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The Escape Time in Nonpotential Systems

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A generalisation of Kramer's method is developed for computing the escape time in non potential systems. The method is applied to i) moderate friction case in the Kramers problem; ii) a certain two dimensional system treated by Caroli et. al. using a perturbative method.

KEY WORDS: Kramers equation; escape time; bistability; stochastic processes; Fokker–Planck equations.

1. INTRODUCTION

In this paper I give an account of a method by which the asymptotic relaxation time of a bistable system may be computed. This method was given in a preliminary version in Ref. 1, and is essentially a generalization of the method of Kramers,[2] to multidimensional nonpotential systems. It bears a strong affinity to methods developed by Landauer and Swanson[3] and Langer.[4] In the preliminary version, no applications of the method were given, and since the method is at first glance somewhat intricate, I have chosen two examples to demonstrate its application, which in practice turns out to be relatively straightforward. These are as follows.

(i) Kramers' Equation.[2] Here a particle with position x, and momentum p (and unit mass) moves according to the stochastic differential equations

$$\begin{aligned} dx &= p\,dt \\ dx &= \left[-U'(x) - \gamma p \right] dt + (2\gamma T)^{1/2} dW(t) \end{aligned} \tag{1.1}$$

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and $U(x)$ is a two-welled potential with a central barrier at $x = 0$. In the high friction limit ($\gamma \to \infty$) the escape time can be computed using Kramers' method. My method, for finite γ, gives the escape time $\tau(\gamma)$ in the form

$$\tau(\gamma) = \tau_0 \left\{ \frac{1}{2} + \left(\frac{1}{4} + \frac{U_2}{\gamma^2} \right)^{1/2} \right\} \tag{1.2}$$

where

$$U_2 = -U''(0) \tag{1.3}$$

and τ_0 is the escape time computed using Kramers' method.

(ii) A Class of Two-Dimensional Models described by

$$d\mathbf{x} = \begin{pmatrix} 1 & a \\ -a & 1 \end{pmatrix} \nabla U(\mathbf{x})\, dt + \varepsilon \begin{pmatrix} dW_1(t) \\ dW_2(t) \end{pmatrix} \tag{1.4}$$

which corresponds to a potential system when $a = 0$, but otherwise not. The relaxation time is found to be

$$\tau(a) = \tau(0) \left\{ \frac{2\mu\lambda}{\left[(\lambda + \mu)^2 + 4\mu\lambda a^2 \right]^{1/2} - \lambda + \mu} \right\} \tag{1.5}$$

where it is assumed that for small $\mathbf{x}$,

$$U(\mathbf{x}) = U_0 + \tfrac{1}{2}(-\mu x^2 + \lambda y^2) \tag{1.6}$$

For small a this result reduces to the result of Caroli *et al.*,[5] who have recently applied perturbation theory to this problem. The result (1.5) is valid, however, for finite a (but small ϵ), while theirs requires small a.

Simulations are presented for both of these systems, and good agreement is found between theory and simulations.

In order to make the work reasonably complete, I first state in Section 2 the method of Kramers, in a formulation of my own, to illustrate its essential points. Section 3 presents the method of computing relaxation times for arbitrary bistable systems, and the two applications are presented in Section 4. Section 5 contains a summary and comparison with other methods.

2. ONE-VARIABLE BISTABLE SYSTEMS

2.1. Fokker–Planck Equation

Kramers[2] was the first to write down a Fokker–Planck equation for a bistable system, in the form

$$\partial_t P(x,t) = \partial_x\big[\, U'(x)P(x,t)\big] + D\,\partial_x^2 P(x,t) \tag{2.1}$$

where $U(x)$ is a double well potential of the form illustrated in Fig. 1. The questions which it is considered of interest to pose about such a system are the following:

(i) Given the potential $U(x)$, what is the stationary distribution function $P_s(x)$? In the case of the one-variable system (2.1) we know

$$P_s(x) = \mathcal{N} \exp\big[-U(x)/D\big] \tag{2.2}$$

In multivariable systems this question cannot always be answered.

(ii) If the particle is one well (say around a) how long does it stay there? An essentially definitive answer to this question was given by Kramers[2] and has been elaborated by others.[3,6,8] I will review Kramers'

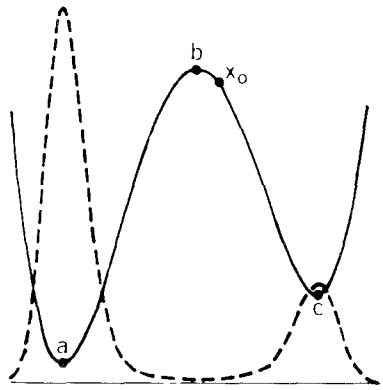

Fig. 1. Double well potential (full curve) and stationary distribution (dashed line). Points a, c, are local minima of the potential and b is a local maximum. The point x_0 is close to the local maximum.

method in a formulation which makes the assumption and their importance clear, and which enables extensions to multivariable systems possible.

2.2. Kramers' Method Reformulated

Using the notation of Fig. 1, define

$$M(x,t) = \int_{-\infty}^{x} dx' P(x',t) \tag{2.3}$$

$$N_a(t) = 1 - N_c(t) = M(b,t) \tag{2.4}$$

$$N_0(t) = (c-a)P(x_0,t) \tag{2.5}$$

and define also the corresponding stationary quantities by

$$n_a = 1 - n_c = \int_{-\infty}^{b} P_s(x)\,dx \tag{2.6}$$

$$n_0 = (c-a)P_s(x_0) \tag{2.7}$$

We now solve as follows: from the Fokker–Planck equation (2.1) follows

$$\dot{M}(x,t) = DP_s(x)\frac{\partial}{\partial x}\{P(x,t)/P_s(x)\} \tag{2.8}$$

which is integrated to give

$$\int_a^{x_0} dx\, \dot{M}(x,t)/P_s(x) = D\big[P(x_0,t)/P_s(x_0) - P(a,t)/P_s(a)\big] \tag{2.9}$$

