

First Passage Time and Extremum Properties of Markov and Independent Processes

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It was shown by Newell in 1962 that the extreme value and first passage time distributions of various types of common Markov processes asymptotically approach those for independent random variables. In view of the great simplification this occasions in the calculation of a number of important properties of Markov processes, it is clearly of interest to determine in some detail the conditions on both the time and space variables under which this equivalence holds. In this paper we investigate and establish these conditions for Markov processes described by the Fokker-Planck equation and express them in simple analytic forms which are directly related to the coefficients of the Fokker-Planck equation. To demonstrate the usefulness of these conditions, we apply them to two representative examples of Fokker-Planck equations, the Ornstein-Uhlenbeck process and the Montroll-Shuler model for harmonic oscillator dissociation. It is shown very clearly in these examples that the extreme value and first passage time

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distributions, and thus the mean extreme and mean first passage times, of these Markov processes approach very closely those for independent random variables at finite values of the time and space variables.

KEY WORDS: Markov processes; independent random variables; Fokker–Planck equation; Ornstein–Uhlenbeck equation; extreme value distributions; first passage time distributions; mean maxima; mean first passage times.

1. INTRODUCTION

Most previous work on the theory of extremes in probability theory deals with independent random variables in discrete time.⁴ Physical processes, however, frequently involve *dependent* random variables in *continuous* time. It is thus of interest and importance to extend the theory of extremes to dependent variables in continuous time. This paper is concerned with such an extension to a specific class of Markov processes.

The theory of extremes is the study of the distribution of the extreme values (maximum or minimum) of a random variable within a given time interval. The distribution of extreme values is closely related to the distribution of first passage times of the random variable to a prescribed boundary.

Some properties of extreme value distributions for Markov processes have been investigated previously.^(3–7) In Ref. 4, Newell discusses the asymptotic extreme value distribution for one-dimensional processes, addressing himself particularly to the question “as to which of the common types of Markov processes give rise to extreme value distributions like those obtained for independent identically distributed random variables.”

The calculation of extreme value distributions and their moments for Markov dependent variables is invariably a much more difficult task than the calculation of these properties for independent random variables. It is reasonable to expect, however, that the extreme values of a Markov dependent random variable within a given time interval themselves form a set of independent random variables if the time interval is sufficiently long. This assumption has been adopted by Gumbel⁽¹⁾ and other workers. Thus, for instance, when considering the problem of maxima of levels in a river over a period of many years, Gumbel makes the assumption that the set of observations of these maxima in a given interval of time forms a set of independent random variables if this time interval is sufficiently long, say one year. This is certainly a reasonable assumption. Even though the maximum heights of the river are strongly correlated variables if observations are made within 10-min inter-

⁴ Gumbel⁽¹⁾ gives a very useful survey of the subject and its history through 1958. See David⁽²⁾ for more recent work.

vals, one would certainly expect that this correlation has completely disappeared as the observation interval is extended to one year. It is of interest to know how rapidly these correlations decay in a Markov process so that one can calculate, rather than guess, time intervals for which the assumption of independent random variable behavior of the extreme values is valid.

A stochastic process with independent random variables can be characterized by the simple functional form of the probability $F(\xi, t)$ that the process stays below ξ throughout the time t . This form is $F(\xi, t) = \exp[-\lambda(\xi)t]$, where the function $\lambda(\xi)$ is related to the statistical distribution of the random variables and is hence dependent on the details of the process. From this distribution, moment properties can be calculated. The mean first passage time to ξ , for instance, is given by $T_1(\xi) = [\lambda(\xi)]^{-1}$. The mean maximum of the process is also simply related to $F(\xi, t)$. The probability $F(\xi, t)$ and its moments for a Markov process are much more complicated and in general difficult to calculate. After a sufficiently long time t and for sufficiently large values of the variable ξ , the Markovian probability function $F(\xi, t)$ is well approximated by $\exp[-\lambda_0(\xi)t]$, the simple form characteristic of an independent random variable process. The function $\lambda_0(\xi)$ depends on the details of the Markov process but is much simpler to evaluate than the exact probability $F(\xi, t)$. Approximate moment properties can again readily be obtained; for instance, the mean first passage time to ξ is $T_1(\xi) \simeq [\lambda_0(\xi)]^{-1}$.

It is thus of importance to determine conditions on both the time and space variables for which extreme value distributions and their moments in Markov processes approach the behavior characteristic of processes of independent random variables, since calculations are then greatly simplified. In this paper we investigate and establish such conditions for the class of Markov processes that obey a Fokker–Planck equation. We find such conditions and express them in forms which can be directly related to the coefficients in the Fokker–Planck equation. These conditions are then tested for two particular processes, namely the Ornstein–Uhlenbeck (OU) process⁽⁸⁾ and the Montroll–Shuler model⁽⁹⁾ for harmonic oscillator dissociation in the high-temperature limit.^(10,11) It is shown in these examples that the extreme value and first passage time distributions of these Markov processes approach very closely those for independent random variables at finite values of the time and space variables.

In Section 2 we present the necessary definitions and general expressions for first passage time and extreme value distributions and their moments. In Section 3 results for independent random variables are briefly reviewed. In Section 4 we consider the general Fokker–Planck equation and establish conditions for approach to independent random variable behavior. These conditions are tested on the Ornstein–Uhlenbeck equation, for which detailed

numerical calculations are presented in Section 5, and on the harmonic oscillator dissociation equation in Section 6.

2. DEFINITIONS

In this section we define the functions and processes to be studied in the body of this paper.

We limit our considerations to one-dimensional Markov processes with random variables $X(t)$ defined for continuous time. Let $f(x, t|x_0) dx$ be the probability that $X(t)$ lies within $(x, x + dx)$ without ever having crossed $x = \xi$ in time $(0, t)$, given $X(0) = x_0$. As will be seen below, all quantities relevant to the theory of extremes can be expressed in terms of the probability density $f(x, t|x_0)$.

Define a new random variable

$$Z(t) \equiv \max\{X(\tau), 0 \leq \tau \leq t\} \quad (1)$$

Then the cumulative distribution function, defined by

$$F(\xi, t|x_0) \equiv \int_r^\xi dx f(x, t|x_0) \quad (2a)$$

has the probabilistic meaning

$$F(\xi, t|x_0) = \text{Prob}\{Z(t) < \xi | X(0) = x_0\} \quad (2b)$$

where $x = r$ denotes a reflecting boundary; r may be finite or negative infinite, with $r \leq x_0 < \xi$. The function F is useful when treating maxima problems. Minima problems can be treated similarly but then $\xi < x_0 \leq r$ with r finite or positive infinite.

An important random variable is the time τ when the process crosses $x = \xi$ for the first time, i.e., the first passage time

$$T(\xi) \equiv \min\{\tau | X(\tau) = \xi\} \quad (3)$$

Since $F(\xi, t|x_0)$ is the probability that $X(\tau)$ never crosses $x = \xi$ during the time $0 \leq \tau \leq t$, it can be related to the first passage time. From Eqs. (2b) and (3) we find

$$F(\xi, t|x_0) = \text{Prob}\{T(\xi) > t | X(0) = x_0\} \quad (4)$$

Two more useful definitions are

$$\begin{aligned} \Psi(\xi, t|x_0) d\xi &\equiv [(\partial/\partial\xi)F(\xi, t|x_0)] d\xi \\ &= \text{Prob}\{\xi < Z(t) < \xi + d\xi | X(0) = x_0\} \end{aligned} \quad (5)$$

$$\begin{aligned} \Phi(\xi, t|x_0) dt &\equiv -[(\partial/\partial t)F(\xi, t|x_0)] dt \\ &= \text{Prob}\{t < T(\xi) \leq t + dt | X(0) = x_0\} \end{aligned} \quad (6)$$

The functions f , F , Ψ , and Φ are Green's functions for processes with arbitrary initial distributions. They can be averaged over any initial distribution $\eta(x_0)$:

$$\begin{aligned}
 F(\xi, t) &\equiv \int_{\tau}^{\xi} dx_0 \eta(x_0) F(\xi, t | x_0) \\
 &= \text{Prob}\{T(\xi) > t\} = \text{Prob}\{Z(t) < \xi\}
 \end{aligned}
 \tag{7}$$

$$\Psi(\xi, t) \equiv \int_{\tau}^{\xi} dx_0 \eta(x_0) \Psi(\xi, t | x_0) = (\partial/\partial \xi) F(\xi, t)
 \tag{8}$$

$$\Phi(\xi, t) \equiv \int_{\tau}^{\xi} dx_0 \eta(x_0) \Phi(\xi, t | x_0) = -(\partial/\partial t) F(\xi, t)
 \tag{9}$$

Using these distribution functions, one can now write down moments, i.e., various mean properties, such as, for instance, the mean maximum of the variable $X(t)$ in a given time interval $(0, t)$ or the mean first passage time to $x = \xi$. We define the n th moments of $Z(t)$ and $T(\xi)$ by

$$\begin{aligned}
 Z_n(t | x_0) &\equiv \int_{\tau}^{\infty} d\xi \xi^n \Psi(\xi, t | x_0) \\
 &= r^n + n \int_{\tau}^{\infty} d\xi \xi^{n-1} [1 - F(\xi, t | x_0)]
 \end{aligned}
 \tag{10}$$

$$T_n(\xi | x_0) \equiv \int_0^{\infty} dt t^n \Phi(\xi, t | x_0) = n \int_0^{\infty} dt t^{n-1} F(\xi, t | x_0)
 \tag{11}$$

Moments with respect to an initial distribution $\eta(x_0)$ will be denoted by $Z_n(t)$ and $T_n(\xi)$. The quantity $Z_1(t)$ is then the mean maximum of the process in the time interval $(0, t)$; the variance of the maximum in this time interval is $Z_2(t) - Z_1^2(t)$. The mean first passage time to $x = \xi$ is $T_1(\xi)$ and its variance is $T_2(\xi) - T_1^2(\xi)$. The corresponding conditional quantities are similarly defined.

