

Optimal paths and the calculation of state selection probabilities

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The addition of noise to a dynamical system means that initial states near points of instability may no longer decay to a unique stable state. A common example of this behavior occurs in a dynamical system with two degrees of freedom and with two or more stable states. If the initial state of the system is near the separatrices bounding the basins of attraction of these stable states, then the addition of noise to the system means that there is a nonzero probability that the stable state selected is in a different basin of attraction to that of the initial state. We discuss a method of calculating these state-selection probabilities based on a path-integral representation of the stochastic dynamics. The relationship of this approach to a method based on the solution of the backward Fokker-Planck equation is particularly stressed, since this was used in previous studies of problems of this type. However, while the method based on the backward Fokker-Planck equation is a powerful one for systems with one degree of freedom, in systems with more degrees of freedom it is much less useful. Since the standard method of solution in this case involves a series of mappings onto a deterministic dynamics which is simply the classical dynamics associated with the path-integral formulation, we argue that for systems with more than one degree of freedom, the path-integral method is a very natural way of calculating state-selection probabilities. We illustrate this on a simple example taken from population biology, and find that the state-selection probabilities are in excellent agreement with Monte Carlo simulations.

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I. INTRODUCTION

This paper is concerned with the phenomenon of state selection: if a system is initially near a point of instability, and more than one stable state is available to it, with what probabilities are each of these final states chosen? It is immediately clear that this is a question in stochastic dynamics since noise will obviously be crucially dependent for the selection of the final state. The simplest example of this phenomenon is a one-dimensional (1D) system consisting of an overdamped particle moving in a potential $V(x)$. The deterministic dynamics is described by the equation $\dot{x} = -V'(x)$, where time has been rescaled so that the coefficient of \dot{x} is unity and the dot denotes differentiation with respect to time. If the initial condition imposed on the system is that the particle begins at a local maximum of $V(x)$, then infinitesimally small noise will cause the particle to move either to the right or to the left of the maximum with a probability of $1/2$. If the particle is initially near the maximum, e.g., slightly to the right of it, then in the presence of infinitesimally small noise the particle will move to the right with probability 1. However, if the noise strength is increased, there will be a nonzero probability that fluctuations will carry the particle over the maximum and its final state will be to the left of the maximum. The goal is to develop a mathematical framework that will allow us to calculate the probability of ending up to the right or left of the maximum as a function of the initial position, noise strength, nature of the potential, or any other parameters that may be relevant. The noise will be taken to be Gaussian and white with zero mean and strength D . Therefore, the dynamics will be described by $\dot{x} = -V'(x)$

+ $\eta(t)$, where $\langle \eta(t) \rangle = 0$ and $\langle \eta(t) \eta(t') \rangle = 2D \delta(t - t')$.

An important point which needs to be emphasized at the outset is that when we talk about selection of final states, we mean this on relatively short time scales. On these time scales, the system will have moved to a local minimum of the potential (if it exists) or to plus or minus infinity (if no boundaries or minima exist). Of course, once the system has reached a local minimum it will fluctuate about it and on longer time scales will have a probability of escaping to another minimum. These transitions between states, which are stable in the deterministic dynamics and metastable in the stochastic dynamics, are of no interest to us here. We need to emphasize this, since by far the majority of studies of decay to (meta)stable states in stochastic dynamics have focused on the transitions between such states [1]. In this paper we will be interested in systems that are initially near an unstable state rather than a stable state. For example, in the one-dimensional potential $V(x) = -(1/2)\alpha x^2 + (1/4)\beta x^4$, there is an unstable state at $x=0$ and two stable states at $x = \pm(\alpha/\beta)^{1/2}$. Our interest only focuses on initial conditions near $x=0$. If $|x| < (\alpha/\beta)^{1/2}$ but some way from $x=0$, the particle will reach one of the minima on a relatively short time scale. The result is similar if $|x| > (\alpha/\beta)^{1/2}$. Once the particle has reached one of the minima, or if it starts there, a new set of questions, not of interest to us here, can be asked concerning transitions between the two stable states. On extremely long time scales, many transitions will take place between these states and eventually the particle will be found at the position x with a probability given by the Boltzmann distribution $\exp[-V(x)/D]$.

While the one-variable case is useful for describing the phenomenon of state selection, the possible types of behavior

are rather limited. The basic phenomenon can be understood qualitatively by the study of any potential with a single extremum which is in the form of a maximum. The simplest example is the case $V(x) = -(1/2)\alpha x^2$. In two dimensions, a rather richer structure is found. There are two distinct situations: type I, where the initial point is near the separatrix between the basins of attraction of two stable states, and type II, where the initial point is near an unstable point. When a potential exists, this unstable point will be a local maximum. In the first case, i.e., type I, the system will have the greatest probability of moving to the stable state which lies in the same basin of attraction as the initial position, but also a nonzero probability of reaching the other stable states. The process of reaching the stable state on the “other side” of the separatrix can be thought of as a generalized “barrier crossing” event. During the last decade, several applications of this phenomenon have been discussed, particularly in the biological sciences [2–5]. In the second case, i.e., type II, there are no barriers to cross at all, as the paths that connect the initial position with any of the local minima are entirely “downhill” [6,7]. In both of these cases, we wish to understand how one calculates these probabilities and to develop a framework for developing an intuition about the underlying mathematical framework. In three and higher dimensions the number and type of transitions increase further. In this paper we will be primarily concerned with a discussion of the relative merits of the mathematical techniques that can be used to calculate the state-selection probabilities, and so will not consider these higher-dimensional situations. Instead we will use one-dimensional examples to describe the techniques and build intuition, and then apply them to two-dimensional examples.

The two main techniques that have been used to calculate state-selection probabilities are the solution of the backward Fokker-Planck equation (BFPE) [8,9] and the use of optimal paths in the path-integral formulation of the stochastic process [10,11]. Both methods have advantages and disadvantages, and one of the aims of this paper is to highlight these. To our knowledge, type I state selection has only been investigated using the BFPE approach and related methods from classical asymptotic analysis [12–15,2], and type II using only the path-integral approach [6,7]. In this paper we will apply the path-integral method to type I problems and compare the method with the BFPE approach. As we will see, the BFPE method is very efficient for one-dimensional problems, less so for higher dimensions, and the path-integral approach is more intuitive than BFPE, leading to a deeper understanding of the phenomenon under study.

