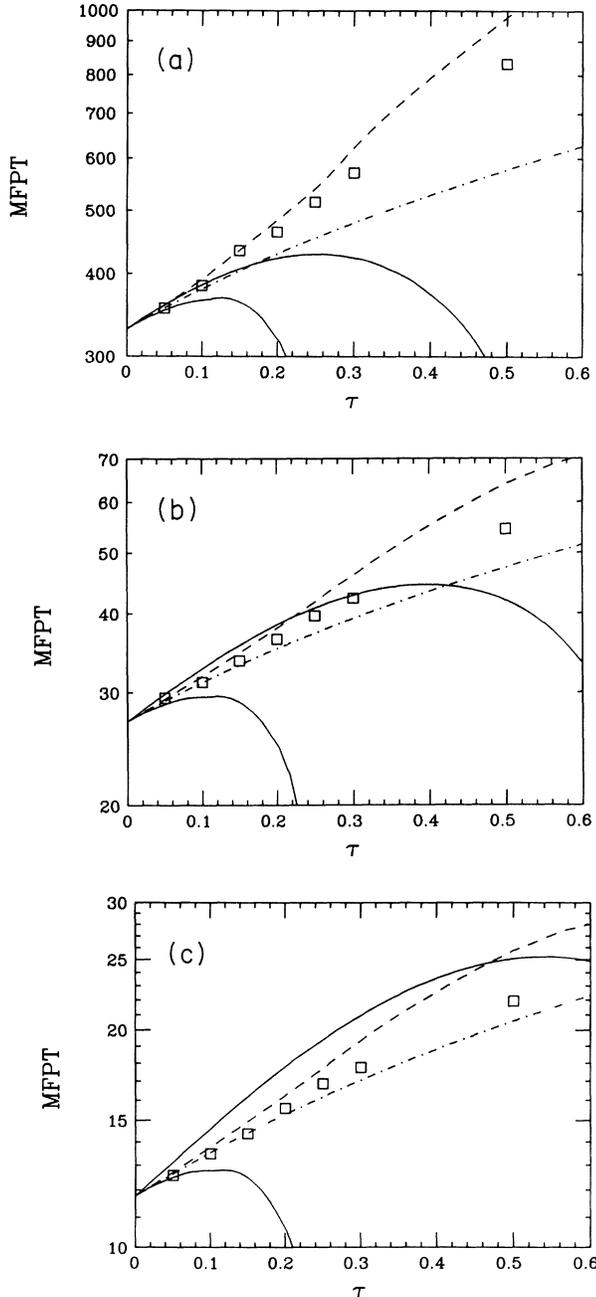


FIG. 5. T_{sep} (MFPT) vs τ for (a) $D=0.05$, (b) $D=0.1$, and (c) $D=0.15$. The upper solid curve is Eq. (2.14), the lower solid curve is Eq. (2.13), the dash-dotted curve is Eq. (2.12), and the dashed line is the path-integral approach prediction. The symbols are obtained from the numerical simulations.

theoretical approach of Ref. 12 based on the path integral formalism. We believe that this is probably the most powerful and most useful approach to the understanding of the escape mechanism. Having said this, we would like to add a few comments. Let us go back to the way the action in Eq. (2.4) is calculated. One has to compute the action along the path which extremizes the action itself, extremal path derived solving the Euler-Lagrange equations associated to the action. Now, from the differential equations of the extremal path it would be possible to write an effective Fokker-Planck operator which, at lowest order in the time derivatives, coincides with the Fokker-Planck operator obtained within the UCNA approach. However, we believe that one thing is the extremizing path used to evaluate the action and another thing is the most probable path in the space of the real trajectories. Though we do not have a formal proof of this and, even if our conjecture might be true, a formal proof could be probably difficult to obtain, we would like to argue that our simulations strongly support our viewpoint. Before introducing our argument, we remind the reader that in the path-integral approach the path extremizing the action starts from $\{x=-1, y=0\}$ and ends in $\{x=1, y=0\}$ going through the point $\{x=0, y=0\}$ [see also inset of Fig. 2 in Ref. 12(c)]. We are going to show that the most probable path in the trajectories space does *not* go through $\{x=0, y=0\}$.