We will also consider processes for which $f(x, t | x_0) dx$ is the probability that the random variable $X(t)$ lies within $(x, x + dx)$ without ever having crossed $x = \pm \xi$ ($\xi \geq 0$) in time $(0, t)$, given $X(0) = x_0$. This case is of interest, for instance, in the study of largest deviations of the random variable from equilibrium. All definitions given so far can be suitably modified to cover this situation. We define the random variable

$$Y(t) \equiv \max\{|X(\tau)|, 0 \leq \tau \leq t\}
 \tag{12}$$

as the greatest excursion of the random variable X from zero in the time interval $(0, t)$. The appropriate cumulative distribution function for this problem is

$$F(\xi, t | x_0) \equiv \int_{-\xi}^{\xi} dx f(x, t | x_0)
 \tag{13}$$

The probabilistic definitions in Eqs. (2b) and (4) hold here with $Y(t)$ as defined in Eq. (12) and $T(\xi)$ given by

$$T(\xi) \equiv \min\{\tau | X(\tau) = \pm \xi\} \tag{14}$$

Equations (5)–(9) and (11) remain unchanged except for the replacement $r \rightarrow -\xi$ in the lower limits of integration. In place of Eq. (10) we now have

$$Y_n(t|x_0) \equiv \int_0^\infty d\xi \xi^n \Psi(\xi, t|x_0) = n \int_0^\infty d\xi \xi^{n-1} [1 - F(\xi, t|x_0)] \tag{15}$$

With $F(\xi, t|x_0)$ defined in (13), the quantities $Y_1(t|x_0)$ and $Y_1(t)$ are now mean extrema; $T_1(\xi|x_0)$ and $T_1(\xi)$ are mean first passage times to $x = \pm \xi$. It should be noted that in the frequently occurring situations in which $F(\xi, t)$ is an even function of ξ , the moments $T_n(\xi)$ and $Y_n(t)$ here are identical with the moments $T_n(\xi)$ and $Z_n(t)$ discussed earlier with a reflecting boundary at $r = 0$.

We restrict our discussion to Markov processes in continuous time. We believe that many of our conclusions are valid for a large class of master equations of the form

$$(\partial/\partial t)f(x, t|x_0) = \int dx' K(x, x')f(x', t|x_0) \tag{16}$$

where $K(x, x')$ is the transition rate from state x' to state x . However, we will concern ourselves only with a special case of Eq. (16), namely the Fokker-Planck equation

$$\frac{\partial}{\partial t}f(x, t|x_0) = \frac{\partial}{\partial x} \left\{ -m_1(x)f(x, t|x_0) + \frac{1}{2} \frac{\partial}{\partial x} [m_2(x)f(x, t|x_0)] \right\} \tag{17}$$

with the initial condition $f(x, 0|x_0) = \delta(x - x_0)$ and appropriate boundary conditions to be discussed in Section 4.

3. RESULTS FOR INDEPENDENT RANDOM VARIABLES

Since it is one of the objectives of this paper to compare the results for extreme value distributions of Markov processes with those for independent random variables, we collect here the relevant results for the latter case.^(1,2,12) The statistics of extremes for independent random variables are traditionally dealt with in terms of variables defined for discrete times. We will thus state results in terms of processes in discrete time and then take limits to continuous time where appropriate.

Let X_1, X_2, \dots, X_n be n sequential observations of a process. The X_i are taken to be identically and continuously distributed independent random

variables. Let $Z(n)$ be a new random variable defined by

$$Z(n) \equiv \max\{X_m, 1 \leq m \leq n\} \tag{18}$$

in analogy with Eq. (1). In further analogy with the equations in Section 2 we can define probabilities and probability densities such as, for example,

$$F(\xi, n) \equiv \text{Prob}\{Z(n) < \xi\} \tag{19}$$

[cf. Eq.(7)] and

$$\Psi(\xi, n) d\xi = [(\partial/\partial\xi)F(\xi, n)] d\xi = \text{Prob}\{\xi < Z(n) < \xi + d\xi\} \tag{20}$$

[cf. Eq. (8)]. The moments can then be determined as in Section 2. Here the probabilities and probability densities are independent of the initial condition since we are dealing with independent random variables.

Let $P(x)$ be the cumulative distribution function for each x_i and $p(x)$ be its probability density function:

$$P(x) \equiv \text{Prob}\{X < x\} \tag{21}$$

$$p(x) \equiv (d/dx)P(x) \tag{22}$$

The function $P(x)$ [or $p(x)$] is all that is needed to determine every property of the process. Thus, for instance, the probability $F(\xi, n)$ that the maximum of n observations is below ξ is equal to the probability that each of the X_i , $i = 1, \dots, n$, is less than ξ so that

$$F(\xi, n) = [P(\xi)]^n \tag{23}$$

from which it follows that

$$\Psi(\xi, n) = n[P(\xi)]^{n-1}p(\xi) \tag{24}$$

Moments can also be given immediately. Let Δt be the time between observations and let $t = n \Delta t$ be the time of the n th observation. Time is introduced here so that comparison with continuous time processes can be made later; we could of course continue our discussion in terms of "observation" or "step number" and never introduce time. The mean first passage time to $x = \xi$ [cf. Eq. (11)] is now given by the infinite series

$$\begin{aligned} T_1(\xi) &= \Delta t\{[1 - P(\xi)] + 2P(\xi)[1 - P(\xi)] + 3P^2(\xi)[1 - P(\xi)] + \dots\} \\ &= \frac{\Delta t}{1 - P(\xi)} \end{aligned} \tag{25}$$

For the independent process we define an upcrossing rate $\lambda(\xi)$ so that $\lambda(\xi) \Delta t$ is the probability that the process crosses the level $x = \xi$ from below in time Δt . Then

$$\lambda(\xi) \Delta t = 1 - P(\xi) \tag{26}$$

and the probability $F(\xi, t)$ that the process stays below ξ throughout the time $t = n \Delta t$ can, instead of Eq. (23), be written as

$$F(\xi, t) = [1 - \lambda(\xi) \Delta t]^n \quad (27)$$

In the limit of many observations such that $n \rightarrow \infty$, $\Delta t \rightarrow 0$, $n \Delta t = t$,

$$F(\xi, t) \rightarrow e^{-\lambda(\xi)t} \quad (28)$$

In this limit, the first passage time moments are then given by [cf. Eq. (11)]

$$T_n(\xi) = n!/\lambda^n(\xi) \quad (29)$$

and the mean maxima are [cf. Eq. (10)]

$$Z_n(t) = r^n + n \int_r^\infty d\xi \xi^{n-1} [1 - e^{-\lambda(\xi)t}] \quad (30)$$

The results of Eqs. (28) and (29), summarized as

$$F(\xi, t) \rightarrow e^{-t/T_1(\xi)} \quad (31)$$

are characteristic of independent processes. The form of $\lambda(\xi)$ or $T_1(\xi)$ of course depends on the particular process one is considering, i.e., on $P(\xi)$.

Equations (28), (29), and (31) also hold with some changes in definitions when one considers first arrival at $x = \pm \xi$. In place of Eq. (21) one now has

$$P(x) \equiv \text{Prob}\{|X_i| < x\} \quad (32)$$

The quantity $\lambda(\xi) \Delta t$ is the probability that the process crosses the level $x = \xi$ from below, or the level $x = -\xi$ from above, in time Δt . The moments $Y_n(t)$ now are

$$Y_n(t) = n \int_0^\infty d\xi \xi^{n-1} [1 - e^{-\lambda(\xi)t}] \quad (33)$$

Depending on the form of the cumulative distribution function of Eq. (21), and hence of the mean first passage time $T_1(\xi)$, one obtains in the limit as $t \rightarrow \infty$ (equivalent to $n \rightarrow \infty$) one of the three familiar stable asymptotic distributions of $F(\xi, t)$.^(12,13) The most familiar of the three, known as the asymptotic distribution of the exponential class,⁽¹⁴⁾ is

$$\lim_{t \rightarrow \infty} F(\xi, t) \sim \exp[-\exp(-Z)] \quad (34)$$

with

$$Z \equiv \alpha_n(\xi - \beta_n) \quad (35)$$

and α_n, β_n defined by the relations

$$P(\beta_n) = 1 - \frac{1}{n}; \quad \alpha_n = n \left. \frac{dP(x)}{dx} \right|_{x=\beta_n} \quad (36)$$

This asymptotic distribution holds for a wide class of probability density functions $p(x)$ for which, as $x \rightarrow \infty$,

$$\frac{P''(x)}{P'(x)} \sim \frac{P'''(x)}{P''(x)} \sim \frac{P^{(4)}(x)}{P'''(x)} \sim \dots \tag{37}$$

Exponential and Gaussian density functions are members of this class. The quantity β_n is the expected extreme value of X and becomes equal to the most probable extreme value when $n \rightarrow \infty$. The quantity α_n is a measure of the variation of β_n with n . The mean first passage time to $x = \xi$ corresponding to the asymptotic distribution (34) is

$$\frac{T_1(\xi)}{\Delta t} \sim \{1 - \exp[-\exp(-Z)]\}^{-1} \sim \exp Z \quad \text{for large } Z \tag{38}$$

It has been shown^(4,5) that in the limit $\xi \rightarrow \infty, t \rightarrow \infty$, the distribution $F(\xi, t)$ for Markov processes tends to the asymptotic independent random variable form, Eqs. (28) and (29). We will show in this paper by detailed analysis of some specific Markov processes that first passage time and extreme value distributions and moments are given to a very good approximation by the independent variable formulas also for finite times and finite boundaries. The criteria for this agreement and the errors involved will be discussed in detail in the next few sections.

4. SOLUTIONS OF THE FOKKER-PLANCK EQUATION WITH BOUNDARIES

In this section we formulate the solution of the Fokker-Planck equation

$$\begin{aligned} & \frac{\partial}{\partial t} f(x, t | x_0) \\ &= \frac{\partial}{\partial x} \left\{ -m_1(x) f(x, t | x_0) + \frac{1}{2} \frac{\partial}{\partial x} [m_2(x) f(x, t | x_0)] \right\} \end{aligned} \tag{39}$$

in the presence of boundaries. In Eq. (39) the coefficients $m_1(x)$ and $m_2(x)$ are given by the conditional expectation values of the change ΔX of the random variable X in time Δt :

$$\begin{aligned} E[\Delta X | X(t) = x] &= m_1(x) \Delta t + o(\Delta t) \\ E[(\Delta X)^2 | X(t) = x] &= m_2(x) \Delta t + o(\Delta t) \\ E[(\Delta X)^r | X(t) = x] &= o(\Delta t), \quad r \geq 2 \end{aligned} \tag{40}$$

The probability density also satisfies the backward Kolmogorov equation

$$\begin{aligned} & \frac{\partial}{\partial t} f(x, t | x_0) \\ &= m_1(x_0) \frac{\partial}{\partial x_0} f(x, t | x_0) + \frac{1}{2} m_2(x_0) \frac{\partial^2}{\partial x_0^2} f(x, t | x_0) \end{aligned} \quad (41)$$

There exists a large literature dealing with equations of the form of Eq. (39). Most of the literature can roughly be divided into three (overlapping) categories.^{(15–27),5} One category^(8,15,16) deals with the Ornstein–Uhlenbeck (OU) process [$m_1(x) = -\mu x$, $m_2(x) = 2D$, μ and D constant] as a description of Brownian motion, where the velocity distribution of Brownian particles is the distribution of interest.⁶ The OU equation is solved, but not for extreme value distributions, and only specialized boundary conditions are considered. The second category^(3–7,17–22) deals with first passage time or extreme value distributions of diffusion processes. In this group are the papers that are concerned with formal rather than detailed solutions of Eq. (39) with general boundary conditions and with asymptotic properties of these distributions. Finally, there are many papers concerned with specific applications that involve various particular forms of Eq. (39), for which we only give a few typical references.^(10,23–25) Of all these many papers only the work on the Fokker–Planck equation described in Refs. 4–6 deals with the problem of the asymptotic equivalence of the extremum properties of the FP equation and independent random variable processes. The recent numerical work of Keilson and Ross⁽²⁶⁾ on passage time distributions for the OU process is also related to the calculations presented here.