The outline of the paper is as follows. In Sec. II, we will calculate the state-selection probabilities for the one-dimensional potential $V(x) = -(1/2)\alpha x^2$. The calculation will be carried out exactly using both the BFPE and path-integral techniques. In Sec. III the nature of the optimal paths used in the path-integral approach will be described and the connection between the two methods of calculation will be explained. This relation between the two methods will be explored further for two dimensional, type I situations in Sec. IV. In Sec. V we conclude by summarizing the available calculational approaches, comparing them, and commenting on possible further work. There are two appendixes. In Ap-

pendix A, a brief outline of the path-integral formulation of stochastic processes and the use of optimal paths in the weak-noise limit is given. In Appendix B, the nature of the optimal paths which govern state selection in a general one-dimensional potential are analyzed in some detail.

II. STATE SELECTION IN A SIMPLE 1D SYSTEM

In this section we will study the evolution of the system

$$\dot{x}(t) = \alpha x(t) + \eta(t), \quad x(0) = x_0, \quad (1)$$

where $\eta(t)$ is a Gaussian noise such that

$$\langle \eta(t) \rangle = 0, \quad \langle \eta(t) \eta(t') \rangle = 2D \delta(t - t'). \quad (2)$$

This simple problem can be solved exactly on the infinite interval $-\infty < x < \infty$. There are many ways to do this [8,9], but probably the easiest method is to use Eq. (1) to calculate $\langle x(t) \rangle$ and $\langle x^2(t) \rangle$ and then note that since $x(t)$ is linearly related to $\eta(t)$ and $\eta(t)$ has a Gaussian distribution, so will $x(t)$. Doing this one finds that the probability distribution that the system is at x_f at time T given that it began at x_0 at time $t=0$ is

$$p(x_f, T | x_0, 0) = \left(\frac{\alpha}{2\pi D} \right)^{1/2} \frac{1}{(e^{2\alpha T} - 1)^{1/2}} \times \exp - \left\{ \frac{\alpha(x_0 - x_f e^{-\alpha T})^2}{2D(1 - e^{-2\alpha T})} \right\}. \quad (3)$$

The probability that the system has selected the states with $x_f > X$ is

$$P(X, T | x_0, 0) = \int_X^\infty dx_f p(x_f, T | x_0, 0). \quad (4)$$

Here $X > 0$ is some position far enough away from the origin so that once the system has reached this point there is negligible probability of it crossing back to $x_f < 0$, at least on the time scales of interest here. The integral in Eq. (4) may be carried out exactly by changing variables to $z = x_f e^{-\alpha T} - x_0$, so that

$$P(X, T | x_0, 0) = \left(\frac{\alpha}{2\pi D} \right)^{1/2} \frac{e^{\alpha T}}{(e^{2\alpha T} - 1)^{1/2}} \times \int_{X e^{-\alpha T} - x_0}^\infty dz \exp - \left\{ \frac{\alpha z^2}{2D(1 - e^{-2\alpha T})} \right\}. \quad (5)$$

An important point to notice is that the change of variable has brought out a factor of $e^{\alpha T}$ which makes it manifestly obvious that Eq. (5) has a finite nonzero limit as $T \rightarrow \infty$. Although we need not take $T \rightarrow \infty$ (or more precisely $T \gg \alpha^{-1}$, so that terms $e^{-\alpha T}$ can be neglected), the results simplify considerably in this limit, so it is convenient to do so. If we choose to work at finite T , we need to choose X appropriately to ensure that the state-selection process has occurred. On the other hand, in the limit that $T \rightarrow \infty$ the probability (5) becomes independent of X , as we would expect. From Eq. (5)

$$\begin{aligned} \lim_{T \rightarrow \infty} P(X, T | x_0, 0) &= \left(\frac{\alpha}{2\pi D} \right)^{1/2} \int_{-x_0}^{\infty} dz \exp - \left\{ \frac{\alpha z^2}{2D} \right\} \\ &= \frac{1}{2} [1 + \operatorname{erf}(x_0/\ell)], \end{aligned} \quad (6)$$

where $\ell \equiv (2D/\alpha)^{1/2}$ is a characteristic diffusion length and erf is the error function [16]. This is the probability that the state at large positive x is selected. If $x_0=0$ then this probability is $1/2$, if $x_0>0$ it is greater than $1/2$ and approaches unity for $x_0 \gg \ell$. Similarly, if $x_0<0$ the state-selection probability is less than $1/2$ and approaches zero for $|x_0| \gg \ell$, again as we would expect. Clearly the probability that the state at large negative x is selected can be obtained by subtracting Eq. (6) from 1 to give $(1/2)[1 - \operatorname{erf}(x_0/\ell)]$. This can be obtained directly by beginning with Eq. (4), but with the range of integration now being $(-\infty, -X)$, where $X>0$. This leads to an integration range in Eq. (6) of $(-\infty, -x_0)$. Since erf is an odd function, we may combine these two results and write the probability of the state at large positive (negative) x being selected as $P_+(P_-)$ where

$$P_{\pm} = \frac{1}{2} [1 + \operatorname{erf}(\pm x_0/\ell)]. \quad (7)$$

This is one of the few problems in which we have the luxury of calculating state-selection probabilities exactly. In all other cases approximation schemes have to be used. As discussed in Sec. I, the two methods applied to date are the BFPE and path integrals. Therefore, the remainder of this section will be devoted to the derivation of the state-selection probability, i.e., Eq. (6), using these methods.

To formulate the problem using the BFPE, let us first denote the solution of the (forward) Fokker-Planck equation for a potential $V(x) = -(1/2)\alpha x^2$ with absorbing boundary conditions at $x_f = \pm X$, by $\tilde{p}(x_f, T | x_0, 0)$. This function also satisfies the BFPE [8,9],

$$\frac{\partial \tilde{p}}{\partial T} = -V'(x_0) \frac{\partial \tilde{p}}{\partial x_0} + D \frac{\partial^2 \tilde{p}}{\partial x_0^2}. \quad (8)$$

By integrating Eq. (8) over x_f , it follows that the probability that the system is still in the interval $(-X, X)$ at time T , that is, the survival probability,

$$Q(X, T | x_0, 0) = \int_{-X}^X dx_f \tilde{p}(x_f, T | x_0, 0), \quad (9)$$

also satisfies this equation. In addition, it is clear that the probability of absorption before time T , given by

$$P(X, T | x_0, 0) = 1 - Q(X, T | x_0, 0), \quad (10)$$

also satisfies the BFPE. Since $P(X, T | x_0, 0)$ has a finite limit as $T \rightarrow \infty$ we may take this limit at the outset. Once again, there is no need in principle to do this; we could keep T finite. Taking $T \rightarrow \infty$, the stationary problem reads

$$0 = \alpha x_0 \frac{du}{dx_0} + D \frac{d^2 u}{dx_0^2}, \quad u(x_0) = \lim_{T \rightarrow \infty} P(X, T | x_0, 0). \quad (11)$$