Evidence that supports our conjecture is the success of the fluctuating potential approach in describing the dynamics in the case of very colored noise: when x crosses the boundary $\{x=0, y \text{ anything}\}$ the noise is by definition different from zero [it is roughly order⁸ of $y_c=2\sqrt{3}/3$, but see Ref. 9(a)]. Also, some numerical evidence that this is the case (at least for finite values of D) can be found in the numerical work of Ref. 10.

We have calculated the average value y_{av} of the noisy term y when x crosses the boundary $\{x=0, y \text{ anything}\}$, for different values of D and τ . First of all, we have noticed (Fig. 6) that for large enough values of τ [for the force of Eq. (2.3), values of τ larger than something order of 1; in general, we guess, if ω_{top} is the frequency at the top of the potential barrier, τ greater than $1/\omega_{\text{top}}$] y_{av} value for different D and τ scale on a universal curve when plotted against the scaling parameter first introduced in Ref. 9. To make contact with the theory, we should make D very small, which means that the scaling parameter must go to infinity: in Fig. 6 the scaling parameter is still finite, though very large, but clearly the universal curve one can draw through our data points seems to asymptotically approach the straight line $y_{\text{av}}=y_c$, where $y_c=2\sqrt{3}/3$ is the critical value for the noise derived from a fluctuating potential approach. We think that this is a strong proof that for any value of τ , as long as τ is large enough, the most probable path in the trajectories space goes through the point $\{x=0, y=y_c\}$ in the limit of vanishing D . To further support our view, we have plotted in the inset of Fig. 6 values of y_{av} as function of D only, for some values of τ . Again, it is clear that the extrapolation to $D=0$ of a line drawn through the data points cuts the ordinate axis at a value very close to y_c , a value markedly different from $y=0$.

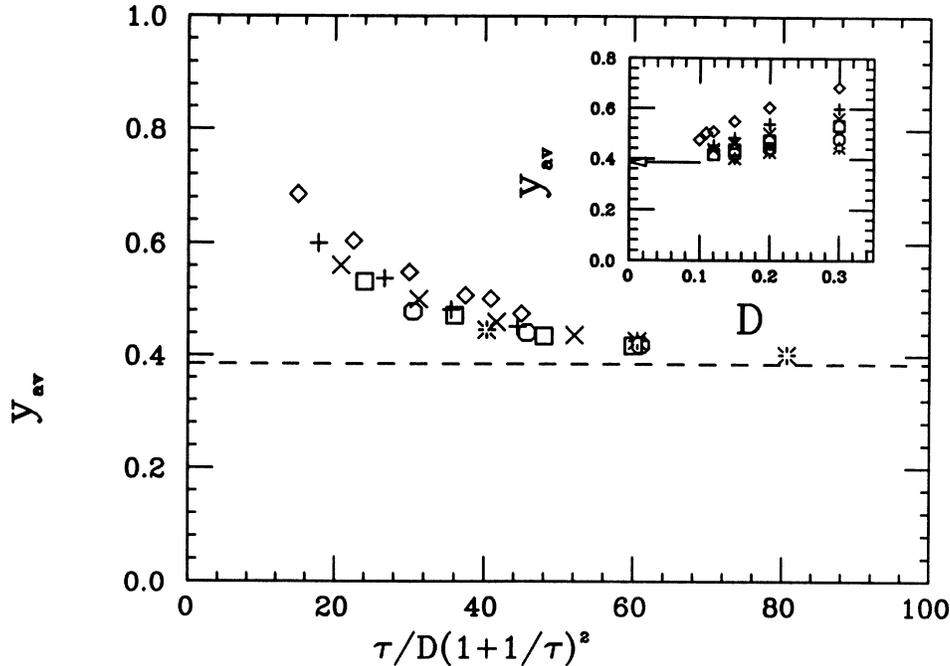


FIG. 6. Average value of y (y_{av}) when x crosses the boundary $x=0$ vs the scaling parameter introduced in Ref. 9. The same symbol identifies values of y_{av} corresponding to the same value of τ (different D). Note that even for quite different values of D and τ , the data points almost scale when plotted as function of $\tau/D(1+1/\tau)^2$. The dashed line is the value predicted by the fluctuating potential approach of Ref. 8. In the inset, values of y_{av} as a function of D only, for different τ values. Note that a line through the points would cut the ordinate axis close to the arrow, pointing to the value of y_{av} predicted by the fluctuating potential.