A number of different mathematical techniques have been used to solve Eq. (39) and to find properties related to $f(x, t | x_0)$. The two most common ones are Laplace transforms^(18,19,26) and eigenfunction expansions.^(4,20) The former are inconvenient for numerical work because of difficult inverse transforms that must be performed, and become tractable only for certain specialized boundary conditions. We therefore chose the method of eigenfunction expansions.

Equation (39) is a parabolic partial differential equation whose solution can be expressed as the eigenfunction expansion

$$f(x, t | x_0) = \sum_{k=0}^{\infty} \rho(x) \frac{U_k(x) U_k(x_0)}{N_k} e^{-\lambda_k t} \quad (42)$$

⁵ References 15–27 are by no means a complete list, particularly with regard to applications. We limit ourselves to some representative examples.

⁶ We show in Appendix A that the OU process is equivalent to a stationary autoregressive process of first order (in the terminology of time series analysis) under the assumption of continuous time and delta correlated Gaussian noise.

Here the weight function $\rho(x)$ is the equilibrium solution of the Fokker-Planck equation (39) with or without reflecting boundaries, but without *absorbing* boundaries,

$$\rho(x) = \frac{2h(a)}{m_2(x)} \exp \left[\int_a^x dx' \frac{2m_1(x')}{m_2(x')} \right] \quad (43)$$

with $h(a)$ determined by the normalization condition

$$\int_a^\infty \rho(x) dx = 1 \quad (44)$$

The constant a is left undefined at this point, and will be chosen later to conform to the particular boundary conditions to be considered. The eigenfunctions U_k and eigenvalues λ_k satisfy the differential equation

$$\frac{1}{2} m_2(x) \frac{d^2 U_k(x)}{dx^2} + m_1(x) \frac{dU_k(x)}{dx} + \lambda_k U_k(x) = 0 \quad (45)$$

In addition, two boundary conditions for $U_k(x)$ must be specified. The normalization constants N_k also depend on the boundary conditions. To deduce some properties of the eigenvalues λ_k , it is convenient to rewrite Eq. (45) in the self-adjoint form

$$\frac{d}{dx} \left[\sigma(x) \frac{dU_k(x)}{dx} \right] + \lambda_k \rho(x) U_k(x) = 0 \quad (46)$$

where

$$\sigma(x) \equiv \frac{1}{2} m_2(x) \rho(x) \quad (47)$$

Since this equation is of the Sturm-Liouville type, the eigenvalues λ_k are real and nondegenerate. For $m_2(x) > 0$, which is required in order that the FP equation (39) describe a physical system, the roots are nonnegative and

$$\lambda_0 < \lambda_1 < \lambda_2 < \dots \quad (48)$$

4.1. Reflecting Boundary at $x = r$, Absorbing Boundary at $x = \xi$

We impose a reflecting boundary condition at $x = r$, where r may be finite or negative infinite. For definiteness we consider here maxima problems; for minima problems r is finite or positive infinite. The boundary condition is

$$\left\{ \frac{\partial}{\partial x} \left[\frac{m_2(x)}{2} f(x, t | x_0) \right] - m_1(x) f(x, t | x_0) \right\}_{x=r} = 0 \quad (49)$$

for all $t \geq 0$. This condition ensures (provided m_1 and m_2 are physically

reasonable) that the process is conservative, i.e., for $\xi = \infty$

$$\int_r^\infty dx f(x, t | x_0) = 1 \quad (50)$$

The second boundary condition is obtained directly from the definition of $f(x, t | x_0) dx$ given in Section 2 as the probability that the random variable $X(t)$ lies within $(x, x + dx)$ *without ever having crossed* $x = \xi$ in time $(0, t)$, given $X(0) = x_0$. We can thus impose the absorbing boundary condition

$$f(x, t | x_0)|_{x=\xi} = 0 \quad (51)$$

It should be stressed here that the condition at $x = \xi$ *does not necessarily imply the presence of a physical boundary*. It simply represents the value ξ of x at which we “watch” for the first passage, or crossing, of the random variable $X(t)$. The initial value x_0 of $X(t)$ is bounded by $r \leq x_0 < \xi$.

For these boundary conditions we take $a = r$ as the lower limit for the normalization equation (44). The normalization constants N_k in Eq. (42) are given by

$$\delta_{k,m} N_k = \int_r^\xi dx \rho(x) U_k(x) U_m(x) \quad (52)$$

The boundary conditions on the eigenfunctions are

$$\rho(x) \frac{dU_k(x)}{dx} \Big|_{x=r} = 0 \quad (53)$$

$$\rho(\xi) U_k(\xi) = 0 \quad (54)$$

4.2. Absorbing Boundaries at $x = \pm \xi$

We now consider the case of symmetric (about $x = 0$) absorbing boundaries at $x = \pm \xi$. The boundary conditions are

$$f(x, t | x_0)|_{x=\pm\xi} = 0 \quad (55)$$

and the normalization constants N_k are

$$\delta_{k,m} N_k = \int_{-\xi}^\xi dx \rho(x) U_k(x) U_m(x) \quad (56)$$

with $a = -\infty$ in Eqs. (43) and (44). The boundary conditions on the eigenfunctions are

$$\rho(\pm \xi) U_k(\pm \xi) = 0 \quad (57)$$

4.3. First Passage Times

To obtain first passage times for the boundary conditions considered above we utilize the backward Kolmogorov equation (41). The first passage time moments $T_n(\xi|x_0)$ satisfy the differential difference equations, obtained from Eq. (41),

$$\begin{aligned}
 T_0(\xi|x_0) &= 1 \\
 \frac{1}{2} m_2(x_0) \frac{d^2 T_n(\xi|x_0)}{dx_0^2} + m_1(x_0) \frac{dT_n(\xi|x_0)}{dx_0} &= -nT_{n-1}(\xi|x_0) \quad (58) \\
 n &= 1, 2, \dots
 \end{aligned}$$

with appropriate boundary conditions.^(17,27) For first passage to $x = \xi$ with a reflecting boundary at $x = r$, the boundary conditions on T_n are

$$T_n(\xi|x_0)|_{x_0=\xi} = 0 \quad (59)$$

$$\frac{d}{dx_0} T_n(\xi|x_0)|_{x_0=r} = 0 \quad (60)$$

For first passage to $x = \pm \xi$,⁷

$$T_n(\xi|x_0)|_{x_0=\pm\xi} = 0 \quad (61)$$

Rewriting Eq. (58) in self-adjoint form and integrating twice yields

$$T_n(\xi|x_0) = \int_{x_0}^{\xi} \frac{dz}{\sigma(z)} \int_c^z nT_{n-1}(\xi|y)\rho(y) dy \quad (62)$$

with $c = r$ for boundaries at $x = r, \xi$ (case 4.1), and $c = 0$ for boundaries at $x = \pm \xi$ (case 4.2).

To obtain the mean first passage time $T_1(\xi)$ for the initial distribution $\eta(x_0) = \rho(x = x_0)$, we multiply Eq. (62), with $n = 1$, by $\rho(x_0)$ and integrate between the boundaries. With boundaries at r and ξ ,

$$T_1(\xi) = \int_r^{\xi} \frac{[\chi(z) - \chi(r)]^2}{\sigma(z)} dz \quad (63)$$

where

$$\chi(z) \equiv \int_0^z \rho(y) dy \quad (64)$$

⁷ In the interest of simplicity, when dealing with two absorbing boundaries we will henceforth assume that $m_1(x)$ is odd and $m_2(x)$ is even.

With boundaries at $\pm \xi$,

$$T_1(\xi) = \int_{-\xi}^{\xi} \frac{\chi^2(z)}{\sigma(z)} dz \tag{65}$$

Equation (63) reduces to Eq. (65) when $r = 0$, as noted earlier.

4.4. Asymptotic Results

We now present asymptotic results for the cumulative distribution functions $F(\xi, t|x_0)$ and $F(\xi, t)$, the first passage time moments $T_n(\xi)$, and the extremum moments $Z_n(t)$ and $Y_n(t)$ for the Fokker–Planck equation discussed above. It is useful to define new functions $A_k(\xi)$ and $B_k(\xi)$ by

$$F(\xi, t|x_0) = \sum_{k=0}^{\infty} A_k(\xi) U_k(x_0) e^{-\lambda_k t} \tag{66}$$

$$F(\xi, t) = \sum_{k=0}^{\infty} B_k(\xi) e^{-\lambda_k t} \tag{67}$$

from which it follows that [see Eqs. (2a), (13), and (42)]

$$A_k(\xi) = \frac{1}{N_k(\xi)} \int_b^{\xi} dx \rho(x) U_k(x) \tag{68}$$

with $b = r$ or $-\xi$, depending upon the nature of the boundaries. We consider in this paper only initial probability densities $\eta(x)$ that are identical with the equilibrium weight function $\rho(x)$ defined in Eq. (43). It then follows that

$$B_k(\xi) = A_k(\xi) \int_b^{\xi} dx U_k(x) \rho(x) = N_k(\xi) A_k^2(\xi) \tag{69}$$

4.4.1. Cumulative Distribution Functions. For large ξ , $\lambda_0(\xi) \rightarrow 0$. With the proper choice of normalization, $U_0(x_0) \rightarrow 1$ for $x_0 \ll \xi$, and $N_0(\xi) \rightarrow 1$. In these limits, indicated by the symbol \sim , with one reflecting and one absorbing boundary it follows from Eqs. (68) and (69) that

$$A_0(\xi) \sim \int_r^{\xi} dx \rho(x) = 1 - \int_{\xi}^{\infty} dx \rho(x) \tag{70}$$

and

$$B_0(\xi) \sim \left[\int_r^{\xi} dx \rho(x) \right]^2 = \left[1 - \int_{\xi}^{\infty} dx \rho(x) \right]^2 \tag{71}$$

With absorbing boundaries at $x = \pm \xi$ one finds

$$A_0(\xi) \sim \int_{-\xi}^{\xi} dx \rho(x) = 1 - 2 \int_{\xi}^{\infty} dx \rho(x) \tag{72}$$

and

$$B_0(\xi) \sim \left[\int_{-\xi}^{\xi} dx \rho(x) \right]^2 = \left[1 - 2 \int_{\xi}^{\infty} dx \rho(x) \right]^2 \tag{73}$$

It now follows from Eqs. (66) and (67), for large ξ and t , independently of boundary conditions and initial conditions, that

$$F(\xi, t | x_0) \sim F(\xi, t) \sim e^{-\lambda_0(\xi)t} \tag{74}$$

a result which has been derived previously.⁽⁴⁻⁷⁾

Since $B_k(\xi) \geq 0$ for all k and ξ [cf. Eq. (69)] while $A_k(\xi)U_k(x_0)$ may be positive or negative, one can be more specific about the approach to asymptotic behavior of $F(\xi, t)$ than one can for $F(\xi, t | x_0)$. From the initial condition

$$F(\xi, t = 0) = \sum_{k=0}^{\infty} B_k(\xi) = \int_b^{\xi} dx \rho(x) \equiv \varepsilon(\xi) \tag{75}$$

and Eqs. (48) and (67) it follows that for all ξ and t

$$B_0(\xi)e^{-\lambda_0(\xi)t} \leq F(\xi, t) \leq \varepsilon(\xi)e^{-\lambda_0(\xi)t} \tag{76}$$

Hence Eqs. (71), (73), and (75) imply that, for all times t ,

$$F(\xi, t) \simeq e^{-\lambda_0(\xi)t} \tag{77}$$

for ξ sufficiently large, so that

$$\int_{\xi}^{\infty} \rho(x) dx \ll 1 \tag{78a}$$

It should be noted that the condition (78a) implies

$$B_0(\xi) \simeq \varepsilon(\xi) \simeq 1 \tag{78b}$$

from which (77) follows immediately.