We are interested in the probability of absorption through one boundary. If we choose this to be the boundary at X , then

Eq. (11) has to be solved subject to the absorbing boundary conditions $u(X)=1$ and $u(-X)=0$. The solution is

$$u(x_0) = \frac{\int_{-X/\ell}^{x_0/\ell} dz e^{-z^2}}{\int_{-X/\ell}^{X/\ell} dz e^{-z^2}}. \quad (12)$$

The residual dependence on X only gives exponentially small terms, which are related to the very rare chance of recrossing the maximum. As explained in Sec. I, these very long time phenomena are not of interest here, and so we may take $X \rightarrow \infty$ in Eq. (12) giving

$$u(x_0) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{x_0/\ell} dz e^{-z^2} = \frac{1}{2} [1 + \operatorname{erf}(x_0/\ell)], \quad (13)$$

as in Eq. (6). We see that the method based on the use of the BFPE gets the result very quickly in this simple example. The weakness of the method becomes apparent when investigating higher dimensional situations. Then the ordinary differential equation (11) becomes a partial differential equation and so is much more difficult to solve.

The path-integral approach consists of calculating $p(x_f, T | x_0, 0)$ when D is small. This is achieved by finding the optimal paths, which is analogous to making a semiclassical approximation in quantum mechanics or finding instanton solutions in field theory. In this simple example, it is possible to find the exact result (3) using this method. In more complicated problems only the exponential term, and perhaps the prefactor, can be calculated. However, for the values of D that we are interested in, the leading contribution provided by the exponential factor is sufficient.

An overview of the method is given in Appendix A. Here we will simply indicate how the exponential factor may be obtained. The starting point is the action functional

$$S[x] = \frac{1}{4} \int_0^T dt (\dot{x} - \alpha x)^2. \quad (14)$$

The extrema of $S[x]$ are found by setting $\delta S / \delta x(t) = (1/2) \times (-\ddot{x} + \alpha^2 x)$ equal to zero, and solving the resulting differential equation subject to the boundary conditions $x(0) = x_0$ and $x(T) = x_f$. This is the path of least action, also called the optimal path or classical path. In this case, it is easily found by solving the equation $\ddot{x} = \alpha^2 x$ to be

$$x_c(t) = x_0 e^{\alpha t} + (x_f - x_0 e^{\alpha T}) \frac{\sinh \alpha t}{\sinh \alpha T}. \quad (15)$$

Substituting Eq. (15) into Eq. (14) gives the action for the classical path,

$$S_c = \frac{1}{4} \int_0^T dt (\dot{x}_c - \alpha x_c)^2 = \frac{\alpha(x_0 - x_f e^{-\alpha T})^2}{2(1 - e^{-2\alpha T})}. \quad (16)$$

As explained in Appendix A, the leading contribution to the path integral is $e^{-S_c/D}$, and we see that using Eq. (16) the exponential factor in Eq. (3) is recovered.

III. COMPARISON OF THE TWO METHODS

The two methods of calculating the state-selection probabilities in Sec. II look very different. First, the BFPE involves time-independent quantities, whereas in the path integral, the temporal dynamics is central. Second, in the BFPE the error function arises directly, whereas in the path integral the quantity which naturally arises is the exponential factor $e^{-S/D}$. How are these seemingly different methods related? Our aim in this section is to answer this question.

Let us begin by asking why in the BFPE approach we can take $T \rightarrow \infty$ at an early stage, but why, at least in Sec. II, we do not do so in the path integral. The reason rests on the fact that, while the probability distributions p or \bar{p} vanish as $T \rightarrow \infty$ (there is no stationary probability distribution), the probability of absorption before time T , which is P , does have a finite nonzero limit as $T \rightarrow \infty$. Since P also satisfies the BFPE, we may work with it directly, but when using path integrals we have first to calculate p , then perform an integration to find P . From the specific example shown in Eq. (5), it is clear that carrying out the integration over x_f brings out a factor which makes P nonzero in the limit $T \rightarrow \infty$. It is also clear that the $T \rightarrow \infty$ limit must be finite, since P is a probability, and so is less than or equal to unity. We would therefore like to find a way of taking the limit $T \rightarrow \infty$ at an earlier stage in the path-integral method, and so simplifying the calculation.

To do this, we return to our explicit example. As we noted when discussing Eq. (5), the $e^{\alpha T}$ factor which appears in the change of variable $x_f = e^{\alpha T}(z + x_0)$ is crucial in that for large T it cancels the $(e^{2\alpha T} - 1)^{-1/2}$ term in the prefactor, thus yielding a finite nonzero result for $P(X, T | x_0, 0)$ as $T \rightarrow \infty$. This means that we cannot take the limit $T \rightarrow \infty$ in the definition of z . To understand the change of variable $z = x_f e^{-\alpha T} - x_0$ in terms of the optimal paths, we define a new path $w(t)$ as

$$w(t) = x_f e^{-\alpha(T-t)} - x_c(t). \quad (17)$$

Since both the terms on the right-hand side of this equation satisfy $\ddot{x} = \alpha^2 x$, so does $w(t)$. Furthermore, since the first term actually satisfies $\dot{x} = \alpha x$, the action for the classical path can be written entirely in terms of $w(t)$:

$$S_c = \frac{1}{4} \int_0^T dt (\dot{w} - \alpha w)^2. \quad (18)$$

The boundary conditions $x(0) = x_0$ and $x(T) = x_f$ on $x_c(t)$ now become conditions $w(0) = z$ and $w(T) = 0$ on the path $w(t)$. Taking $T \rightarrow \infty$ with z fixed, then gives a path which begins at z and ends at the origin. The required solution of $\ddot{w} = \alpha^2 w$ which satisfies these conditions is $w(t) = z e^{-\alpha t}$. Substituting this function into Eq. (18) yields $(1/2)\alpha z^2$, which gives the leading term $\exp -\alpha z^2/2D$ in Eq. (6), and hence the error function as a result. Further insight into the meaning of the transformation (17) can be gained by looking at the case of a more general potential $V(x)$, considered in Appendix B.