Assumption I. We wish to consider only *long time* behavior, so that $P(x,t)$ has attained the stationary shape in each well, but the relevant weights of the two peaks have not reached the stationary value. Quantitatively this means we can set

$$\begin{aligned} P(x,t) &\simeq P_s(x)N_a(t)/n_a \qquad (x < b) \\ &\simeq P_s(x)N_c(t)/n_c \qquad (x > b) \end{aligned} \tag{2.10}$$

Substituting in the right-hand side of the relaxation equation (2.9), for $x_0 < b$ we find

$$\kappa(x_0)\dot{N}_a(t) = D\big[N_0(t)/n_0 - N_a(t)/n_a\big] \tag{2.11a}$$

$$\mu(x_0)\dot{N}_c(t) = D\big[N_0(t)/n_0 - N_c(t)/n_c\big] \tag{2.11b}$$

with

$$\kappa(x_0) = \int_a^{x_0} dx\, P_s(x)^{-1}\big[1 - \psi(x)\big] \tag{2.12a}$$

and

$$\mu(x_0) = \int_{x_0}^{a} dx\, P_s(x)^{-1}\left[1 - \psi(x)\right] \tag{2.12b}$$

and

$$\begin{aligned} \psi(x) &= n_a^{-1} \int_x^b P_s(z)\, dz \qquad (x < b) \\ &= n_c^{-1} \int_b^x P_s(z)\, dz \qquad (x > b) \end{aligned} \tag{2.13}$$

Notice that $\kappa(x_0) + \mu x_0)$ is independent of x_0.

Assumption II. $P_s(x)$ must have a sharp minimum at $x = b$—thus the two states are well separated. As Van Kampen[8] points out, the very concept of a two-state system requires this. This means that (i) $P_s(x)^{-1}$ has a sharp maximum at $x = b$ and (ii) $\psi(x)$ is extremely small in the vicinity of $x = b$. In this case one can write approximately

$$\kappa(x_0) \simeq \int_a^{x_0} dx\, P_s(x)^{-1} \tag{2.14}$$

2.3. Three-State Interpretation

Equations (2.11) correspond to a process symbolically able to be written as

$$N_a \rightleftharpoons N_0 \rightleftharpoons N_c \tag{2.15}$$

except that there is no equation for N_0. However, by noting that $N_a + N_c = 1$, we find that

$$N_0(t) = n_0\left[\mu(x_0)N_a(t) + \kappa(x_0)N_c(t)\right]/\left[\kappa(x_0) + \mu(x_0)\right] \tag{2.16}$$

This is the same solution as would be obtained by adiabatically eliminating the variable $N_0(t)$ from the differential equation for $N_0(t)$:

$$\begin{aligned} \dot{N}_0(t) = D\Big\{ & N_a(t)/\left[n_a\kappa(x_0)\right] + N_c(t)/\left[n_c\mu(x_0)\right] \\ & - N_0(t)\left[(n_0\kappa(x_0))^{-1} + (n_0\mu(x_0))^{-1}\right]\Big\} \end{aligned} \tag{2.17}$$

which is implied by the reaction scheme (2.5) and the other two equations (2.11). Such a procedure is valid when the rate constant for $N_0(t)$ is much larger than the other two, and, it can be seen that the ratio is of the order of n_a/n_0, which is very large, since n_a is of the order of 1, and n_0 is proportional to the very small probability of being at x_0.

This three-state interpretation is essentially the transition state theory of Eyring.[9]

2.4. Elimination of Intermediate States

Eliminating $N_0(t)$ from (2.11) we get

$$\dot{N}_a(t) = -\dot{N}_c(t) = r_a N_a(t) - r_c N_c(t) \tag{2.18}$$

with

$$r_a = D\left\{n_a \int_a^c dx\, P_s(s)^{-1}\left[1 - \psi(x)\right]\right\}^{-1} \tag{2.19a}$$

$$r_c = D\left\{n_c \int_a^c dx\, P_s(x)^{-1}\left[1 - \psi(x)\right]\right\}^{-1} \tag{2.19b}$$

where it is noted that r_a and r_c are independent of x_0: thus the precise choice of x_0 does not affect the interpeak relaxation.

2.5. Splitting Probabilities

Van Kampen[8] has considered the probability that the system, started at x_0, will reach the vicinity of a or c. The picture (2.15) indicates that the ratio of these two probabilities, π_a and π_c, must be the ratio of the rates at which N_0 decays, respectively, to N_a and N_c. Thus we deduce

$$\pi_a = \mu(x_0)/\left[\kappa(x_0) + \mu(x_0)\right], \qquad \pi_b = \kappa(x_0)/\left[\kappa(x_0) + \mu(x_0)\right] \tag{2.20}$$

which is in agreement with his exact results if we make Assumption II.

2.6. Escape Probability

The escape probability per unit time for a particle initially near a, to reach x_0, is the decay rate of $N_a(t)$ under the condition that an absorbing barrier is at x_0. This means that in (2.9) we set $P(x_0, t) = 0$ [but note that $P_s(x)$ is defined by (2.2)]. Similar reasoning gives us

$$\dot{N}_a(t) = -DN_a(t)/\left[n_a \kappa(x_0)\right] \tag{2.21}$$

so that the mean exit time is given by

$$\tau_a = n_a D^{-1} \int_a^{x_0} dx\, P_s(x)^{-1}\left[1 - \psi(x)\right] \tag{2.22}$$

This result is exact for $x_0 < b$, and both it and the exact result differ very little from the approximation obtained from Assumption II, which sets $\psi(x) = 0$, and is valid for x_0 near b.

3. MULTIVARIATE SYSTEMS

The multidimensional case was first treated by Landauer and Swanson[12] and restated by Langer.[4] In the following we generalize and formalize Landauer and Swanson's method to nonpotential situations.