The relations (74) and (77) are identical in form with $F(\xi, t)$ for independent random variables as given in Eq. (28). It is in this sense that the extremum properties of Markov processes approach those of independent processes, even for finite values of the variables. For the Markov process, as is the case for independent random variables, the specific form of $\lambda_0(\xi)$ depends on the details of the process under consideration.

4.4.2. First Passage Time Moments. From Eqs. (11) and (67) it follows that the first passage time moments are given by

$$T_n(\xi) = n! \sum_{k=0}^{\infty} \frac{B_k(\xi)}{\lambda_k^n(\xi)} \tag{79}$$

Asymptotically, when Eqs. (77) and (78a) are applicable, this reduces to

$$T_n(\xi) \simeq n!/\lambda_0^n(\xi) \quad (80)$$

which is identical to the result of Eq. (29) for independent random variables. In particular, $\lambda_0(\xi)$ is again the reciprocal of the mean first passage time to ξ or $\pm \xi$, depending upon the boundary conditions. It should be noted that for fixed ξ , Eq. (80) is more accurate as the order n of the moment increases since the ratio of the $(k + 1)$ th to the k th term in the sum (79) decreases with increasing n . This is a consequence of the fact that the accuracy of the approximation (77) improves for fixed ξ as t increases. This is an important observation for both Markov and independent random variables since the mean first passage time by itself is a very inaccurate measure of the time dependence of any process with an exponential cumulative distribution of the form (77).

Indeed, in the asymptotic limits where (77) and hence (80) are valid, the dispersion of the mean first passage time is unity, i.e.,

$$\lim_{\xi \rightarrow \infty} \{[T_2(\xi) - T_1^2(\xi)]/T_1^2(\xi)\}^{1/2} = 1 \quad (81)$$

The utility of these results [Eq. (80) *et seq.*] lies in the simplicity with which one can calculate $\lambda_0(\xi) \simeq 1/T_1(\xi)$ from Eq. (63) or Eq. (65). This in turn permits one to obtain very readily the asymptotic distribution function (74) and (77).

4.4.3. Extremum Moments. It is more difficult to make general statements about the asymptotic behavior of extremum moments than of first passage time moments. The latter involve integrations over time of a function with a simple time dependence which is known *for all* t . On the other hand, it does not seem possible to establish an equation for $F(\xi, t)$ analogous to Eq. (77), i.e., one involving ξ only via $\lambda_0(\xi)$, *valid for all* ξ . Even if such a relation were to exist, it would be necessary to determine the analytic form of $\lambda_0(\xi)$ for the specific process under consideration in order to carry out the required integration over ξ .

It is nevertheless possible to conclude that for $t \gtrsim t_c$, with t_c defined below, the mean maximum and higher moments are approximately given by

$$Z_n(t) \simeq r^n + n \int_r^\infty d\xi \xi^{n-1} [1 - e^{-\lambda_0(\xi)t}] \quad (82)$$

i.e., that for $t \gtrsim t_c$, the distribution $F(\xi, t)$ in Eq. (10) can be replaced by the asymptotic form $\exp[-\lambda_0(\xi)t]$ averaged over the initial distribution $\rho(x_0)$. The time t_c is given by the relation

$$t_c \simeq T_1(\xi_0) \simeq 1/\lambda_0(\xi_0) \quad (83)$$

where ξ_0 is the smallest value of ξ for which the condition (78a) holds. We assume here that $\lambda_0(\xi)$ is a monotonically nonincreasing function of ξ , which would appear to be true in physically interesting cases. Equation (82) can be justified as follows. If $t \geq t_c$, then for $\xi \ll \xi_0$, it follows from the definition of $F(\xi, t)$ in Eq. (7) that $F(\xi, t) \ll 1$. Therefore $F(\xi, t)$ makes a negligible contribution to the integrand $\xi^{n-1}[1 - F(\xi, t)]$ of Eq. (10). The detailed form of $F(\xi, t)$ in this region of integration is thus unimportant. It is only when $\xi \geq \xi_0$ that the form of $F(\xi, t)$ is important. With ξ_0 defined in Eq. (83), Eqs. (76) and (77) then allow us to replace $F(\xi, t)$ with its asymptotic form. Hence if $t \geq t_c$, it is again sufficient to know only $\lambda_0(\xi) \simeq 1/T_1(\xi)$ to obtain the mean maximum and higher moments. It should be noted that for fixed $t \geq t_c$, the first moment $Z_1(t)$ obtained from the asymptotic form (82) is expected to be more accurate than the higher moments $Z_n(t)$, $n \geq 2$. This is because the largest contributions to $Z_1(t)$ come from small values of ξ where $\exp[-\lambda_0(\xi)t] \ll 1$, so that errors introduced through use of the asymptotic form are less important than in the evaluation of the higher moments. It should also be observed that for large t the mean maximum $Z_1(t)$ is a good measure of the distribution of maxima. It can readily be shown via Eq. (82) that the dispersion of the maximum $Z_1(t)$ tends to zero, i.e.,

$$\lim_{t \rightarrow \infty} \{[Z_2(t) - Z_1^2(t)]/Z_1^2(t)\}^{1/2} = 0 \tag{84}$$

This is in marked contrast to the mean first passage time $T_1(\xi)$, which, as shown by its dispersion [Eq. (81)], is not a good measure for the distribution of first passage times in the limit as $\xi \rightarrow \infty$.

The asymptotic approximations to the extremum moments $Y_n(t)$ for $t \geq t_c$ are given by Eq. (82) with $r = 0$.

5. THE ORNSTEIN-UHLENBECK EQUATION

In order to make some progress beyond the above formalism, it is necessary to consider some particular Fokker-Planck equation. For our first example we turn to the Ornstein-Uhlenbeck (OU) equation⁽⁸⁾

$$\frac{\partial}{\partial t} f(x, t|x_0) = \frac{\partial}{\partial x} \left[\mu x f(x, t|x_0) + D \frac{\partial}{\partial x} f(x, t|x_0) \right] \tag{85}$$

where the general coefficients $m_1(x)$ and $m_2(x)$ of the FP equation (39) now take the form $m_1(x) = -\mu x$ and $m_2(x) = 2D$ with μ and D constant. After defining the dimensionless variables

$$\mu t \rightarrow \tau \tag{86}$$

$$(\mu/2D)^{1/2} x \rightarrow y \tag{87}$$

we can rewrite the eigenfunction equation (45) as

$$\frac{d^2 U_k(y)}{dy^2} - 2y \frac{dU_k(y)}{dy} + 2\lambda_k U_k(y) = 0 \quad (88)$$

where the eigenvalues λ_k of Eq. (88) are dimensionless ones related to those of Eq. (45) by $\lambda_k \rightarrow \lambda_k/\mu$. All variables and functions from here on are understood to be in dimensionless form, even when the same symbols are used for them as in earlier sections. The weight function $\rho(y)$ normalized with respect to y is

$$\rho(y) = \frac{2}{\sqrt{\pi}} \frac{\exp(-y^2)}{1 - \operatorname{erf} a} \quad (89)$$

where the value of a depends on the boundary conditions.

We now consider the solution for each type of boundary condition separately.

5.1. Reflecting Boundary at $y = r$, Absorbing Boundary at $y = \xi$

The solutions of the eigenfunction equation (88) with boundary conditions (53) and (54) are combinations of confluent hypergeometric functions⁽²⁸⁾:

$$U_k(y) = M\left(-\frac{\lambda_k}{2}, \frac{1}{2}, y^2\right) + \frac{2\lambda_k r y M(1 - \frac{1}{2}\lambda_k, \frac{3}{2}, r^2) M(\frac{1}{2} - \frac{1}{2}\lambda_k, \frac{3}{2}, y^2)}{M(\frac{1}{2} - \frac{1}{2}\lambda_k, \frac{1}{2}, r^2)} \quad (90)$$

The eigenvalues are obtained numerically from the boundary condition (51) as will be discussed below. Our choice of normalization makes the lowest eigenfunction $U_0(y) \rightarrow 1$ for any finite y as $\xi \rightarrow \infty$.

Equation (90) simplifies in a number of special cases. When $r \rightarrow -\infty$ the eigenfunctions reduce to⁽²⁸⁾

$$U_k(y) = M\left(\frac{-\lambda_k}{2}, \frac{1}{2}, y^2\right) + \frac{2\Gamma(\frac{1}{2} - \frac{1}{2}\lambda_k)}{\Gamma(-\frac{1}{2}\lambda_k)} y M\left(\frac{1}{2} - \frac{\lambda_k}{2}, \frac{3}{2}, y^2\right) \quad (91)$$

where $\Gamma(y)$ is the gamma function. For the special case $r \rightarrow -\infty$ and $\xi = 0$ the eigenfunctions are the odd Hermite polynomials, $U_k(y) = H_{2k+1}(y)$, and the eigenvalues are the odd positive integers, $\lambda_k = 2k + 1$. In this case the full probability density function $f(y, \tau|y_0)$ can be written in closed form as⁽²⁹⁾

$$f(y, \tau|y_0) = [\pi(1 - \exp -2\tau)]^{-1/2} \left\{ \exp - \frac{(y - y_0 e^{-\tau})^2}{1 - e^{-2\tau}} \right. \\ \left. - \exp - \frac{(y + y_0 e^{-\tau})^2}{1 - e^{-2\tau}} \right\} \quad (92)$$

with $-\infty < y_0 < 0$. The cumulative distribution function is

$$F(\xi = 0, \tau|y_0) = \operatorname{erf} \frac{-y_0 e^{-\tau}}{(1 - e^{-2\tau})^{1/2}} \quad (93)$$

If $r \rightarrow -\infty$ and $\xi \rightarrow \infty$, the eigenfunctions are all the Hermite polynomials, $U_k(y) = H_k(y)$, and the eigenvalues are the nonnegative integers, $\lambda_k = k$.⁽²⁸⁾ The probability density function in this case is⁽²⁹⁾

$$f(y, \tau | y_0) = \{\pi[1 - (\exp - 2\tau)]\}^{-1/2} \exp - \frac{(y - y_0 e^{-\tau})^2}{1 - e^{-2\tau}} \tag{94}$$

and the cumulative distribution function $F(\xi \rightarrow \infty, \tau | y_0)$ is of course unity.