In addition to this discussion of the mathematical structure of the optimal paths in the limit $T \rightarrow \infty$, it is useful to examine how the form of the paths changes as T moves from

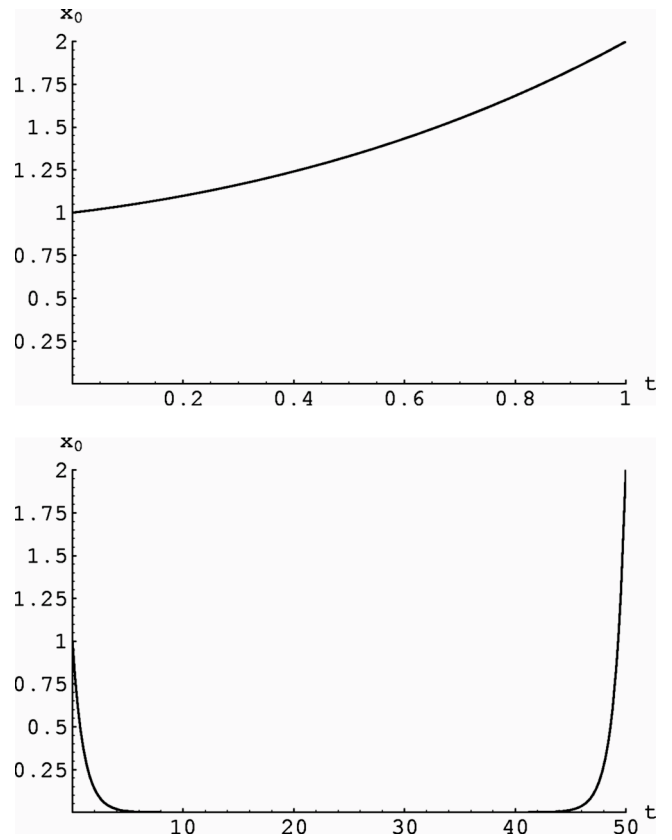


FIG. 1. The optimal paths for $T=1$ and $T=50$ with $\alpha=1$.

a value on the order of α^{-1} (the time scale associated with the potential) to values much greater than α^{-1} . We will see that a consideration of the nature of the paths in this case will give us a key insight into the type of paths that dominate the functional integral for type I state selection.

The optimal path for the problem considered in Sec. II is given by Eq. (15), and plotted out in Fig. 1 for two values of T : $T=1$ and $T=50$. The paths for these two values of T look very different. The reason is that if the specified time interval is short, e.g., $T=1$, the path taken in space and time is direct. This is a consequence of the constraint imposed by the initial and final conditions. On the other hand, as T gets larger the system has to take an increasingly indirect route in order to reach the final point at the specified time T . In the case where $T=50$, shown in Fig. 1, it is apparent that the system moves back to very near the origin, spends most of the time in the vicinity of the origin, and then moves back to $x_f = x$ relatively quickly. In the limit $T \rightarrow \infty$, the particle will move back to the origin in a time set by α^{-1} , spend an infinite amount of time in the vicinity of the maximum, and then move to $x_f = x$ in a time again set by α^{-1} .

Our aim in this section was to show how the BFPE and path-integral approaches are connected. In the BFPE approach the $T \rightarrow \infty$ limit is taken at the outset. Using the path integral, T may be chosen large, but at first sight it appears as if it has to be kept finite to ensure that a meaningful result is obtained. However, a transformation (17) can be made which allows the limit to be taken at an earlier stage. The nature of the optimal path for T large shows the importance of the maximum of the potential for state selection, which will be

important when investigating two-dimensional examples. The resulting form for S , and the identification of the variable z , leads to the error function, which in the BFPE approach is obtained by solution of the differential equation (11).

The discussion in this section has been concerned with the linear evolution equation (1). More generally, we can ask whether the same ideas apply to the case

$$\dot{x}(t) = -V'[x(t)] + \eta(t), \quad x(0) = x_0, \quad (19)$$

where $V(x)$ is a potential with a maximum at $x=0$ which also includes nonlinear terms. In this case, the stationary problem as defined in Eq. (11) generalizes by replacing the αx_0 factor with $-V'(x_0)$, which can be solved to give

$$u(x_0) = \frac{\int_{-X}^{x_0} dz e^{V(z)/D}}{\int_{-X}^X dz e^{V(z)/D}}. \quad (20)$$

Clearly, the error function only arises when $V(x)$ is a quadratic function of x . In the nonlinear case, if we change variables to $\zeta = \sqrt{-V(x)}/D$ we see that the nontrivial Jacobian of this transformation means that the resulting integral is not an error function. However, the dominant contribution can be approximated as an error function [2]. The description of the optimal path which leads to the result (20) is given in Appendix B.

IV. STATE SELECTION IN 2D SYSTEMS

We now turn our attention to 2D systems. For concreteness, we will focus on the following system:

$$\begin{aligned} \dot{x}(t) &= \alpha x(t) - \gamma x(t)y(t) + x(t)\eta_1(t), \\ \dot{y}(t) &= \beta y(t) - \gamma x(t)y(t) + y(t)\eta_2(t), \end{aligned} \quad (21)$$

where $\eta_i(t)$ is a Gaussian noise such that

$$\langle \eta_i(t) \rangle = 0, \quad \langle \eta_i(t) \eta_j(t') \rangle = 2D \delta_{ij} \delta(t - t'). \quad (22)$$

This is a simplified version of a model considered in Ref. [17] to describe the competition between two species in a fluctuating environment. In this paper we will use this model to illustrate the essential points necessary to understand state selection in dimensions higher than one. Although the deterministic equations cannot be derived from a potential, this poses no problems for the method. The connection between state selection and population dynamics will be made in a forthcoming paper. The deterministic equivalent of Eq. (21) has two fixed points, one at the origin and one at $(x, y) = (\beta/\gamma, \alpha/\gamma)$. In this model, no stable coexistence between the two species exists. Consequently, there is a separatrix that divides the x - y plane into two regions, one where the x species dominates the y species, and the other where the y species dominates the x species. The separatrix begins at the origin, passes through the nontrivial fixed point, and continues on to infinity. The detailed shape of this curve will de-

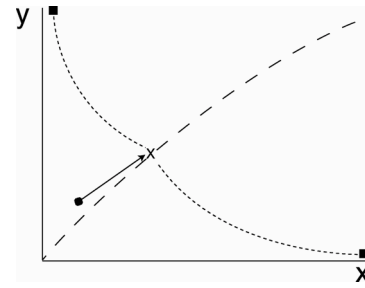


FIG. 2. A schematic representation of optimal paths that start near the separatrix at the solid circle, move to the vicinity of the saddle point indicated by an X, and move to either one of the end points indicated by a solid square. The separatrix is indicated by the large-dashed line.

pend on the parameters α , β , and γ . The state-selection problem in this case can be formulated by asking: given an initial condition (x_0, y_0) , what is the probability that a given species dominates? If the initial condition is sufficiently far from the separatrix, when the noise is weak the species that will dominate will be the one that has the same basin of attraction as the initial condition. However, if the initial condition is close to the separatrix, then there is a nonzero probability that the system will cross the separatrix and end up in the other basin of attraction. It is this probability that we wish to calculate. Clearly, this process is what we have called type I state selection.