3.1. Fokker–Planck Equation

We consider a completely general Fokker–Planck equation in l dimensions

$$\partial_t P = \nabla \cdot \left[-\mathbf{v}(\mathbf{x})P + \epsilon \mathsf{D}(\mathbf{x}) \cdot \nabla P \right] \tag{3.1}$$

[For computational convenience we write the diffusion matrix $\mathsf{D}(x)$ to the right of the gradient, so that $\mathbf{v}(x)$ is not exactly the usual drift velocity.] The stationary solution of (3.1) is to be called $P_s(\mathbf{x})$, and can only be exhibited explicitly if (3.1) satisfies potential conditions. We assume that $P_s(\mathbf{x})$ has two well-defined maxima at **a** and **c**, and well-defined saddle point at **b** (see Fig. 2), and that the value at the saddle point is very much smaller than the values at **a** and **c**. We introduce a family of $(l-1)$-dimensional planes $\mathbf{S}(w)$, where w is a parameter which labels the planes. We choose $\mathbf{S}(a)$ to pass through **a**, $\mathbf{S}(b)$ through **b**, and $\mathbf{S}(c)$ through **c**. The planes $\mathbf{S}(w)$ are assumed to be oriented in such a way that $P_s(\mathbf{x})$ has a unique maximum when restricted to any one of them. We define, similarly to the treatment in Section 2,

$$M\left[\mathbf{S}(w)\right] = \int_{L(w)} d\mathbf{x}\, P(\mathbf{x}) \tag{3.2}$$

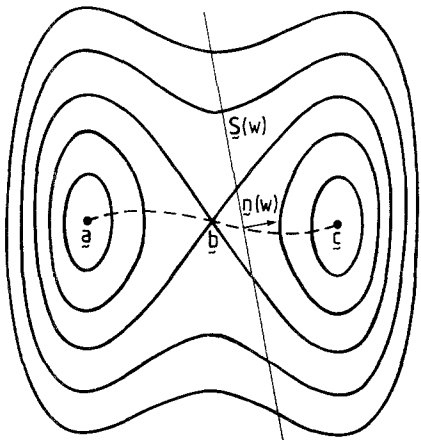

Fig. 2. Contours of the stationary distribution function $P_s(\mathbf{x})$. The plane $\mathbf{S}(w)$ is oriented so that $P_s(\mathbf{x})$ has a unique maximum there and the curve $\mathbf{x} = \mathbf{u}(w)$ is the locus of these maxima (dashed line).

where $L(w)$ is the region of space to the left of the plane $\mathbf{S}(w)$. Then

$$\dot{M}[\mathbf{S}(w)] = \int_{\mathbf{S}(w)} d\mathbf{S} \cdot [-\mathbf{v}(\mathbf{x})P + \epsilon \mathsf{D}(x) \cdot \nabla P] \tag{3.3}$$

3.2. Current in Stationary State

The current in the stationary state is defined by

$$\mathbf{J}_s = -\mathbf{v}(\mathbf{x})P_s + \mathsf{D}(\mathbf{x}) \cdot \nabla P_s \tag{3.4}$$

Assumption I. We exclude cases in which finite currents $\mathbf{J}_s$ occur where P_s is very small. Because of $\nabla \cdot \mathbf{J}_s = 0$, we can always write

$$\mathbf{J}_s = -\epsilon \nabla \cdot (\mathsf{A} P_s) \tag{3.5}$$

where A is an antisymmetric tensor. We require that $\mathsf{A}(\mathbf{x})$ be a slowly varying function of $\mathbf{x}$ in comparison to $P_s(\mathbf{x})$.

3.3. Relaxation Equations

Relaxation equations are derived in two stages. Define a quantity $\beta(\mathbf{x})$ by

$$\begin{aligned} \beta(\mathbf{x}) = P(\mathbf{x}, t)/P_s(\mathbf{x}) &\simeq N_a(t)/n_a \qquad (\mathbf{x} \text{ near } \mathbf{a}) \\ &\simeq N_c(t)/n_c \qquad (\mathbf{x} \text{ near } \mathbf{c}) \end{aligned} \tag{3.6}$$

This is the assumption that all relaxation within peaks has ceased and that only equilibration of the total populations in each peak is taking place. Substitute now in (3.3), integrate by parts discarding terms at infinity, and obtain

$$\dot{M}[\mathbf{S}(w)] = \epsilon \int_{\mathbf{S}(w)} dS \cdot [\mathfrak{D}(\mathbf{x}) \cdot \nabla \beta] P_s(\mathbf{x}) \tag{3.7}$$

with

$$\mathfrak{D}(\mathbf{x}) = \mathsf{D}(\mathbf{x}) + \mathsf{A}(\mathbf{x}) \tag{3.8}$$

Assumption II. $P_s(x)$ is sharply singly peaked on $\mathbf{S}(w)$, so we may make the approximate evaluation

$$\dot{M}[\mathbf{S}(w)] = \{[\mathbf{n}(w) \cdot \mathfrak{D}(\mathbf{x}) \cdot \nabla \beta]_{\mathbf{u}(w)} + \delta(w)\} \left| \int_{\mathbf{S}(w)} d\mathbf{S} P_s(\mathbf{x}) \right| \tag{3.9}$$

where $\delta(w)$ is expected to be very much smaller than the term in square brackets. Here $\mathbf{u}(w)$ is the position at which $P_s(x)$ has its maximum value

when restricted to $\mathbf{S}(w)$. The validity of (3.9) depends on the validity of Assumption I, that $\mathbf{A}$ is slowly varying compared to $P_s(\mathbf{x})$.