VII. CONCLUSIONS

To summarize, we have carried out a refined simulation of a bistable system driven by colored (strongly colored) noise. The algorithm used, faster and more precise than any algorithm previously used, to our knowledge, particularly when a MFPT is concerned, allowed for very good statistics even for large correlation times and small intensities of the noise. We have found a previously unknown scaling relation between the MFPT and the noise intensity which allowed us to obtain the activation energies for the system under study in the limit of vanishing diffusion coefficients, after fitting the logarithm of the MFPT with a constant plus a linear term in D . In turn, it has been possible to compare different (and in some sense, conflicting) theories in the limit when they should become exact: we have clearly demonstrated that as far as activation energies are concerned, the results obtained in Ref. 12 via a path-integral approach are extremely good. This should settle a long-standing problem in stochastic nonlinear physics. We have also studied the problem of the activation rate (not simply the activation energy) in the limit of small τ and for several values of D . Again, the results obtained via the path-integral formalism are in satisfactory agreement with the simulations, though the other theoretical approach considered, based on a two-dimensional Fokker-Planck operator, is also reasonable in the appropriate region of applicability. We

have also extensively commented on the possibility that the path used to compute the external action within the path-integral approach might have little to do with the trajectories in the real space. The proof goes through the evaluation of the average value of the noise when the system crosses a particular boundary in the phase space. Finally, we would like to say that our tabulated values for the activation-energy fitting parameters could be used to obtain mean first-passage times even for intermediate values of D not covered in the simulations, via appropriate interpolations, given the very good agreement between fit and actual data. We believe that this will be very useful to researchers in the field, saving them from repeating the simulations from the very beginning, and making available data in the most interesting region, i.e., very small diffusion coefficients and intermediate to large noise correlation times; it should be noted that we have quoted values also for the linear term, which should make it possible to obtain reliable values even for the pre-factor (to a logarithmic accuracy) for small enough D .

ACKNOWLEDGMENTS

We would like to thank A. Bray for making available the values of $S_{\text{theor}}(\tau)$ reported in Table III and M. San Miguel and A. J. McKane for copies of their works before publication. We also thank J. M. Sancho for drawing our attention to Ref. 22.