In the path-integral approach to this problem we will once again take T to be large. In the one-dimensional case we saw that the optimal path was such that it spent most of the time in the vicinity of the maximum. This was necessary in order for the path to satisfy the conditions that it end up at the final point at precisely the time T . In the population dynamics model, the only way that an optimal path can be of arbitrarily long duration, is that it spend most of its time in the vicinity of the saddle point. It is this feature that makes the large T regime so convenient.

A typical optimal path, as illustrated schematically in Fig. 2, will move to the vicinity of the saddle point, remain there for a long period, and then move into either one of the basins of attraction. Of course, actual stochastic paths as seen in a Monte Carlo simulation, will display characteristics that are quite different from the optimal paths; see Appendix A for a discussion of this point.

The calculation now proceeds in a manner completely analogous to the 1D case discussed previously. The optimal path naturally decomposes into two distinct pieces. The first originates near the separatrix and ends in the vicinity of the saddle point, corresponding to the uphill path in the 1D problem. The second begins near the saddle point and moves to the final position in one of the basins, corresponding to the downhill path. As in the 1D case, no stationary probability distribution exists. Therefore, to calculate the state-selection probability we need to integrate over all final positions in the relevant basin of attraction.

To illustrate these ideas we take $\alpha = \beta$. The advantage of this choice is that the equation for the separatrix is simply $y = x$. We define coordinates parallel and perpendicular to the separatrix by

$$\begin{aligned}
r &\equiv y - x, \\
s &\equiv \frac{1}{2}(x + y) - \frac{\alpha}{\gamma}.
\end{aligned}
\tag{23}$$

The required integration over (x_f, y_f) now becomes an integration over (r_f, s_f) . The integration over s_f converts the probability distribution function in two variables to a function in one variable. The remaining coordinate r_f is analogous to x_f in the one-dimensional problem. The integration over r_f is performed by changing variables to the analog of z in the one-dimensional case. With this change of variables, we can take the $T \rightarrow \infty$ limit before performing the integration. The state-selection probability is now in the form of an integral that runs from $-r_0$ to ∞ . The leading contribution in the integrand is $e^{-S/D}$, where S is essentially the action for the first part of the optimal path, i.e., the part that connects the initial point with the saddle point. More specifically, it is the action calculated in the limit that $T \rightarrow \infty$ but with the parameter r_0 replaced with the variable $-z$, just as in the one-dimensional case.

We can take advantage of the fact that we are only interested in points near the separatrix to calculate S . Linearizing the extremal equations about the separatrix yields two coupled, linear ordinary differential equations. This process involves first solving for the nonlinear dynamics along the separatrix and then linearizing about this solution. The details of this calculation will be provided in a forthcoming publication [18]. The result for S is

$$S(z) = \frac{(\alpha - \gamma s_0)^2 z^2}{8s_0^2 [\alpha \ln(\alpha/\gamma s_0) - (\alpha - \gamma s_0)]} \equiv S z^2. \tag{24}$$

Putting these components together we find that the probability of ending up in the basin of attraction where r is large and positive (the y species dominates) is

$$\int_{-r_0}^{\infty} dz \exp \{-S z^2/D\}. \tag{25}$$

This expression is exactly of the form (6) and can be written, after normalization, as

$$\frac{1}{2}[1 + \operatorname{erf}(r_0 \sqrt{S/D})] = \frac{1}{2}[1 + \operatorname{sgn}(r_0) \operatorname{erf}(\sqrt{S(r_0)/D})]. \tag{26}$$

As in Sec. II, the probability that the state with large negative r is selected (the x species dominates) is 1 minus this quantity, that is,

$$\frac{1}{2}[1 - \operatorname{sgn}(r_0) \operatorname{erf}(\sqrt{S(r_0)/D})]. \tag{27}$$

So the final result for the probability of state selection is

$$\frac{1}{2}[1 + \operatorname{erf}(\pm \sqrt{S(r_0)/D})], \tag{28}$$

where the plus or minus sign is taken depending on whether the value of r in the selected state is the same or different to the sign of r_0 .

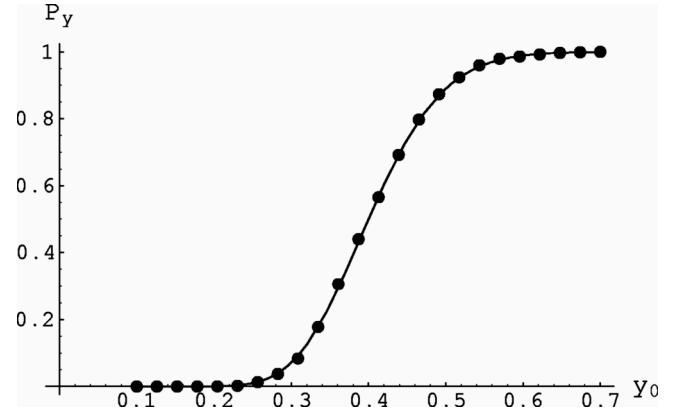


FIG. 3. Comparison of calculated state-selection probability (solid line) using Eq. (28) and Monte Carlo results (closed circles) with $D=0.01$, $x_0=0.4$, and $\alpha=\beta=\gamma=1$.

As can be seen in Figs. 3 and 4, these results are in remarkably good agreement with Monte Carlo simulations. Given that the result (25) was obtained via a linearization about the separatrix, it is somewhat surprising that the calculated probability agrees so well with the simulated probability for relatively large values of r_0 . Presumably, the small values of D ensure that we are still in the linear regime.