When $r = 0$, the second term on the r.h.s. of Eq. (90) vanishes. If in this case $\xi \rightarrow \infty$, the eigenfunctions are the even Hermite polynomials, $U_k(y) = H_{2k}(y)$, and the eigenvalues are the even nonnegative integers, $\lambda_k = 2k$. The probability density function is as in (94) with $-y_0$ replacing y_0 , and the cumulative distribution function is again unity.

5.2. Absorbing Boundaries at $y = \pm \xi$

The solutions of Eq. (88) with boundary conditions (57) are either even or odd functions of y :

$$U_{2k}(y) = M(-\frac{1}{2}\lambda_{2k}, \frac{1}{2}, y^2), \quad k = 0, 1, 2, \dots \tag{95a}$$

$$U_{2k+1}(y) = yM(\frac{1}{2} - \frac{1}{2}\lambda_{2k+1}, \frac{3}{2}, y^2), \quad k = 0, 1, 2, \dots \tag{95b}$$

Again $U_0(y) \rightarrow 1$ as $\xi \rightarrow \infty$. The eigenvalues are obtained from the conditions

$$U_{2k}(\xi) = U_{2k+1}(\xi) = 0 \tag{96}$$

The odd eigenfunctions do not contribute to the cumulative distribution function $F(\xi, \tau)$ with $\rho(y)$ as the initial distribution, and they also do not contribute to $F(\xi, \tau | y_0 = 0)$. When $\xi \rightarrow -\infty$, the eigenfunctions and eigenvalues are the same as those of the $r \rightarrow -\infty, \xi \rightarrow \infty$ case.

Expressions for the mean first passage time $T_1(\xi)$ in terms of the auxiliary function $\chi(z)$ of Eq. (64) can readily be evaluated for the equilibrium weight function $\rho(y)$ of Eq. (89). They are

$$T_1(\xi) = \frac{\sqrt{\pi}}{1 - \operatorname{erf} r} \int_r^\xi dy (\exp y^2)(\operatorname{erf} y - \operatorname{erf} r)^2 \tag{97}$$

for a single absorbing boundary, and

$$T_1(\xi) = \sqrt{\pi} \int_r^\xi dy (\exp y^2) \operatorname{erf}^2 y \tag{98}$$

for two absorbing boundaries. Note that Eq. (98) is identical to Eq. (97) with $r = 0$. When ξ is very large, asymptotic expansion of Eq. (97) yields⁽⁴⁾

$$T_1(\xi) \xrightarrow{\xi \rightarrow \infty} \sqrt{\pi}(1 - \operatorname{erf} r)(\exp \xi^2)/2\xi \tag{99}$$

5.3. Results and Discussion

To obtain the desired results for more general boundary conditions on the approach of the Markov properties to those of independent random variables it is necessary to calculate numerically the eigenfunction $U_k(y)$ and the eigenvalues λ_k . These calculations were performed on a Burroughs 6700

Table I. First Four Eigenvalues for the OU Process with Symmetric Absorbing Boundaries at $\pm \xi$

ξ	$\lambda_0(\xi)$	$\lambda_1(\xi)$	$\lambda_2(\xi)$	$\lambda_3(\xi)$
0.5	0.445113E + 01	0.192745E + 02	0.439521E + 02	0.784969E + 02
0.6	0.295044E + 01	0.132586E + 02	0.303985E + 02	0.543889E + 02
0.7	0.204971E + 01	0.964021E + 01	0.222360E + 02	0.398627E + 02
0.8	0.146932E + 01	0.730094E + 01	0.169484E + 02	0.304452E + 02
0.9	0.107570E + 01	0.570653E + 01	0.133337E + 02	0.239993E + 02
1.0	0.798460E + 00	0.457558E + 01	0.107588E + 02	0.193997E + 02
1.1	0.597622E + 00	0.374838E + 01	0.886452E + 01	0.160077E + 02
1.2	0.449103E + 00	0.312881E + 01	0.743473E + 01	0.134391E + 02
1.3	0.337658E + 00	0.265619E + 01	0.633313E + 01	0.114517E + 02
1.4	0.253228E + 00	0.229061E + 01	0.547028E + 01	0.988641E + 01
1.5	0.188932E + 00	0.200498E + 01	0.478549E + 01	0.863542E + 01
1.6	0.139902E + 00	0.178027E + 01	0.423645E + 01	0.762354E + 01
1.7	0.102597E + 00	0.160282E + 01	0.379285E + 01	0.679701E + 01
1.8	0.743660E - 01	0.146254E + 01	0.343257E + 01	0.611662E + 01
1.9	0.531815E - 01	0.135183E + 01	0.313908E + 01	0.555318E + 01
2.0	0.374612E - 01	0.126482E + 01	0.289979E + 01	0.508464E + 01
2.1	0.259540E - 01	0.119689E + 01	0.270497E + 01	0.469404E + 01
2.2	0.176634E - 01	0.114434E + 01	0.254692E + 01	0.436817E + 01
2.3	0.117959E - 01	0.110416E + 01	0.241944E + 01	0.409659E + 01
2.4	0.772308E - 02	0.107388E + 01	0.231744E + 01	0.387090E + 01
2.5	0.495410E - 02	0.105142E + 01	0.223669E + 01	0.368426E + 01
2.6	0.311200E - 02	0.103508E + 01	0.217356E + 01	0.353099E + 01
2.7	0.191369E - 02	0.102342E + 01	0.212496E + 01	0.340626E + 01
2.8	0.115180E - 02	0.101529E + 01	0.208819E + 01	0.330593E + 01
2.9	0.678437E - 03	0.100976E + 01	0.206092E + 01	0.322634E + 01
3.0	0.391083E - 03	0.100608E + 01	0.204113E + 01	0.316422E + 01
3.1	0.220632E - 03	0.100370E + 01	0.202711E + 01	0.311665E + 01
3.2	0.121826E - 03	0.100220E + 01	0.201743E + 01	0.308098E + 01
3.3	0.658439E - 04	0.100128E + 01	0.201093E + 01	0.305487E + 01
3.4	0.348370E - 04	0.100072E + 01	0.200667E + 01	0.303624E + 01
3.5	0.180448E - 04	0.100040E + 01	0.200397E + 01	0.302330E + 01
3.6	0.915147E - 05	0.100022E + 01	0.200230E + 01	0.301458E + 01
3.7	0.454455E - 05	0.100011E + 01	0.200130E + 01	0.300887E + 01
3.8	0.221000E - 05	0.100006E + 01	0.200072E + 01	0.300525E + 01
3.9	0.105251E - 05	0.100003E + 01	0.200038E + 01	0.300302E + 01
4.0	0.490869E - 06	0.100002E + 01	0.200020E + 01	0.300169E + 01

Table II. First Four Eigenvalues for the OU Process with Boundaries at $r = -1, \gamma = \xi$

ξ	$\lambda_0(\xi)$	$\lambda_1(\xi)$	$\lambda_2(\xi)$	$\lambda_3(\xi)$
0.1	0.147597E + 01	0.972635E + 01	0.260467E + 02	0.505187E + 02
0.2	0.122134E + 01	0.817342E + 01	0.218882E + 02	0.424516E + 02
0.3	0.101603E + 01	0.696016E + 01	0.186473E + 02	0.361691E + 02
0.4	0.847714E + 00	0.599455E + 01	0.160732E + 02	0.311816E + 02
0.5	0.707917E + 00	0.521405E + 01	0.139955E + 02	0.271570E + 02
0.6	0.590656E + 00	0.457490E + 01	0.122951E + 02	0.238633E + 02
0.7	0.491601E + 00	0.404575E + 01	0.108870E + 02	0.211348E + 02
0.8	0.407545E + 00	0.360364E + 01	0.970891E + 01	0.188505E + 02
0.9	0.336059E + 00	0.323145E + 01	0.871463E + 01	0.169201E + 02
1.0	0.275266E + 00	0.291621E + 01	0.786905E + 01	0.152755E + 02
1.1	0.223672E + 00	0.264793E + 01	0.714525E + 01	0.138643E + 02
1.2	0.180066E + 00	0.241882E + 01	0.652226E + 01	0.126457E + 02
1.3	0.143434E + 00	0.222273E + 01	0.598356E + 01	0.115876E + 02
1.4	0.112905E + 00	0.205478E + 01	0.551603E + 01	0.106645E + 02
1.5	0.877131E - 01	0.191099E + 01	0.510907E + 01	0.985584E + 01
1.6	0.671669E - 01	0.178814E + 01	0.475413E + 01	0.914487E + 01
1.7	0.506356E - 01	0.168356E + 01	0.444421E + 01	0.851801E + 01
1.8	0.375368E - 01	0.159498E + 01	0.417352E + 01	0.796401E + 01
1.9	0.273328E - 01	0.152049E + 01	0.393728E + 01	0.747357E + 01
2.0	0.195302E - 01	0.145840E + 01	0.373149E + 01	0.703891E + 01
2.1	0.136819E - 01	0.140722E + 01	0.355276E + 01	0.665351E + 01
2.2	0.939049E - 02	0.136557E + 01	0.339823E + 01	0.631187E + 01
2.3	0.631072E - 02	0.133220E + 01	0.326540E + 01	0.600932E + 01
2.4	0.415080E - 02	0.130591E + 01	0.315210E + 01	0.574190E + 01
2.5	0.267130E - 02	0.128561E + 01	0.305636E + 01	0.550620E + 01
2.6	0.168182E - 02	0.127027E + 01	0.297640E + 01	0.529928E + 01
2.7	0.103579E - 02	0.125893E + 01	0.291053E + 01	0.511858E + 01
2.8	0.624041E - 03	0.125076E + 01	0.285715E + 01	0.496186E + 01
2.9	0.367814E - 03	0.124503E + 01	0.281467E + 01	0.482708E + 01
3.0	0.212110E - 03	0.124111E + 01	0.278158E + 01	0.471238E + 01
3.1	0.119693E - 03	0.123851E + 01	0.275641E + 01	0.461600E + 01
3.2	0.661000E - 04	0.123682E + 01	0.273773E + 01	0.453624E + 01
3.3	0.357286E - 04	0.123576E + 01	0.272426E + 01	0.447139E + 01
3.4	0.189044E - 04	0.123512E + 01	0.271481E + 01	0.441975E + 01
3.5	0.979233E - 05	0.123473E + 01	0.270839E + 01	0.437956E + 01
3.6	0.496628E - 05	0.123451E + 01	0.270415E + 01	0.434910E + 01
3.7	0.246628E - 05	0.123438E + 01	0.270145E + 01	0.432666E + 01
3.8	0.119931E - 05	0.123431E + 01	0.269977E + 01	0.431062E + 01
3.9	0.571186E - 06	0.123427E + 01	0.269876E + 01	0.429953E + 01
4.0	0.266407E - 06	0.123425E + 01	0.269818E + 01	0.429211E + 01