- ¹(a) K. Lindenberg, B. J. West, and J. Masoliver, in *Noise in Nonlinear Dynamical Systems*, edited by F. Moss and P. V. E. McClintock (Cambridge University Press, Cambridge, 1989), Vol. 1; (b) K. Lindenberg, B. J. West, and G. P. Tsironis (unpublished).
- ²R. Mannella and V. Palleschi, *Phys. Lett. A* **129**, 317 (1988).
- ³P. Hanggi, T. J. Mroczkowski, F. Moss, and P. V. E. McClintock, *Phys. Rev. A* **32**, 695 (1985).
- ⁴(a) Th. Leiber, F. Marchesoni, and H. Risken, *Phys. Rev. Lett.* **59**, 1381 (1987); **60**, 659 (1988); *Phys. Rev. A* **38**, 982 (1988); (b) Th. Leiber and H. Risken, *ibid.* **38**, 3789 (1988).
- ⁵P. Jung and H. Risken, *Z. Phys. B* **59**, 469 (1985).
- ⁶P. Jung and P. Hanggi, *Phys. Rev. A* **34**, 4464 (1987).
- ⁷R. S. Larson and M. D. Kostin, *J. Chem. Phys.* **69**, 4821 (1978).
- ⁸G. Tsironis and P. Grigolini, *Phys. Rev. Lett.* **61**, 7 (1988); *Phys. Rev. A* **38**, 3749 (1988).
- ⁹(a) F. J. de la Rubia, E. Peacock-Lopez, G. P. Tsironis, K. Lindenberg, L. Ramirez-Piscina, and J. M. Sancho, *Phys. Rev. A* **38**, 3827 (1988); (b) K. Lindenberg, L. Ramirez-Piscina, J. M. Sancho, and F. J. de la Rubia, *ibid.* **40**, 4157 (1989); (c) L. Ramirez-Piscina, J. M. Sancho, F. J. de la Rubia, K. Lindenberg, and G. P. Tsironis, *ibid.* **40**, 2120 (1989).
- ¹⁰R. Mannella and V. Palleschi, *Phys. Rev. A* **39**, 3751 (1989).
- ¹¹For a comparison between T_{bottom} , lowest eigenvalues of a Fokker-Planck operator, and mean first-passage times to particular boundaries in the phase space, see R. F. Fox, *Phys. Rev. Lett.* **62**, 1205 (1989). Similarly, for T_{top} see C. R. Doering, P. S. Hagan, and C. D. Levermore, *Phys. Rev. Lett.* **59**, 2129 (1987); C. R. Doering, R. J. Bagley, P. S. Hagan, and C. D. Levermore, *ibid.* **60**, 2805 (1988); P. Hanggi, P. Jung, and P. Talkner, *ibid.* **60**, 2804 (1988).
- ¹²(a) A. J. Bray and A. J. McKane, *Phys. Rev. Lett.* **62**, 493 (1988); (b) A. J. McKane, H. C. Luckock, and A. J. Bray, *Phys. Rev. A* **41**, 644 (1990); (c) A. J. Bray, A. J. McKane, and T. J. Newman, *ibid.* **41**, 657 (1990); (d) H. C. Luckock and A. J. McKane, *ibid.* **42**, 1982 (1990).
- ¹³(a) J. F. Luciani and A. D. Verga, *Europhys. Lett.* **4**, 255 (1987); (b) *J. Stat. Phys.* **50**, 567 (1988).
- ¹⁴P. Colet, H. S. Wio, M. San Miguel, L. Pesquera, M. Rodriguez, and A. Verga (unpublished); P. Colet, H. S. Wio, and M. San Miguel (unpublished); M. San Miguel, P. Colet, H. S. Wio, L. Pesquera, and M. A. Rodriguez (unpublished); H. S. Wio, P. Colet, M. San Miguel, L. Pesquera, and M. A. Rodriguez (unpublished).
- ¹⁵See, for instance, R. Graham, in *Quantum Statistics in Optics and Solid-State Physics*, Vol. 66 of *Springer Tracts in Modern Physics*, edited by G. Höhler (Springer, Berlin, 1973).
- ¹⁶H. A. Kramers, *Physica* **7**, 284 (1940).
- ¹⁷(a) P. Jung and P. Hanggi, *Phys. Rev. Lett.* **61**, 11 (1988); (b) P. Hanggi, P. Jung, and F. Marchesoni, *J. Stat. Phys.* **54**, 1367 (1989).
- ¹⁸P. Jung, P. Hanggi, and F. Marchesoni, *Phys. Rev. A* **40**, 5447 (1989).
- ¹⁹M. M. Klosek-Dygas, B. J. Matkowsky, and Z. Shuss, *Phys. Rev. A* **38**, 2605 (1988); *J. Stat. Phys.* **54**, 1309 (1989).
- ²⁰R. F. Fox, *Phys. Rev. A* **37**, 911 (1988).
- ²¹R. Mannella and V. Palleschi, *Phys. Rev. A* **40**, 3381 (1989).
- ²²W. Rumelin, *SIAM J. Numer. Anal.* **19**, 604 (1982).
- ²³L. Lapidus and J. H. Seinfeld, *Numerical Solution of Ordinary Differential Equations* (Academic, New York, 1971).
- ²⁴R. Der, *Phys. Lett. A* **135**, 430 (1989).
- ²⁵P. Hanggi, F. Marchesoni, and P. Grigolini, *Z. Phys. B* **56**, 333 (1984).