V. CONCLUSION

If noise is added to a deterministic system with two or more stable states, various phenomena are initiated. For example, on very long time scales there may be activation over the barrier separating any two of these stable states. In this paper we have been interested in a process which occurs on a shorter time scale: calculating the probability that the various stable states are “selected” by the system, given a particular initial condition. For the vast majority of initial states, one particular stable state will be selected with probability 1, and this is the state that would be predicted as the final state in the corresponding deterministic system. However, if the initial state is near a point of instability, such as a saddle

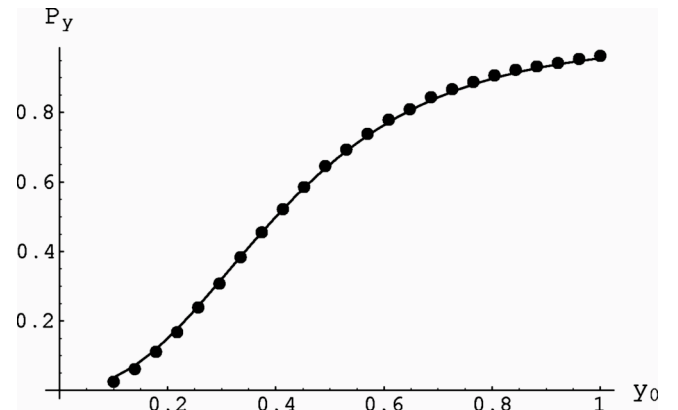


FIG. 4. Comparison of calculated state-selection probability (solid line) using Eq. (28) and Monte Carlo results (closed circles) with $D=0.1$, $x_0=0.4$, and $\alpha=\beta=\gamma=1$.

point, a separatrix, or an unstable point, the answer to the question of which stable state is “selected” is not so clear-cut; only probabilities of the various stable states being selected can be given. This paper has been concerned with the calculation of these probabilities.

In Sec. I we introduced a nomenclature to differentiate between different types of state selection. In one-dimensional problems only one type of state selection exists, but in two dimensions the system may start from the vicinity of the separatrix separating the basin of attraction of two stable states, or from the vicinity of a completely unstable state. We denoted these two kinds of state selection as type I and type II, respectively. In this paper, we restricted our attention to the former type, the latter having been explored previously [6,7]. Our concern was with the potential analytical approaches to the calculation of state-selection probabilities for type I systems, rather than the elucidation of any particular system. As is common in the field of stochastic nonlinear dynamics, there are two main approaches to the analysis: the asymptotic analysis of differential equations, typified in this context by the use of the BFPE, and the use of the path-integral formalism. This latter approach is the one favored by physicists, largely because of the intuitive insights it affords.

Although the BFPE is extremely powerful for one-dimensional problems, in higher dimensions a partial differential equation must be solved. The method of solution proceeds via a series of mappings resulting in a problem in two-dimensional classical dynamics. It has been known for many years that there is a classical dynamics associated with stochastic equations of the Langevin type and the solution of this dynamics in the weak noise limit allows the calculation of mean first passage times [19]. In the path-integral method, the optimal paths are the least-action solutions of this classical dynamics. In this sense, the path-integral method is more direct. One of the main aims of this paper has been to develop an intuition that will enable us to understand progressively more difficult state-selection problems. For example, we have shown how the error function is a direct consequence of integrating over the final positions in the relevant basin of attraction, but only when the potential transverse to the separatrix is quadratic. Another example concerns the nature of the optimal path in the large T limit. In order that the system arrives at the final point at time T , it needs to spend a long period in the vicinity of the saddle point. This is the fundamental reason why the saddle point is so important, even though typical Monte Carlo paths make transitions across any point along the separatrix.

This paper has stressed the technical aspects of the type I problem at the expense of making contact with applications. However, this does not mean that there is a lack of applications. In fact, the generic nature of the phenomenon implies that it will exist in a wide variety of situations, and some references to these applications were given in Sec. I. In a forthcoming publication [18] we will use the method of analysis outlined in this paper to explore some of these problems in more detail.

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APPENDIX A

In this appendix we review the formulation of stochastic differential equations, such as Eqs. (1), (19), or (21), as functional integrals and obtain the dominant contribution to the conditional probability we wish to determine in the limit where the noise strength tends to zero. We will limit our detailed discussion to the one-variable case, and simply state the results for an example in two dimensions, since the formalism generalizes in an obvious way. The use of path integrals in the solution of stochastic differential equations was described by Onsager and Machlup [20] in the case of linear equations and later extended to nonlinear equations by many authors, principally Graham [21,22]. An introduction to these ideas can be found in some of the standard textbooks on path integrals and quantum field theory [23,24]. An outline of the use of optimal paths in problems of this kind can be found in our earlier papers [7,25].

The conditional probability that the system is in the state x_f at time T , given it was initially in the state x_0 at $t=0$ is

$$p(x_f, T|x_0, 0) = \langle \delta[x_f - x(T)] \rangle_{\text{IC}}, \quad (\text{A1})$$

where IC denotes the initial condition $x(0)=x_0$ on the stochastic process and $x(T)$ is the solution of the differential equation (19) describing this process at time T . The average in Eq. (A1) is over Gaussian white noise $\eta(t)$ with zero mean and correlation function given by Eq. (2). In terms of functional integrals Eq. (A1) equals

$$\mathcal{C} \int_{\text{IC}} D\eta \delta[x_f - x_\eta(T)] \exp \left\{ -\frac{1}{4D} \int_0^T dt [\eta^2(t)] \right\}, \quad (\text{A2})$$

where \mathcal{C} is a normalization constant and the subscript η on $x(T)$ is to emphasize that it depends on $\eta(T)$ through Eq. (19). Using these equations to perform a functional change of variable from η to x yields, up to a normalization constant,

$$\int_{\text{IC}} Dx J \delta[x_f - x(T)] \exp \left\{ -\frac{1}{4D} \int_0^T dt [\dot{x} + V'(x)]^2 \right\}, \quad (\text{A3})$$

where J is the Jacobian of the transformation. Expressed as a path integral

$$p(x_f, T|x_0, 0) = \mathcal{C} \int_{x(0)=x_0}^{x(T)=x_f} Dx J[x] \exp \{-S[x]/D\}. \quad (\text{A4})$$

The action $S[x]$ and the Jacobian $J[x]$ are functionals which are given by

$$S[x] = \frac{1}{4} \int_0^T dt [\dot{x} + V'(x)]^2 \quad (\text{A5})$$

and [24]

$$J[x] = \det \left[\frac{\delta \eta}{\delta x} \right] \propto \exp \left\{ \frac{1}{2} \int_0^T dt [V''(x)] \right\}. \quad (\text{A6})$$

For $D \rightarrow 0$, the path integral (A4) is dominated by solutions of the Euler-Lagrange equations $\delta S / \delta x(t) = 0$, which satisfy the boundary conditions $x(0) = x_0$ and $x(T) = x_f$. Let the solution of least action be denoted by $x_c(t)$. Then writing $x(t) = x_c(t) + \delta x(t)$, scaling δx by $D^{1/2}$, and performing the Gaussian functional integral yields

$$p(x_f, T | x_0, 0) = C' \exp \{-S[x_c]/D\} J[x_c] \times \det \left[\frac{\delta^2 S}{\delta x(t') \delta x(t'')} \Big|_{x=x_c} \right]^{-1/2}. \quad (\text{A7})$$

The new overall constant C' is determined by normalization and there are higher corrections in the form of a power series in D multiplying Eq. (A7) which have been omitted.