Assumption III. The direction of $\mathbf{n}(w)$ can be chosen so that $\mathfrak{D}^T(x) \cdot \mathbf{n}(w)$ is parallel to the tangent at w to the curve $\mathbf{x} = \mathbf{u}(w)$—without violating the other assumptions. Hence

$$\mathfrak{D}^T[\mathbf{u}(w)] \cdot \mathbf{n}(w) = d(w)\, \partial_w \mathbf{u}(w) \tag{3.10}$$

This equation, if it has any solutions, gives a way of determining $\mathbf{n}(w)$ and hence the planes $\mathbf{S}(w)$. We show how to use it in two examples given in Section 4. The quantity $d(w)$ is thus defined by (3.10).

Define now

$$p(w) = \left| \int_{\mathbf{S}(w)} d\mathbf{S}\, P_s(\mathbf{x}) \right| \tag{3.11}$$

which is (up to a slowly varying factor) the probability density for the particle to be on the plane $\mathbf{S}(w)$, and is expected to have a two-peaked shape, with maxima at $w = a$ and $w = c$, and a minimum at $w = b$.

Assumption IV. These are assumed to be sharp maxima and minima. Neglecting $\delta(w)$, making the choice (3.11), and noting

$$\partial_w \mathbf{u}(w) \cdot \nabla \beta[\mathbf{u}(\mathbf{w})] = \partial_w \beta[\mathbf{u}(\mathbf{w})] \tag{3.12}$$

we find

$$\int_a^{w_0} dw \left\{ M[\mathbf{S}(w)] / [p(w)\, d(w)] \right\} = \beta(w_0) - \beta(a) \tag{3.13}$$

and using the sharp peaked nature of $p(w)^{-1}$, (3.13) can now be approximated by taking the value at the peak, using (3.6) and,

$$N(a,t) = M[\mathbf{S}(b), t] \tag{3.14}$$

as well as defining

$$\kappa(w_0) = \int_a^{w_0} [p(w)]^{-1} dw \tag{3.15a}$$

$$\mu(w_0) = \int_{w_0}^{c} [p(w)]^{-1} dw \tag{3.15b}$$

to obtain the relaxation equations

$$\kappa(w_0) \dot{N}_a(t) = d(w_0)[N_0(t)/n_0 - N_a(t)/n_a] \tag{3.16a}$$

$$\mu(w_0) \dot{N}_c(t) = d(w_0)[N_0(t)/n_0 - N_c(t)/n_c] \tag{3.16b}$$

which are of exactly the same for as those in the one variable case, and can be interpreted similarly to secs. 2.3–2.5.

The escape time from well a is obtained by setting $N_0(t) = 0$ in Eq. (3.16a), and is

$$\tau = \frac{n_a}{d(w_0)} \kappa(w_0) \tag{3.17}$$

4. APPLICATIONS

This section considers two quite different two-dimensional problems; firstly Kramers' equation, which is of classic interest, and which does not have a nontrival limit with a potential solution, and secondly, a model in which an explicit nonpotential term is added to a drift arising from a potential. We show how the method of Section 3 can be used to calculate explicitly the escape times from both of these systems.

4.1. Kramers' Equation

We consider Brownian motion in velocity and position as initially introduced by Kramers.[2] Thus, we consider the Fokker–Planck equation

$$\frac{\partial P(x,p,t)}{\partial t} = -p\frac{\partial P}{\partial x} + U'(x)\frac{\partial P}{\partial p} + \gamma\left(\frac{\partial P}{\partial p}pP + T\frac{\partial^2 P}{\partial p^2}\right) \tag{4.1}$$

In the notation of Eq. (3.1) we have

$$\mathbf{x} = (x, p) \tag{4.2}$$

$$\mathbf{v}(\mathbf{x}) = (p, -U'(x) - \gamma p) \tag{4.3}$$

$$\epsilon = T \tag{4.4}$$

$$\mathsf{D}(\mathbf{x}) = \begin{pmatrix} 0 & 0 \\ 0 & \gamma \end{pmatrix} \tag{4.5}$$

$$P_s(\mathbf{x}) = \mathcal{N}_2 \exp\left[-\frac{p^2}{2T} - \frac{U(x)}{T}\right] \tag{4.6}$$

$$\mathcal{N}_2 = [2\pi]^{-1/2}\mathcal{N}_1 \tag{4.7}$$

$$\mathcal{N}_1 = \left\{\int_{-\infty}^{\infty} dx \exp\left[\frac{-U(x)}{T}\right]\right\}^{-1} \tag{4.8}$$

Hence we can write

$$\mathbf{v}(\mathbf{x}) = T\begin{pmatrix} 0 & -1 \\ 1 & \gamma \end{pmatrix} \cdot \nabla[\log P_s] \tag{4.9}$$

and the current in the stationary state is

$$\mathbf{J}_s = -\mathbf{v}P_s + T\mathsf{D}\cdot\nabla P_s = -T\nabla\cdot\left\{\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}P_s\right\} \tag{4.10}$$

so that A exists, and

$$\mathsf{A} = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \tag{4.11}$$

Thus Assumption I is satisfied.

The plane $\mathbf{S}(w)$ can be written in the form of

$$\lambda x + p = w \tag{4.12}$$

Assumption II requires us to maximize $P_s(\mathbf{x})$ on this plane, i.e., to maximize $-\frac{1}{2}p^2 - U(x)$ on this plane. Using standard methods, we find that maxima must lie along the curve $\mathbf{u}(w)$ given by

$$\mathbf{u}(w) = \begin{pmatrix}x(w)\\ p(w)\end{pmatrix} = \begin{pmatrix}x(w)\\ w - \lambda x(w)\end{pmatrix} \tag{4.13}$$

where $x(w)$ satisfies

$$U'\big[x(w)\big] + \lambda^2 x(w) - \lambda w = 0 \tag{4.14}$$

Whether $P_s(x)$ is sharply peaked depends on the nature of $U(x)$.

We now implement Assumption III.