Table III. First Four Eigenvalues for the OU Process with Boundaries at $r = -\infty, y = \xi$

ξ	$\lambda_0(\xi)$	$\lambda_1(\xi)$	$\lambda_2(\xi)$	$\lambda_3(\xi)$
-1.0	0.253720E + 01	0.510382E + 01	0.752665E + 01	0.987880E + 01
-0.9	0.234546E + 01	0.485571E + 01	0.723644E + 01	0.955350E + 01
-0.8	0.216238E + 01	0.461611E + 01	0.695468E + 01	0.923661E + 01
-0.7	0.198788E + 01	0.438498E + 01	0.668133E + 01	0.892809E + 01
-0.6	0.182190E + 01	0.416228E + 01	0.641635E + 01	0.862791E + 01
-0.5	0.166436E + 01	0.394795E + 01	0.615971E + 01	0.833604E + 01
-0.4	0.151516E + 01	0.374194E + 01	0.591135E + 01	0.805243E + 01
-0.3	0.137424E + 01	0.354419E + 01	0.567125E + 01	0.777706E + 01
-0.2	0.124147E + 01	0.335466E + 01	0.543935E + 01	0.750989E + 01
-0.1	0.111677E + 01	0.317328E + 01	0.521562E + 01	0.725088E + 01
0.1	0.891046E + 00	0.283475E + 01	0.479246E + 01	0.675720E + 01
0.2	0.789767E + 00	0.267746E + 01	0.459294E + 01	0.652246E + 01
0.3	0.696010E + 00	0.252808E + 01	0.440141E + 01	0.629573E + 01
0.4	0.609609E + 00	0.238653E + 01	0.421781E + 01	0.607697E + 01
0.5	0.530383E + 00	0.225274E + 01	0.404210E + 01	0.586615E + 01
0.6	0.458133E + 00	0.212663E + 01	0.387423E + 01	0.566323E + 01
0.7	0.392642E + 00	0.200813E + 01	0.371415E + 01	0.546817E + 01
0.8	0.333671E + 00	0.189716E + 01	0.356182E + 01	0.528094E + 01
0.9	0.280963E + 00	0.179364E + 01	0.341718E + 01	0.510150E + 01
1.0	0.234234E + 00	0.169746E + 01	0.328019E + 01	0.492981E + 01
1.1	0.193179E + 00	0.160855E + 01	0.315081E + 01	0.476585E + 01
1.2	0.157467E + 00	0.152678E + 01	0.302898E + 01	0.460958E + 01
1.3	0.126744E + 00	0.145205E + 01	0.291467E + 01	0.446097E + 01
1.4	0.100634E + 00	0.138421E + 01	0.280783E + 01	0.431999E + 01
1.5	0.787399E - 01	0.132313E + 01	0.270840E + 01	0.418663E + 01
1.6	0.606492E - 01	0.126863E + 01	0.261634E + 01	0.406085E + 01
1.7	0.459393E - 01	0.122048E + 01	0.253159E + 01	0.394264E + 01
1.8	0.341851E - 01	0.117845E + 01	0.245408E + 01	0.383199E + 01
1.9	0.249672E - 01	0.114224E + 01	0.238373E + 01	0.372886E + 01
2.0	0.178817E - 01	0.111151E + 01	0.232044E + 01	0.363324E + 01
2.1	0.125495E - 01	0.108586E + 01	0.226408E + 01	0.354512E + 01
2.2	0.862483E - 02	0.106484E + 01	0.221448E + 01	0.346446E + 01
2.3	0.580188E - 02	0.104797E + 01	0.217140E + 01	0.339122E + 01
2.4	0.381882E - 02	0.103472E + 01	0.213457E + 01	0.332534E + 01
2.5	0.245887E - 02	0.102456E + 01	0.210363E + 01	0.326671E + 01
2.6	0.154860E - 02	0.101697E + 01	0.207815E + 01	0.321520E + 01
2.7	0.953966E - 03	0.101144E + 01	0.205762E + 01	0.317060E + 01
2.8	0.574827E - 03	0.100753E + 01	0.204148E + 01	0.313264E + 01
2.9	0.338838E - 03	0.100483E + 01	0.202912E + 01	0.310095E + 01
3.0	0.195412E - 03	0.100302E + 01	0.201991E + 01	0.307508E + 01
3.1	0.110274E - 03	0.100184E + 01	0.201325E + 01	0.305446E + 01
3.2	0.608996E - 04	0.100110E + 01	0.200858E + 01	0.303847E + 01
3.3	0.329181E - 04	0.100064E + 01	0.200541E + 01	0.302644E + 01
3.4	0.174174E - 04	0.100036E + 01	0.200331E + 01	0.301765E + 01
3.5	0.902211E - 05	0.100020E + 01	0.200198E + 01	0.301145E + 01
3.6	0.457567E - 05	0.100011E + 01	0.200115E + 01	0.300721E + 01
3.7	0.227227E - 05	0.100006E + 01	0.200065E + 01	0.300440E + 01
3.8	0.110500E - 05	0.100003E + 01	0.200036E + 01	0.300261E + 01
3.9	0.526216E - 06	0.100001E + 01	0.200019E + 01	0.300151E + 01
4.0	0.245493E - 06	0.100001E + 01	0.200010E + 01	0.300084E + 01

computer and the plotting was done on a CDC 3600 computer. In Tables I–IV and Figs. 3–7 we present a representative sample of the extensive calculations that were carried out. The complete set of calculations is available upon request.

The quantities of main interest are the eigenvalues, since all subsequent results depend upon them. Since $\rho(y)$ is nonzero for all finite y , the search for the eigenvalues reduces to finding the zeros of the eigenfunctions of Sections 5.1 and 5.2. A “bisection search” method was used to obtain the first four eigenvalues as a function of the absorbing boundary ξ , for various values of the reflecting boundary r and for symmetric absorbing boundaries. The results for some representative cases are given in Tables I–III. It should be noted that the ratio $\lambda_0(\xi)/\lambda_1(\xi)$ decreases rapidly with increasing ξ . For $\xi = 1$, this ratio is already of $O(10^{-1})$ for all the boundary conditions studied by us. It is of course this rapid separation of the lowest and next eigenvalue with increasing ξ which causes the asymptotic results to hold to a very good approximation for finite values of the boundary value ξ . It is also important to note (see Table IV) that the condition (78a), i.e., $\alpha \equiv \int_{\xi}^{\infty} \rho(x) dx \ll 1$, holds for all values of $\xi \geq 1$.

Results for the cumulative probability distribution $F(\xi, t)$ of Eq. (67) are presented in Table IV for reflecting boundaries at $r = 0$, $r = -1$, and $r = -\infty$, for various times $\lambda_0\tau$. As can be seen from the equations and discussions in Sections 5.1 and 5.2, the cumulative distribution function $F(\xi, t)$ for $r = 0$, with an absorbing boundary at $y = \xi$, is identical to $F(\xi, t)$ for symmetric absorbing boundaries at $y = \pm\xi$. The entries in the first row of Table IV thus pertain both to the case $y = r = 0$, $y = \xi$ and to the case $y = \pm\xi$. The results presented in Table IV and all subsequent ones discussed here were obtained by using the first four eigenvalues $\lambda_0(\xi)$ through $\lambda_3(\xi)$.

The asymptotic cumulative distributions $F(\xi, t) \rightarrow \exp[-\lambda_0(\xi)\tau]$, Eq. (77), are also presented for comparison in Table IV. The “exact” distributions, obtained with the use of our eigenvalues λ_0 through λ_3 , and the asymptotic distributions $\exp[-\lambda_0(\xi)\tau]$, are quite close in value (to within 15–20%) already for $\xi \simeq 1$, regardless of the boundary conditions. For $\xi \geq 3$ they are essentially indistinguishable.⁸

Results for the mean first passage time and mean extrema are shown in Figs. 1–6. Figures 1–3 display the natural logarithm of the mean first passage time $T_1(\xi)$ for symmetric absorbing boundaries as discussed in Section 5.2 and for reflecting boundaries with $r = -1$ and $r = -\infty$, as discussed in Section 5.1. The solid curves are the exact mean first passage times obtained from numerical integration of Eq. (97). It is of interest to note that the mean

⁸ It should be noted that the values of $F(1, \tau)$ may have a nonnegligible error for short times due to the truncation of the expansion for $F(\xi, t)$ after four terms.

Table IV. Exact and Asymptotic Cumulative Distributions Functions for the OU Process^a

$\lambda_0(\xi)\tau$	$\exp[-\lambda_0(\xi)\tau]$	$F(1, \tau)$	$F(2, \tau)$	$F(3, \tau)$	$F(4, \tau)$
$\alpha = 7.8650E - 02 \quad \alpha = 2.3389E - 03 \quad \alpha = 1.1045E - 05 \quad \alpha = 7.7089E - 09$					
Symmetric absorbing boundaries	0.1	0.90483	0.89471	0.90479	0.90483
	0.3	0.74081	0.73252	0.74078	0.74081
	0.5	0.60653	0.46214	0.59974	0.60653
	0.7	0.49658	0.37833	0.49102	0.49658
	0.9	0.40657	0.30975	0.40202	0.40656
	1.1	0.33287	0.25360	0.32914	0.33287
	1.3	0.27253	0.20763	0.26948	0.27253
	1.5	0.22313	0.16999	0.22063	0.22313
	1.7	0.18268	0.13918	0.18063	0.18268
	1.9	0.14956	0.11395	0.14789	0.14956
$\alpha = 8.5363E - 02 \quad \alpha = 2.5385E - 03 \quad \alpha = 1.1988E - 05 \quad \alpha = 8.3669E - 09$					
$r = -1$	0.1	0.90483	0.76702	0.89861	0.90481
	0.3	0.74081	0.61798	0.73572	0.74079
	0.5	0.60653	0.50484	0.60235	0.60651
	0.7	0.49658	0.41319	0.49316	0.49657
	0.9	0.40657	0.33827	0.40377	0.40655

r	$\alpha = 7.8650E - 02$	$\alpha = 2.3389E - 03$	$\alpha = 1.1045E - 05$	$\alpha = 7.7089E - 09$
1.1	0.33287	0.27695	0.33058	0.33287
1.3	0.27253	0.22675	0.27065	0.27253
1.5	0.22313	0.18565	0.22159	0.22312
1.7	0.18268	0.15199	0.18142	0.18268
1.9	0.14956	0.12444	0.14854	0.14956
$r = -\infty$				
0.1	0.90483	0.77047	0.89891	0.90483
0.3	0.74081	0.61828	0.73596	0.74081
0.5	0.60653	0.50383	0.60255	0.60653
0.7	0.49658	0.41197	0.49333	0.49658
0.9	0.40657	0.33717	0.40390	0.40656
1.1	0.33287	0.27602	0.33069	0.33287
1.3	0.27253	0.22598	0.27074	0.27253
1.5	0.22313	0.18502	0.22166	0.22313
1.7	0.18268	0.15148	0.18148	0.18268
1.9	0.14956	0.12402	0.14858	0.14956

^a Note: $\alpha(\xi) \equiv \int_{\xi}^{\infty} \rho(y) dy$.