While the above discussion has been carried out for a system with one degree of freedom, it should be clear that it generalizes in an obvious way to systems of more than one degrees of freedom and those where no potential exists [24]. We may summarize the result of performing the functional steepest descent on Eq. (A4) to next-to-leading order by

$$p(\vec{r}_f, T | \vec{r}_0, 0) = p^{(1)}(\vec{r}_f, T) \exp \{-p^{(0)}(\vec{r}_f, T)/D\} [1 + O(D)], \quad (\text{A8})$$

where the leading order contribution $p^{(0)}$ is just the action of the optimal path $\vec{r}_c(t) = [x_c(t), y_c(t), \dots]$ and the next-to-leading order contribution is

$$p^{(1)}(\vec{r}_f, T) = J[\vec{r}_c] (\det L[\vec{r}_c])^{-1/2}. \quad (\text{A9})$$

Here L is the matrix formed from the second order functional derivative of the action functional evaluated at the optimal path,

$$L[\vec{r}_c] = \frac{\delta^2 S}{\delta \vec{r}(t') \delta \vec{r}(t'')} \Big|_{\vec{r}=\vec{r}_c}. \quad (\text{A10})$$

The result (A8) is the starting point for our method: if we can determine the functions $p^{(0)}$ and $p^{(1)}$, then we will have a form for the conditional probability valid when the noise is weak.

To illustrate these ideas, let us use the simplest one variable problem $V(x) = -(1/2)\alpha x^2$, discussed in the main text, as an example. Then $V'(x) = -\alpha x$ and the action (A5) becomes Eq. (14). A variation then leads to the differential equation $\dot{x} = \alpha^2 x$ for the optimal path. The explicit form of the solution and its action are given in the main text by Eq. (15) and (16), respectively. This gives the leading order contribution. The next to leading order contribution [represented by Eq. (A9)] are found from

$$L[x_c] = -\frac{d^2}{dt^2} + \alpha^2, \quad J[x_c] \propto \exp \left\{ \frac{1}{2} \int_0^T dt [-\alpha] \right\}. \quad (\text{A11})$$

The functional determinant of $L[x_c]$ is proportional to $\sinh \alpha T / \alpha$ [26] and the Jacobian to $e^{-\alpha T/2}$. Putting these together gives Eq. (3), up to a normalization constant.

It is important to realize that there are two distinct dynamics associated with problems of this kind. The first is the original stochastic dynamics given by, for instance, Eq. (19). This is the dynamics used in Monte Carlo simulations. The second dynamics is the *deterministic* dynamics, given by a variation of the action (A5), which describes the $D \rightarrow 0$ limit of the stochastic dynamics. They are quite different and it is important not to carry over intuition from one to the other without careful consideration. From (A5),

$$S[x] = \frac{1}{2} \int_0^T dt \left[\frac{1}{2} \dot{x}^2 - U(x) \right] + \frac{1}{2} \int_0^T dt \frac{dV}{dt}, \quad (\text{A12})$$

where

$$U(x) = -\frac{1}{2} [V'(x)]^2. \quad (\text{A13})$$

Since the last term in Eq. (A12) is a constant, and consequently gives zero variation, the Euler-Lagrange equations obtained from Eq. (A12) correspond to classical mechanics in the potential $U(x)$. When considering the optimal paths such as $x_c(t)$, it is the potential $U(x)$, and not $V(x)$, which is relevant.

As we have stressed, all of these ideas generalize immediately to systems with more than one variable. For example, the stochastic differential equations (21) give rise to the action

$$S[x, y] = \frac{1}{4} \int_0^T dt \left[\left(\frac{\dot{x} - \alpha x + \gamma xy}{x} \right)^2 + \left(\frac{\dot{y} - \beta y + \gamma xy}{y} \right)^2 \right], \quad (\text{A14})$$

which when varied leads to the differential equations

$$\frac{1}{x} \frac{d}{dt} \left(\frac{\dot{x}}{x} - \alpha + \gamma y \right) = \gamma \left(\frac{\dot{y}}{y} - \beta + \gamma x \right), \quad (\text{A15})$$

$$\frac{1}{y} \frac{d}{dt} \left(\frac{\dot{y}}{y} - \beta + \gamma x \right) = \gamma \left(\frac{\dot{x}}{x} - \alpha + \gamma y \right).$$

APPENDIX B

In this appendix we explore the path-integral approach to the calculation of state-selection probabilities in a general one-dimensional potential $V(x)$. As we have stressed throughout, such calculations are most straightforwardly carried out using the BFPE. This was shown explicitly in Sec. III, where the result in the case of interest was obtained, and displayed in Eq. (20). However, our interest is not in this one-dimensional problem for its own sake, but instead in using it to gain insights into the path-integral method for other problems of this kind. These insights will turn out to be

valuable in the investigation of higher-dimensional systems where the BFPE method is not so useful, and path-integral methods are.

The potential $V(x)$ will be assumed to have no extrema other than at the origin, where it has a maximum. For all other values of x , $V(x) < 0$: it has a positive slope for negative x and a negative slope for positive x . Obviously, the simple example $V(x) = -(1/2)\alpha x^2$, discussed previously in this paper, satisfies these conditions. We will also use $V(x) = -(1/2n)\alpha x^{2n}$, $n=2,3,\dots$, as another simple example.

The problem is formally defined by Eq. (19) with $\eta(t)$ given by Eq. (2). The path-integral formulation of this problem is given in Appendix A. The optimal paths, found by variation of the action (A5), are solutions of the second order differential equation

$$\ddot{x} = V'(x)V''(x), \quad (\text{B1})$$

which may be integrated once to give

$$\frac{1}{2}\dot{x}^2 = \frac{1}{2}[V'(x)]^2 + k, \quad (\text{B2})$$

where k is a constant of integration. In the, technically similar but conceptually different, study of the problem of activation over a potential barrier, the paths begin and end at an extrema of the potential, and so both $V'(x)$ and \dot{x} are zero as $t \rightarrow \pm\infty$, and so $k=0$ [10,11]. In this case Eq. (B2) reduces to $\dot{x} = \pm V'(x)$. A solution satisfying $\dot{x} = +V'(x)$ is called an ‘‘uphill’’ path [since \dot{x} and $V'(x)$ both have the same sign] and $\dot{x} = -V'(x)$ a ‘‘downhill’’ path [since \dot{x} and $V'(x)$ have different signs] [10]. These solutions again turn out to have important roles to play in the present problem, in the limit $T \rightarrow \infty$.