The parameter λ is a function of w on the particular set of planes which satisfy (3.10). The tangent to $\mathbf{u}(w)$ is parallel to

$$\left(\frac{dx}{dw}, 1 - \lambda\frac{dx}{dw} - x\frac{d\lambda}{dw}\right)$$

and differentiating (4.14), we have

$$\frac{dx}{dw} = \big[U'' + \lambda^2\big]^{-1}\left[\lambda - \frac{d\lambda}{dw}(2\lambda x - w)\right] \tag{4.15}$$

The normal to (4.12) is parallel to $(\lambda, 1)$. Hence

$$\mathcal{P}^T\mathbf{n} = \big[1+\lambda^2\big]^{-1/2}\begin{pmatrix}0 & 1\\ -1 & \gamma\end{pmatrix}\begin{pmatrix}\lambda\\ 1\end{pmatrix} = \big[1+\lambda^2\big]^{-1/2}\begin{pmatrix}1\\ \gamma-\lambda\end{pmatrix} \tag{4.16}$$

and this is parallel to $\partial\mathbf{u}(w)/\partial w$ if

$$\frac{dx}{dw}\Big/1 = \left(1 - \lambda\frac{dx}{dw} - x\frac{d\lambda}{dw}\right)\Big/(\gamma - \lambda) \tag{4.17}$$

Thus, (4.17) is the explicit form of Assumption III, Eq. (3.10). We can now

solve (4.17) and (4.15) simultaneously, to get

$$\frac{dx}{dw} = \frac{1}{\gamma} - \frac{x}{\gamma^2}\left[\frac{U'' - \lambda\gamma + \lambda^2}{x(U'' + \lambda^2) - (2\lambda x - w)}\right] \tag{4.18}$$

$$\frac{d\lambda}{dw} = \frac{1}{\gamma}\left[\frac{U'' - \lambda\gamma + \lambda^2}{x(U'' + \lambda^2) - (2\lambda x - w)}\right] \tag{4.19}$$

These equations are somewhat singular near $x = 0$. Two kinds of solutions exist, depending on whether

$$\lim_{w\to 0}\left\{\frac{U''[x(w)] - \lambda(w)\gamma + \lambda(w)^2}{x(w)\{U''[x(w)] + \lambda(w)^2\} - \{2\lambda(w)x(w) - w\}}\right\} \tag{4.20}$$

is finite or infinite. It is not difficult to show that if $U(x)$ has a power series expansion round $x = 0$, only the case for (4.20) finite occurs. Assuming this, we see that choosing $w = 0 \Leftrightarrow x = 0$, and from (4.18) it follows that

$$x \simeq w/\gamma \qquad \text{as} \quad w \simeq 0 \tag{4.21}$$

Near $x = 0$, we write approximately

$$U[x] \simeq U_0 - \tfrac{1}{2}U_0 x^2 \tag{4.22}$$

And substituting (4.22) and (4.21) in (4.14), we see that

$$\lambda^2 - \gamma\lambda + U''(0) = 0 \tag{4.2.3}$$

which determines

$$\lambda(0) = \frac{\gamma}{2} \pm \left(\frac{\gamma^2}{4} + U_2\right)^{1/2} \tag{4.24}$$

We now see that (4.19) tells us that $d\lambda/dw = 0$ when $w = 0$. Thus, λ will not change significantly from (4.24) around the saddle point, and we shall from now on approximate λ by (4.24).

Only one of the roots is acceptable, and physically, this should be $\lambda \to \infty$ in the high friction limit, which would give Kramers' result, and requires the positive sign. The other root corresponds to taking planes such that we get a minimum of $P_s(x)$ on them.

We now integrate (3.11), and determine $d(w)$. Notice that $d(w)$ must be defined with $\mathbf{n}(w)$ a unit vector. Substituting directly in (4.16) and using (4.21) we find

$$(1 + \lambda^2)^{-1/2} = \frac{dx}{dw}(w = 0)\, d(0) = \frac{1}{\gamma} d(0) \tag{4.25}$$

so that

$$d(0) = \gamma(1 + \lambda^2)^{-1/2} \tag{4.26}$$

Further

$$p(w) = \int_{\mathbf{S}(w)} |d\mathbf{S}\, P_s(\mathbf{x})| = \int_{\mathbf{S}(w)} (dx^2 + dp^2)^{1/2} P_s(x, p)$$

$$= \frac{[1+\lambda^2]^{1/2}}{\lambda} \int dp \exp\left\{ -\left[\frac{1}{2} p^2 + U\left(\frac{w-p}{\lambda} \right) \right] \Big/ T \right\} \quad (4.27)$$

An exact evaluation depends on the choice of $U(x)$. Approximately, we use

$$U(x) \simeq U_0 - \tfrac{1}{2} U_2 x^2 \quad (4.28)$$

and evaluate the result as a Gaussian: we get

$$p(w) = \frac{T(1+\lambda^2)^{1/2}}{\lambda} \mathfrak{N}_2 e^{-U_0/T} \exp\left[\frac{U_2 w^2}{2T(\lambda^2 - U_2)} \right] \quad (4.29)$$

and thus

$$\kappa(0) = \int_{-\infty}^{0} p(w)^{-1} dw = \frac{1}{2} \mathfrak{N}_2^{-1} \frac{\lambda\gamma}{(1+\lambda^2)^{1/2}} \frac{e^{U_0/T}}{\sqrt{U_2}} = \mu(0) \quad (4.30)$$

Thus, from (3.17) we have for the escape time from one well to the plane S(0)

$$\tau_0 = \kappa(0) d(0)^{-1} = \frac{\lambda}{2} e^{U_0/T} \mathfrak{N}_1^{-1} \left(\frac{2\pi}{U_2} \right)^{1/2} \quad (4.31)$$

$$= \frac{1}{2} \left[\frac{\gamma}{2} + \left(\frac{\gamma^2}{4} + U_2 \right)^{1/2} \right] e^{U_0/T} \mathfrak{N}_1^{-1} \left(\frac{2\pi}{U_2} \right)^{1/2} \quad (4.32)$$

4.2. Comparison with Other Methods

In fact, no other methods of computing the mean first passage time to the center have been given, other than Kramers' simple result. However, there are several results which can usefully be compared. We will go through these in order of complexity.