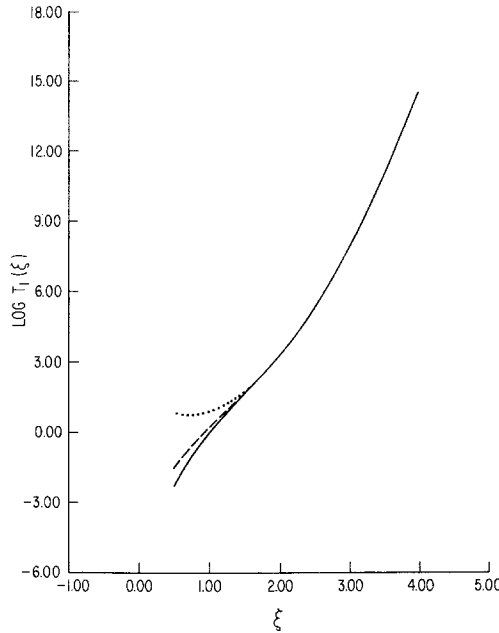


Fig. 1. OU process. Mean first passage time to symmetric absorbing boundaries at $\pm \xi$. Exact result, —. Independent random variable approximation, - -. Asymptotic expansion of exact result, ...

first passage times obtained from the first four terms of Eq. (79) agree closely with these exact results. The dashed curves are the independent random variable approximation $1/\lambda_0(\xi) \simeq T_1(\xi)$. For $\xi \geq 1$ this approximation gives results which are extremely close to the exact $T_1(\xi)$ in all cases. The dotted curves represent the asymptotic expansion (99) of Eq. (97). It is rather a poor approximation for small values of ξ , as expected, but also becomes quite accurate for $\xi > 1$.

We have also evaluated the dispersion of the mean first passage time $(T_2 - T_1^2)^{1/2}/T_1$. It is approximately unity for all values of ξ . This extends to small values of ξ the asymptotic result (81) on the dispersion of the mean first passage time for the general Fokker–Planck equation. This is an interesting and disturbing result. From it one learns that the mean first passage time $T_1(\xi)$ is not a “sharp” measure, and one needs really to calculate the full first passage time distribution, Eq. (9).

The mean extremum $Y_1(\tau)$ as a function of time is shown in Fig. 4. By extremum, we mean here the greatest excursion of the random variable Y above or below $y = 0$. Figures 5 and 6 display the mean maximum $Z_1(\tau)$ as a function of time for processes with reflecting boundaries at $r = -1$ and

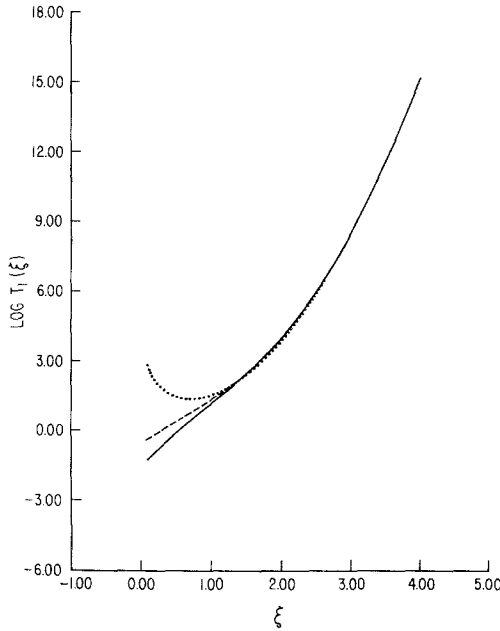


Fig. 2. OU process. Mean first passage time to ξ with reflecting boundary at $r = -1$. Exact result, —. Independent random variable approximation, - -. Asymptotic expansion of exact result, ...

$r = -\infty$, where by maximum we refer to the greatest excursion of the random variable Y above $y = 0$. The dashed curves are the approximate first moments $Z_1(\tau)$ computed from Eq. (82). The solid curves are the exact results, averaged over the initial conditions, obtained from Eqs. (10) and (15) for $n = 1$. The dotted curves are the differences between the exact and approximate results. It will be noted that these differences are very small at all times τ and essentially zero for all times $\tau > \tau_c$, in agreement with our criterion for the validity of (82). From the definition of τ_c in terms of $\lambda_0(\xi_0)$, Eq. (83), one can see from Tables I-III that τ_c is of order unity.

It is interesting to compare this value of τ_c with the characteristic time for decay of correlations in the unbounded OU process. It follows directly from Eq. (85) in terms of the dimensionless variables of Eqs. (86) and (87) that in the absence of boundaries

$$\langle y(\tau)y(0) \rangle \equiv y_0 \int_{-\infty}^{\infty} dy y f(y, \tau | y_0) = y_0^2 e^{-\tau} \tag{100}$$

The characteristic dimensionless decay time, i.e., the time required for the

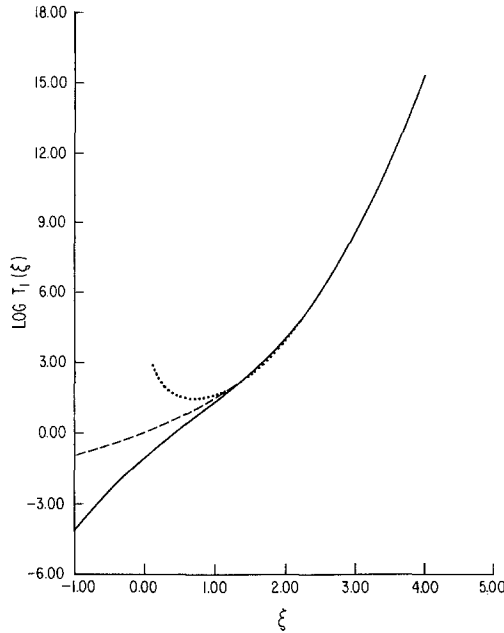


Fig. 3. OU process. Mean first passage time to ξ with reflecting boundary at $r = -\infty$. Exact result, —. Independent random variable approximation, - -. Asymptotic expansion of exact result, ...

correlations to decay to $1/e$ of the initial value, is thus unity. The values of τ_c found here imply the physically reasonable result that mean extrema and maxima of the OU process are well approximated by independent random variable results at times when the correlations of the unbounded OU process have decayed to about $1/e$ of their initial value. Analogous relations for more general Markov processes still need to be developed.

We have also calculated the dispersion of the mean maximum, $(Z_2 - Z_1^2)^{1/2}/Z_1$. For small values of τ it is of $O(1)$; as $\tau \rightarrow \infty$ the dispersion approaches zero, as expected from Eq. (84). In contrast to the relation between the mean first passage time and the first passage time distribution, the mean maximum is thus a useful measure of the distribution of maxima, particularly at large times τ . It is interesting and important to note that one can therefore make a meaningful calculation, i.e., one with a small dispersion, of the most probable maximum excursion of the space random variable for any time interval $(0, \tau)$, but that the calculation of the mean time required for the space variable to reach an extreme value for the first time is not very useful, due to the large dispersion of the mean first passage time.

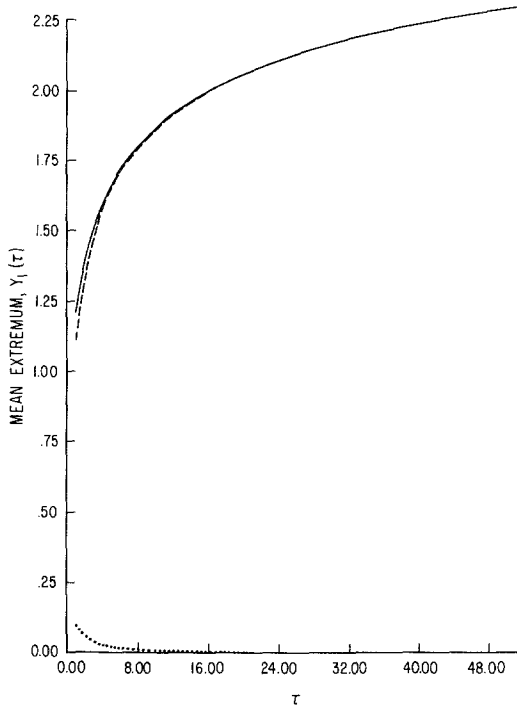


Fig. 4. OU process. Mean extremum. Exact result, —. Independent random variable approximation, - -. Difference,

Finally, we wish to point out that the units in this discussion are scaled dimensionless ones. The absolute values of the time t and the variable x for which independent random variable behavior can be assumed depend on the parameters μ and D of the OU equation, according to Eqs. (86) and (87).

6. HARMONIC OSCILLATOR DISSOCIATION

A specific example to which the developments of Section 4 can readily be applied is the harmonic oscillator dissociation model of Montroll and Shuler in the high-temperature approximation.⁽⁹⁻¹¹⁾

Consider an ensemble of harmonic oscillators in contact with a heat bath at temperature T ; the fundamental frequency of each oscillator is ν . Let

$$\theta \equiv h\nu/kT \tag{101}$$

In the high-temperature limit, $\theta \ll 1$, one can approximate the discrete energy levels of each oscillator by a continuum of energies denoted, in units of $h\nu$, by the dimensionless variable x . The ground state energy is $x = 0$; it is

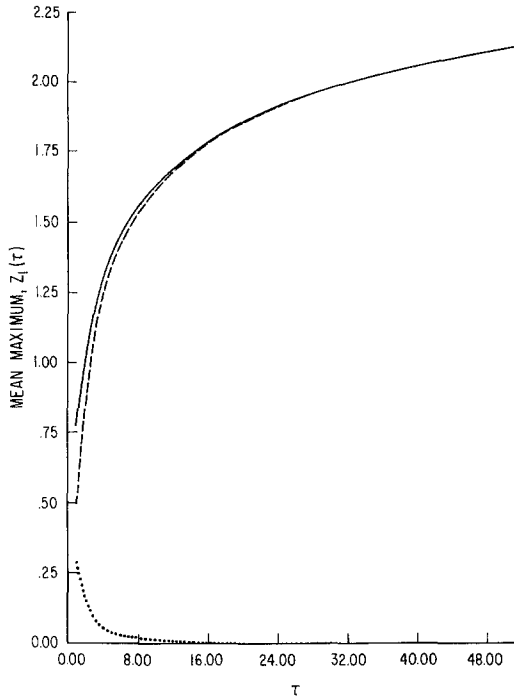


Fig. 5. OU process. Mean maximum with a reflecting boundary at $r = -1$. Exact result, —. Independent random variable approximation, --. Difference,

assumed⁽⁹⁾ that if the energy of an oscillator reaches or exceeds $x = \xi$, the oscillator dissociates irreversibly. The probability that an oscillator has not dissociated at time t then obeys a Fokker-Planck equation with a reflecting boundary at $x = 0$ and an absorbing boundary at $x = \xi$. The coefficients in Eq. (17) are^(10,11)

$$m_1(x) = 1 - \theta x \quad (102)$$

$$m_2(x) = 2x \quad (103)$$

The time t is expressed in units of $1/k_{10}$, where k_{10} is the collisional deactivation rate of the first excited state to the ground state.