To determine the relevant optimal path for general $V(x)$, we first make a change of variable analogous to Eq. (17) in the case $V(x) = -(1/2)\alpha x^2$. The function $x_f e^{-\alpha(T-t)}$ is the downhill solution for this potential which ends up at x_f at time T . Therefore, let $x_d(t; x_f)$ be the solution of $\dot{x} = -V'(x)$ satisfying $x_d(T; x_f) = x_f$. Then the generalization of Eq. (17) is

$$w(t) = x_d(t; x_f) - x_c(t). \quad (\text{B3})$$

Once again $w(t)$ satisfies the boundary conditions $w(0) = z$ and $w(T) = 0$, where z is now defined by

$$z = x_d(0; x_f) - x_0. \quad (\text{B4})$$

For large T , $x_d(0; x_f)$ is very small, since to take a long time to get to x_f requires starting very near to the origin. In particular,

$$\lim_{T \rightarrow \infty} x_d(0; x_f) = 0. \quad (\text{B5})$$

Therefore, from Eq. (B4) we see that $z \approx -x_0$, and from Eq. (B3) that $w(t) \approx -x_c(t)$ for $t \ll T$. This implies that, in the limit $T \rightarrow \infty$, $w(t)$ is a path beginning at z on the other side of the maximum to x_0 and ending at the origin. This implies that it is an uphill path with an initial condition $-z$. We may therefore denote it as $-x_u(t; -z)$. In summary, for large T ,

$$x_c(t) = x_u(t; -z) + x_d(t; x_f). \quad (\text{B6})$$

For the first part of the path ($t \ll T$), the downhill solution is negligible, and the optimal path is entirely made up of the term x_u . For the vast majority of the time, both terms are negligible, and $x_c(t) \approx 0$. For the very last part of the path, the uphill solution is negligible, and the path is entirely made up of the downhill solution. The situation is clearly illustrated in Fig. 1 when $T=50$, for the $n=1$ case. When calculating the action of this path, the time integral in Eq. (A5) may be split up into these three regimes. Since the downhill solution gives zero action [because $\dot{x} + V'(x) = 0$], only the first part of the path gives a nonzero action:

$$S_c = \frac{1}{4} \int_0^{t^*} dt [\dot{x}_c + V'(x_c)]^2 = \int_0^{t^*} dt \dot{x}_c V'(x_c) = \int_{-z}^{x^*} dx_c V'(x_c), \quad (\text{B7})$$

where t^* is the time at which the path reaches x^* , which is so near to the origin that both the uphill and downhill solutions are effectively zero. As $T \rightarrow \infty$, $x^* \rightarrow 0$, and the classical action becomes

$$S_c = \int_{-z}^0 dx_c V'(x_c) = V(0) - V(-z) = -V(-z). \quad (\text{B8})$$

As an explicit example, let us look at the case $V(x) = -(1/2n)\alpha x^{2n}$, $n=1,2,\dots$. When $n=1$,

$$x_u(t; x_0) = x_0 e^{-\alpha t}, \quad x_d(t; x_f) = x_f e^{-\alpha(T-t)}. \quad (\text{B9})$$

When $n=2,3,\dots$, it is straightforward to show that

$$x_u(t, x_0) = \frac{x_0}{[1 + 2(n-1)\alpha t x_0^{2(n-1)}]^{1/2(n-1)}}, \quad (\text{B10})$$

$$x_d(t; x_f) = \frac{x_f}{[1 + 2(n-1)\alpha(T-t)x_f^{2(n-1)}]^{1/2(n-1)}}.$$

It should be clear that the solutions have the properties we have described, and, in particular, when $T \rightarrow \infty$, the time interval may be separated into subintervals where at most one of the solutions is non-negligible.

The dominant contribution to the path integral (A4) is $e^{-S_c/D}$, which by Eq. (B8) gives

$$p(x_f, T | x_0, 0) \sim \exp \{V(-z)/D\}. \quad (\text{B11})$$

Using Eq. (4), the probability that the system has selected the states with $x_f > X$ is

$$P(X, T | x_0, 0) \sim \int_X^\infty dx_f \exp \{V(-z)/D\}. \quad (\text{B12})$$

The \sim sign has been used, since the prefactor $p^{(1)}$ will depend on x_f , and so contribute to the integral. It is also understood that S_c is only exactly equal to $-V(-z)$ in the limit $T \rightarrow \infty$. Changing variables from x_f to z using Eq. (B4), taking $T \rightarrow \infty$, and using Eq. (B5) gives

$$\lim_{T \rightarrow \infty} P(X, T | x_0, 0) \sim \int_{-x_0}^{\infty} dz \exp \{V(-z)/D\}, \quad (\text{B13})$$

in agreement with Eq. (20).

The results of this appendix may be summarized as follows. In order to make a transformation from x_f to a new variable [going from Eq. (4) to Eq. (5) or from Eq. (B12) to Eq. (B13)] we need to keep T finite. This is because as $T \rightarrow \infty$ the dependence of the action on x_f is lost, and the transformation becomes singular. However, since the calculation simplifies considerably in this limit, the idea is to keep T finite only in the combination on the right-hand side of Eq. (B4), and to take the limit elsewhere. This appendix shows that the effect of this is simply to substitute minus this combination (defined to be $-z$) for the initial condition, but to leave the calculation otherwise unchanged. Of course, if T had not been kept finite in Eq. (B4), then $-z$ would have equaled x_0 and the action would simply have been $-V(x_0)$.

This is the result which we would expect from an uphill path in the $T \rightarrow \infty$ limit.

It should be clear that these ideas extend to two, and higher dimensions. A specific two-dimensional calculation is outlined in Sec. IV, and will be presented in more detail in a future publication [18]. The additional feature is that the integration over the final states (the analog of x_f) has to be decomposed into two parts. The first is the coordinate parallel to the separatrix. This is simply integrated over. The second is the coordinate perpendicular to the separatrix. Once the first integration has been carried out, this second integration is of the kind (4) found in one-dimensional problems. The development of the formalism then follows similar lines to that just given.

Finally, several aspects of the formalism discussed in this appendix have the flavor of the BFPE, for instance, the fact that a final condition is imposed on the downhill solution $x_d(t; x_f)$, rather than an initial condition. This connection will be explored in more detail elsewhere [18].

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