(i) Exact One-Dimensional Mean First Passage Time (Smoluchowski's Equation). One reduces Kramers' equation in the large Friction limit[10–15] to the Smoluchowski equation for

$$\hat{P}(x,t) = \int dv\, P(x,v,t) \quad (4.33)$$

namely,

$$\frac{\partial \hat{P}(x,t)}{\partial t} = \frac{1}{\gamma} \frac{\partial}{\partial x} \left\{ U'(x) + T \frac{\partial \hat{P}}{\partial x} \right\} \quad (4.34)$$

and the *exact* result for the mean first passage time from $x = a$ to $x = 0$ for this equation is

$$\tau_1 = \gamma \int_a^0 dx \exp\left[\frac{U(x)}{T} \right] \int_{-\infty}^x dz \exp\left[-\frac{U(z)}{T} \right] \tag{4.35}$$

This result can be evaluated numerically.

(ii) Kramers' Result. This is obtained by applying our method to the one-dimensional Smoluchowski equation (4.34), and making Gaussian approximations to all integrals—it corresponds to (2.14), but evaluated in a Gaussian approximation. The result is

$$\tau_2 = \frac{1}{2} \gamma e^{U_0/T} \mathfrak{U}_1^{-1} \left(\frac{2\pi}{U_2} \right)^{1/2} \tag{4.36}$$

which differs from (4.32) for τ_0 by the replacement $\lambda \to \gamma$, which is valid in a large γ limit. In this limit

$$\tau_0 \simeq (1 + U_2 \gamma^{-2}) \tau_2 \tag{4.37}$$

(iii) Corrected Smoluchowski. Stratonovich,[13] Wilemski,[12] and Titulaer[14] have shown that to next highest order in γ, a more accurate equation than the Smoluchowski equation (4.33) is the *corrected Smoluchowski equation*

$$\frac{\partial \hat{P}}{\partial t} = \frac{1}{\gamma} \frac{\partial}{\partial x} \left\{ \left[1 + \gamma^{-2} U''(x) \right] \left[U'(x) + T \frac{\partial \hat{P}}{\partial x} \right] \right\} \tag{4.38}$$

(A didactic treatment of this problem is given in Ref. 15.) One now calculates the exact mean first passage time for this equation using standard theory; it is

$$\tau_3 = \gamma \int_a^0 dx \left[1 + \gamma^{-2} U''(x) \right] \exp\left[\frac{U(x)}{T} \right] \int_{-\infty}^x dz \exp\left[-\frac{U(z)}{T} \right] \tag{4.39}$$

Note, however, that the principal contribution to the x integral comes from near $x = 0$, so that the small correction term, $\gamma^{-2} U''(x)$, should be sufficiently accurately evaluated by setting

$$U''(x) \simeq U''(0) = -U_2 \tag{4.40}$$

in (4.39). We then find the *corrected Smoluchowski result*,

$$\tau_3 = (1 - \gamma^{-2} U_2)^{-1} \tau_1 \simeq (1 + \gamma^{-2} U_2) \tau_1 \tag{4.41}$$

Notice that in this limit

$$\frac{\tau_3}{\tau_1} = \frac{\tau_0}{\tau_2} \tag{4.42}$$

which means that in the limit that all integrals may be evaluated as sharply peaked Gaussians, our result is in agreement with the corrected Smoluchowski.

(iv) Simulations. By computer simulation of the equivalent stochastic differential equations

$$\begin{aligned} dx &= p\,dt \\ dp &= -\left[\gamma p + U'(x)\right] dt + (2\gamma T)^{1/2} dW(t) \end{aligned} \tag{4.43}$$

we can estimate the mean first passage time *to the plane* $\mathbf{S}_0$—i.e., to the line

$$p = -\lambda x \tag{4.44}$$

The results have to be computed for a given set of potentials. In order to assess the effect of sharpness of peaking, we consider different temperatures, T, and the simulations were performed with the potential

$$U(x) = \tfrac{1}{4}(x^2 - 1)^2 \tag{4.45}$$

The results are shown in Fig. 3. They separate naturally into two sets—curves, or straight lines. The best answer is the corrected Smoluchowski, which agrees with the simulations at all temperatures, and at low temperatures agrees with our method. Thus we confirm the validity of the method in the region of validity expected, since low temperature corresponds to sharply peaked distributions. Notice also that the choice of the plane $\mathbf{S}_0$ as the separatrix is appropriate on another ground. For, near to $x = 0, p = 0$, we can write

$$\begin{aligned} dx &= p\,dt \\ dp &= \left[-\gamma p + U_2 x\right] dt + (2\gamma T)^{1/2} dW(t) \end{aligned} \tag{4.46}$$

The condition that the deterministic part of (dx, dp), namely, $(p, -\gamma p + U_2 x)$ is in the direction connecting the point (x, p) to the origin is clearly

$$\frac{p}{-\gamma p + U_2 x} = \frac{x}{p} \tag{4.47}$$

Putting $p = -x$, we find

$$\lambda^2 + \lambda\gamma - U_2 = 0 \tag{4.48}$$

which is the same as (4.23) near $x = 0$. The two solutions correspond to the deterministic motion pointing towards the origin (positive root) or pointing away from the origin (negative root).

Thus, when the particle is on the separatrix, in the next time interval dt, only the random term $dW(t)$ will move it off this separatrix, and it will move it right or left with equal probability, i.e., this means that the splitting probability, to left or right, should be 1 : 1 on this plane.