The eigenfunctions for this Fokker-Planck equation are confluent hypergeometric functions,^(10,28)

$$U_k(x) = M(-\lambda_k/\theta, 1, \theta x), \quad k = 0, 1, 2, \dots \quad (104)$$

where the λ_k are determined by the absorbing boundary condition $U_k(\xi) = 0$. When $\xi \rightarrow \infty$, the eigenfunctions are the Laguerre polynomials, $U_k(x) = L_k(\theta x)$, with eigenvalues $\lambda_k = k\theta$. The weight function for this problem,

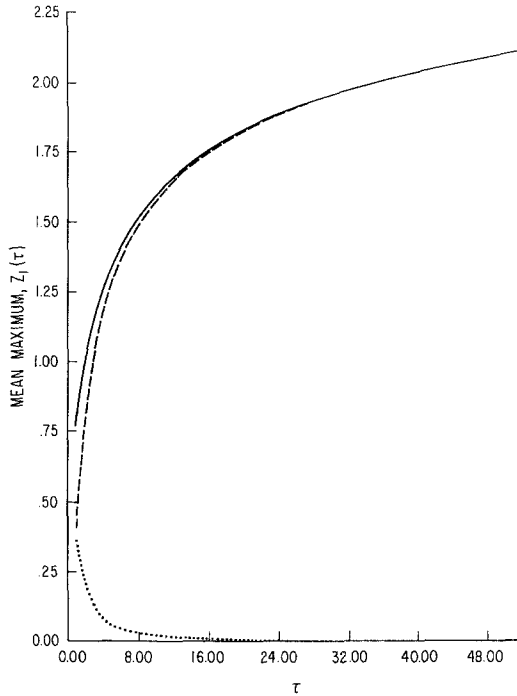


Fig. 6. OU process. Mean maximum with a reflecting boundary at $r = -\infty$. Exact result, —. Independent random variable approximation, - -. Difference, ...

obtained from Eq. (43), is

$$\rho(x) = \theta e^{-\theta x} \tag{105}$$

The mean first passage time to $x = \xi$ with $r = 0$ (i.e., the mean time for dissociation to occur) is given by Eq. (63) as

$$T_1(\xi) = \frac{1}{\theta} \int_0^{\theta \xi} dz \frac{(1 - e^{-z})^2}{ze^{-z}} \xrightarrow{\xi \rightarrow \infty} \frac{e^{\theta \xi}}{\theta^2 \xi} \tag{106}$$

In the limit $\xi \rightarrow \infty$, it then follows from Eqs. (77) and (80), according to which $T_1(\xi) \simeq [\lambda_0(\xi)]^{-1}$, that

$$F(\xi, t) \underset{\xi \rightarrow \infty}{\sim} \exp\{-\theta^2 \xi [\exp(-\theta \xi)] t\} \tag{107}$$

where $F(\xi, t)$ is the probability that $T_1(\xi) < t$. The results in Eqs. (106) and (107) are identical to those obtained from the rigorous discrete energy level treatment of the Montroll-Shuler model⁽⁹⁾ in the high-temperature limit as $N + 1 = \xi \rightarrow \infty$ [Eq. (VII.6) of Ref. 8]. It should be noted that these

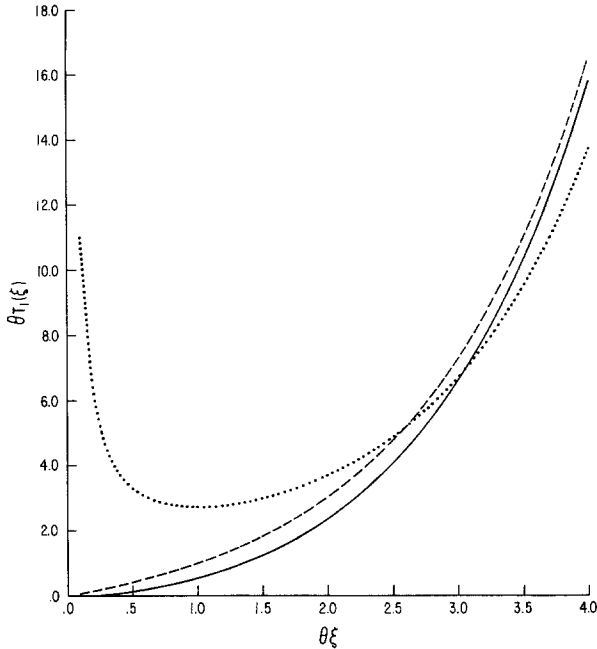


Fig. 7. Harmonic oscillator dissociation. Mean first passage time to ξ . Exact result, —. Independent random variable approximation, - -. Asymptotic expansion of exact result,

results were obtained here with much less effort than in the original papers, Refs. 9 and 10.

Figure 7 shows a comparison of the exact and approximate mean first passage times. The ordinate is in units of $\theta T_1(\xi)$ and the abscissa is in units of $\theta\xi$. The solid curve is the exact mean first passage time obtained from the exact expression in Eq. (106), the dashed curve is $\theta/\lambda_0(\xi)$ evaluated numerically, and the dotted curve is the asymptotic expansion of the exact result of Eq. (106). Beyond $\theta\xi \simeq 3$, we have $T_1(\xi) \simeq 1/\lambda_0(\xi)$ to within 11%. For $\theta\xi = 3$, we have $\int_{\xi}^{\infty} \rho(x) dx = 0.05 \ll 1$, so that the criterion of Eq. (78a) for the validity of Eqs. (77) and (80) is well fulfilled.

APPENDIX A

We illustrate here how a particular Fokker-Planck equation, namely the Ornstein-Uhlenbeck (OU) process, can readily be obtained by starting with a model of a Markov process defined only for the discrete times $t_n \equiv n \Delta t$.

Our starting point is the so-called stationary autoregressive process of first order

$$X(t_{n+1}) = \alpha(\Delta t)X(t_n) + A(t_{n+1}) \tag{A.1}$$

where X is a random variable and A is a “noise” term. Equation (A.1) can be rewritten as

$$X(t_n + \Delta t) = \alpha(\Delta t)X(t_n) + A(t_n + \Delta t) \tag{A.2}$$

We now go over to continuous time, so that t_n becomes the continuous variable t . This permits us to replace the noise term with

$$A(t_n + \Delta t) \rightarrow \int_t^{t+\Delta t} \mathcal{A}(t) dt \tag{A.3}$$

Dividing (A.2) [with (A.3)] by Δt and taking the limit $\Delta t \rightarrow 0$ yields

$$\frac{dX(t)}{dt} = \lim_{\Delta t \rightarrow 0} \left[\frac{\alpha(\Delta t) - 1}{\Delta t} \right] X(t) + \mathcal{A}(t) \tag{A.4}$$

Expansion of $\alpha(\Delta t)$ in a Taylor series about $\Delta t = 0$,

$$\alpha(\Delta t) = 1 + \left. \frac{d\alpha(\Delta t)}{d(\Delta t)} \right|_{\Delta t=0} \Delta t + O[(\Delta t)^2] \tag{A.5}$$

and substitution of (A.5) into (A.4) then gives, to order Δt ,

$$dX(t)/dt = -\mu X(t) + \mathcal{A}(t) \tag{A.6}$$

with

$$\mu \equiv - \left. \frac{d\alpha(\Delta t)}{d(\Delta t)} \right|_{\Delta t=0} \tag{A.7}$$

Equation (A.6) will be recognized as the Langevin equation. If we now assume that $\mathcal{A}(t)$ corresponds to delta-correlated Gaussian noise with

$$\langle \mathcal{A}(t) \rangle = 0, \quad \langle \mathcal{A}(t)\mathcal{A}(t') \rangle = 2D \delta(t - t') \tag{A.8}$$

where D is a constant, then it is easy to show by well-known methods that the Langevin equation (A.6) integrates to the Fokker–Planck equation (17) with $m_1(x) = -\mu x$ and $m_2(x) = 2D$. The stationary autoregressive process of first order, Eq. (A.1), is thus equivalent to the OU process [Eq. (85)] under the assumption of continuous time and delta-correlated Gaussian noise.

APPENDIX B

We present here some of the equations used in the numerical computations for the OU process.

A useful function for these calculations is

$$V_k(y) \equiv (\partial/\partial\lambda_k)U_k(y) \quad (\text{B.1})$$

where the right-hand side represents partial differentiation of the eigenfunctions of Sections 5.1 and 5.2 for fixed y . Some of the quantities that enter the numerical computations can be simply expressed with the use of this auxiliary function.

Normalization constants N_k

Equation (88) in self-adjoint form is

$$\frac{d}{dy} \left[\sigma(y) \frac{dU_k(y)}{dy} \right] + \lambda_k \rho(y) U_k(y) = 0 \quad (\text{B.2})$$

Differentiation of this equation with respect to λ_k yields an inhomogeneous differential equation for $V_k(y)$:

$$\frac{d}{dy} \left[\sigma(y) \frac{dV_k(y)}{dy} \right] + \lambda_k \rho(y) V_k(y) = -\rho(y) U_k(y) \quad (\text{B.3})$$

Multiplying Eqs. (B.2) and (B.3) by $V_k(y)$ and $U_k(y)$, respectively, subtracting them, integrating the difference from b to ξ , and using the appropriate boundary conditions, we obtain

$$N_k(\xi) = \begin{cases} \sigma(\xi) V_k(\xi) U_k'(\xi), & \text{for } b = r \\ 2\sigma(\xi) V_k(\xi) U_k'(\xi), & \text{for } b = -\xi \end{cases} \quad (\text{B.4})$$

where the prime indicates differentiation with respect to y .

Coefficients A_k

Integration of Eq. (B.2) between the boundaries gives

$$\int_b^\xi dy \rho(y) U_k(y) = -[\sigma(\xi) U_k'(\xi) - \sigma(b) U_k'(b)]/\lambda_k(\xi) \quad (\text{B.5})$$

Substitution of Eqs. (B.4) and (B.5) into Eq. (87) results in

$$A_k(\xi) = -[\lambda_k(\xi) V_k(\xi)]^{-1} \quad (\text{B.6})$$

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