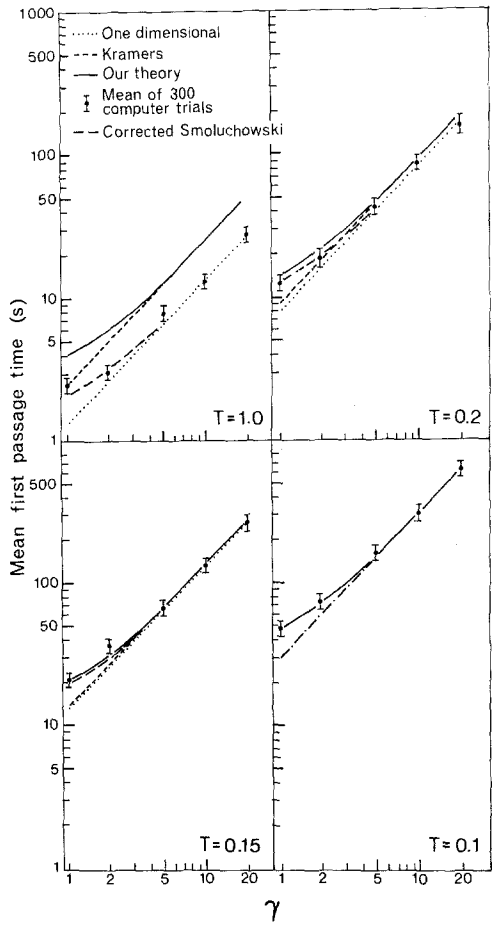

Fig. 3. Mean escape time at various temperatures for a particle moving in a double well $U(x) = \frac{1}{4}(x^2 - 1)^2$ according to Kramers' equation.

4.3. General Two-Dimensional Model

The result (3.5) can be interpreted from quite a different point of view. Supposing we assume that $P_s(\mathbf{x})$ and $\mathsf{D}(x)$ are known; then (3.5) can be used to specify all $\mathbf{v}(\mathbf{x})$ which are compatible with these, through

$$\mathbf{v}(\mathbf{x}) = \frac{\epsilon}{P_s(\mathbf{x})} \nabla \cdot \left[\mathsf{A}(\mathbf{x}) P_s(\mathbf{x})\right] + \frac{\epsilon}{P_s(\mathbf{x})} \mathsf{D}(\mathbf{x}) \cdot \nabla P_s(\mathbf{x}) \qquad (4.49)$$

Viewed this way, we can consider the effect of varying the nonpotential term, [determined by $\mathsf{A}(\mathbf{x})$], while keeping fixed $P_s(\mathbf{x})$ and $\mathsf{D}(\mathbf{x})$. This has recently been carried out by Caroli *et al.*[5] by a perturbation method in

which $\mathsf{A}(\mathbf{x})$ is taken to be small. Our method will obviously be applicable to this situation, provided $\mathsf{A}(\mathbf{x})$ is chosen to satisfy Assumption I, and $P_s(\mathbf{x})$ is chosen to satisfy Assumption II. Assumption III then provides the method of solving the problem.

Let us choose a simple two-dimensional model, like that of Caroli *et al.* We choose

$$\begin{aligned} \mathbf{x} &= (x, y) \\ \mathbf{b} &= (0, 0) \\ \mathsf{D}(\mathbf{x}) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \mathsf{A}(\mathbf{x}) &= \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix} \\ P_s(\mathbf{x}) &= \mathcal{N} \exp\left[-U(\mathbf{x})/\epsilon \right] \end{aligned} \tag{4.50}$$

and we assume that $U(\mathbf{x})$ has a quadratic expansion around the saddle point at $\mathbf{b} = (0, 0)$:

$$U(\mathbf{x}) \simeq U_0 + \tfrac{1}{2}(-\mu x^2 + \lambda y^2) \tag{4.51}$$

We will use the notation

$$\mathsf{G} = \begin{pmatrix} -\mu & 0 \\ 0 & \lambda \end{pmatrix} \tag{4.52}$$

Since all essential quantities depend only on the behavior of quantities near the saddle point, we can use (4.51) in all subsequent calculations.

We take the plane $\mathbf{S}(w)$ to be in the form

$$\mathbf{n} \cdot \mathbf{x} = w \tag{4.53}$$

and determine $\mathbf{u}(w)$, the position of the maximum of $P_s(\mathbf{x})$ on $\mathbf{S}(w)$. Standard methods give

$$\mathbf{u}(w) = \mathsf{G}^{-1} \cdot \mathbf{n} w / (\mathbf{n} \cdot \mathsf{G}^{-1} \cdot \mathbf{n}) \tag{4.54}$$

Assumption III now imposes the condition

$$\mathsf{G} \cdot \mathfrak{D}^T \cdot \mathbf{n} = d(w)\mathbf{n}/(\mathbf{n} \cdot \mathsf{G}^{-1} \cdot \mathbf{n}) \tag{4.55}$$

which means that $\mathbf{n}$ is an eigenvector of $\mathsf{G}\mathfrak{D}^T$, whose eigenvalue is

$$d(w)/(\mathbf{n} \cdot \mathsf{G}^{-1} \cdot \mathbf{n})$$

The eigenvalues of

$$\mathsf{G}\mathfrak{D}^T = \begin{pmatrix} -\mu & \mu a \\ \lambda a & \lambda p \end{pmatrix} \tag{4.56}$$

are

$$z = \frac{\lambda - \mu \pm \left[(\lambda + \mu)^2 + 4\mu\lambda a^2\right]^{1/2}}{2} \tag{4.57}$$

The root corresponding to a maximum of $P_s(\mathbf{x})$ is that such that

$$\mathbf{n} \cdot \mathsf{G}^{-1} \cdot \mathbf{n} < 0 \tag{4.58}$$

We can write

$$\mathbf{n} = (1, \alpha)/(1 + \alpha^2)^{1/2} \tag{4.59}$$

where

$$\alpha = \alpha_{\pm} = \frac{z + \mu}{\mu a} = \frac{(\lambda + \mu) \pm \left[(\lambda + \mu)^2 + 4\mu\lambda a^2\right]^{1/2}}{2\mu a} \tag{4.60}$$

Then

$$\mathbf{n} \cdot \mathsf{G}^{-1} \cdot \mathbf{n} = \frac{\mu\alpha^2 - \lambda}{\mu\lambda(1 + \alpha^2)} \tag{4.61}$$

and hence the appropriate root must satisfy

$$\alpha^2 < \lambda/\mu \tag{4.62}$$

which is the case for the negative root in (4.60), for any a. Hence we now use $\alpha = \alpha_-$, and deduce that

$$d(w) = \epsilon z \mathbf{n} \cdot \mathsf{G}^{-1} \cdot \mathbf{n} = -\epsilon z \left[\frac{\lambda - \mu\alpha^2}{\lambda\mu(1 + \alpha^2)} \right] > 0 \tag{4.63}$$

which is independent of w, a fact that arises from the approximation (4.51).

We now determine

$$p(w) = \left| \int d\mathbf{S} P_s(\mathbf{x}) \right| \tag{4.64}$$

by using the Gaussian approximation to $P_s(\mathbf{x})$ arising from the approximation (4.51) to $U(\mathbf{x})$. The method is similar to that of Section 4.1, and yields

$$p(w) = \left[\frac{2\pi\epsilon(1 + \alpha^2)}{\lambda - \alpha^2\mu} \right]^{1/2} \mathcal{N} e^{-U_0/\epsilon} \exp\left[\frac{w^2}{2\epsilon} \frac{\mu\lambda(1 + \alpha^2)}{\lambda - \alpha^2\mu} \right] \tag{4.65}$$

Hence we can compute

$$\kappa(0) = \int_{-\infty}^{0} dw\, p(w)^{-1} = \frac{1}{2} \mathcal{N}^{-1} e^{U_0/\epsilon} \left(\frac{\lambda - \alpha^2\mu}{1 + \alpha^2} \right) \tag{4.66}$$

The escape time is then given by

$$\tau = n(a)\kappa(0)d(0)^{-1} = \frac{1}{4}\mathfrak{N}^{-1}e^{U_0/\epsilon}\frac{\mu\lambda}{\epsilon|z|}$$

$$= \frac{1}{4}\epsilon\mathfrak{N}^{-1}e^{U_0/\epsilon}\frac{2\mu\lambda}{\left[(\lambda+\mu)^2+4\mu\lambda a^2\right]^{1/2}-(\lambda-\mu)} \tag{4.68}$$

If a is sufficiently small

$$\tau \simeq \frac{1}{2\epsilon}\mathfrak{N}^{-1}e^{U_0/\epsilon}\left(1-\frac{\lambda a^2}{\lambda+\mu}\right) \qquad (a \ll 1) \tag{4.69}$$

which is in complete agreement with the result of Caroli *et al.*[5] The full result, (4.68), is however valid for all a, i.e., all magnitudes of nonpotential force. One finds that if a is very large

$$\tau = \frac{1}{2\epsilon}\mathfrak{N}^{-1}e^{U_0/\epsilon}\left[\frac{(\mu\lambda)^{1/2}}{a}\right] \tag{4.70}$$

which shows that the escape time (in the approximations used) becomes quite small for large enough a.

We have performed simulations using

$$U(\mathbf{x}) = \frac{(x^2-1)}{4} + \frac{y^2}{2} \tag{4.71}$$

(for which $\mu = \lambda = 1$) and $\epsilon = 0.1$ in which case

$$\tau(a) \simeq \frac{\pi}{\sqrt{2}}\exp(1/4\epsilon)(1+a^2)^{-1/2} = \frac{27.06}{(1+a^2)^{1/2}}$$

The comparison with simulations is given in Fig. 4. In this case there does

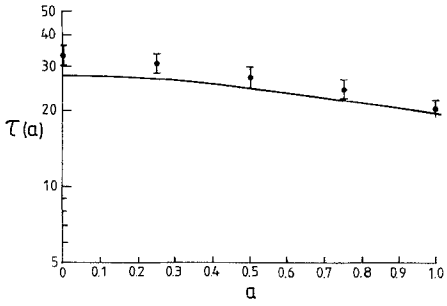

Fig. 4. Comparison of theoretical result (curve) with simulations for the escape time for a system obeying the model of Section 4.3, with potential $U(\mathbf{x}) = \frac{1}{4}(x^2-1)^2 + \frac{1}{2}y^2$.

seem to be a disagreement in absolute normalization, but the $(1 + a^2)^{-1/2}$ dependence is confirmed. The problem must lie in the simulation technique, since for $a = 0$, the x and y equations are quite independent, and the escape problem becomes purely one dimensional. The exact one-dimensional escape time in this situation is very close to 27.06, and disagrees with the $a = 0$ simulation.

5. SUMMARY AND CONCLUSIONS

It has now been demonstrated that the problem of relaxation of a bistable Fokker–Planck system in which a potential solution does not exist is essentially of the same kind as that in which a potential solution does exist. The notable difference is a practical problem—namely, how does one obtain a solution for $P_s(\mathbf{x})$, the stationary distribution.

It is interesting to note that alternative asymptotic methods developed by Schuss and Matkowsky,[16–18] which are more mathematical in nature require the same general assumptions as mine, namely, small noise, and further, also require a knowledge of $P_s(\mathbf{x})$. It is therefore towards a solution of this practical problem that future efforts must be directed.

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NOTE ADDED IN PROOF

It has recently been pointed out (B. J. Matkowsky, Z. Schuss and E. Ben Jacob, *SIAM J. Appl. Math* **42**:835 (1982)) that, in spite of his disclaimers, Kramers did give a value for the escape time is his equation for arbitrary friction, and that this result is identical with eq. 4.32.

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