

Integral equation for the resonant activation rate

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The boundary value problem for the mean first passage time is transformed here into an initial value problem by the shooting method of adjoints. Dichotomous fluctuations between two potentials $V_1(z)$ and $V_2(z)$ are assumed. The activation rate is given by an integral equation whose solutions may be computed iteratively with arbitrary precision. Model calculations are carried out for potentials of the form $V_i(z) = (-1)^i \omega z^\rho$, $\rho \geq 0$, and the strongest resonance of the activation rate is found in the linear case of $\rho = 1$. [S1063-651X(98)06905-0]

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I. INTRODUCTION

The phenomenon of resonant activation over a fluctuating barrier, which was described by Doering and Gadoua [1], has attracted considerable attention over the years. However, very few analytic results are available [1–3] and for general potentials the effect is studied either by numerical simulation [1] or by taking recourse to a non-Markovian kinetic approach [4]. In this work we formulate the problem of a resonant activation rate in terms of an integral equation whose solution may be found iteratively with arbitrary precision.

In the simplest case of dichotomous fluctuations between the two potentials $V_1(z)$ and $V_2(z)$ the mean first passage (MFP) time $\tau(z) = \tau_1(z) + \tau_2(z)$ satisfies the equation [2]

$$\begin{pmatrix} -\gamma + L_1^\dagger & \gamma \\ \gamma & -\gamma + L_2^\dagger \end{pmatrix} \begin{pmatrix} \tau_1 \\ \tau_2 \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (1)$$

where the adjoint Fokker-Planck (Smoluchowski) operators are $L_i^\dagger = -V_i'(z)d/dz + d^2/dz^2$, with $V_i' = dV_i/dz$ (dimensionless units are assumed), and γ is the fluctuation rate. For simplicity we impose initially on Eq. (1) the boundary conditions

$$\tau_i(1) = 0, \quad (2)$$

$$\tau_i'(0) = 0, \quad (3)$$

which, for general potentials $V_i(z)$, represent an absorbing boundary at $z=1$ and a reflecting boundary at $z_0=0$. For symmetric potentials $V_i(z) = V_i(-z)$ Eqs. (2) and (3) correspond also to two absorbing boundaries at $z = \pm 1$.

The minima of the potentials $V_i(z)$ are assumed to be located at the point $z=0$ and the quantity to be determined from Eq. (1) is the MFP time out of the bottom of the well, i.e., the value $\tau(0) = \tau_1(0) + \tau_2(0)$. The activation rate is then defined as $1/\tau(0)$. It is well known that the MFP time $\tau(0)$ is exponentially large [1–3] and, as discussed in Sec. III below, numerical solutions of the discretized differential system (1) yield satisfactory results only if the functions $\tau_i(z)$ are slowly varying, i.e., only if the values of the difference $V_i(1) - V_i(0)$ and of the rate γ are sufficiently small. However, solutions of Eq. (1) at large values of γ are required for the study of the resonant activation rate and in order to find these solutions we employ here the so-called

shooting method of adjoints [5], which we briefly outline in Sec. II. In Sec. III we then use the shooting method to derive an integral equation representing the missing initial conditions $\tau_i(0)$ imposed on Eq. (1). In Sec. III we also propose an iterative algorithm for the numerical solution of this equation and give some illustrative examples. A computation with the general boundary conditions $\tau_i(z_0) = \tau_i(z_1) = 0$ is discussed in Sec. IV.

II. METHOD OF ADJOINTS

Let $A(z)$ be an $(n \times n)$ -dimensional matrix and let $f(z)$ and $y(z)$ be n -dimensional vectors. Further, let the solution of the linear differential system

$$y' = A(z)y + f(z) \quad (4)$$

be sought on the interval $\langle z_0, z_1 \rangle$ subject to the r initial conditions $y_i(z_0) = c_i$ and to the $n-r$ final conditions $y_j(z_1) = c_j$. In the method of adjoints [5] this boundary value problem is transformed into an initial value problem by calculating the missing $n-r$ initial conditions $y_j(z_0)$ from the $n-r$ identities,

$$\begin{aligned} & \sum_{i=1}^n [x_i^{(m)}(z_1)y_i(z_1) - x_i^{(m)}(z_0)y_i(z_0)] \\ &= \sum_{i=1}^n \int_{z_0}^{z_1} dz x_i^{(m)}(z) f_i(z), \end{aligned} \quad (5)$$

where $m = 1, 2, \dots, n-r$. The functions $x^{(m)}(z)$ introduced above are solutions of the adjoint equation

$$dx^{(m)}/dz = -A^T(z)x^{(m)}, \quad (6)$$

$A_{ij} = (A^T)_{ji}$, on which such final conditions $x_i^{(m)}(z_1)$ are imposed that Eq. (5) goes over to a solvable linear system for the $n-r$ missing initial values $y_j(z_0)$.

III. MFP TIME

With the boundary conditions (2) and (3) the sought after MFP time values $\tau_i(0)$ are simply the missing initial condi-

tions on the left of the interval $[0,1]$. In order to determine them from the method of adjoints we first rewrite Eq. (1) in the form (4). With

$$y = (\tau'_1 - \tau'_2, \tau'_1 + \tau'_2, \tau_1 - \tau_2, \tau_1 + \tau_2) \quad (7)$$

the vector f of Eq. (4) becomes

$$f = (0, -1, 0, 0) \quad (8)$$

and writing further $V_i(z) = V(z) - (-1)^i v(z)$ we obtain

$$A = \begin{pmatrix} V' & v' & 2\gamma & 0 \\ v' & V' & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (9)$$

for the matrix $A = A(z)$. From Eqs. (6) and (9) it becomes immediately obvious that $x'_4 \equiv 0$ and the adjoint equation (6) therefore reduces to the 3×3 system

$$\frac{d}{dz} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = - \begin{pmatrix} V' & v' & 1 \\ v' & V' & 0 \\ 2\gamma & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} 0 \\ x_4^{(m)} \\ 0 \end{pmatrix}, \quad (10)$$

where $x_4^{(m)}$ is a constant determined by the final conditions at $z=1$. In order to find the missing initial conditions $y_3(0)$ and $y_4(0)$ from the identities (5) we first impose on Eq. (10) the two sets of final conditions $x^{(1)}(1) = (0, 0, 1, 0)$ and $x^{(2)}(1) = (0, 0, 0, 1)$, respectively. Solving then the 2×2 set of linear equations (5) corresponding to these two sets of final conditions we obtain the expression

$$y_4(0) = \int_0^1 dz x_2^{(2)}(z) - \frac{x_3^{(2)}(0)}{x_3^{(1)}(0)} \int_0^1 dz x_2^{(2)}(z) = \tau(0) \quad (11)$$

for the initial value $y_4(0)$, which equals the sought MFP time $\tau(0)$ by virtue of Eq. (7).

There remains yet the task of finding the two solutions $x^{(1)}(z)$ and $x^{(2)}(z)$. A brief inspection of Eq. (10) shows that, similar to the two functions $\tau_i(z)$, the six functions $x_i^{(m)}(z)$ vary exponentially fast on the interval $[0,1]$ so that direct numerical integration of the initial value problem becomes very difficult. We have tested several explicit and implicit integration schemes [6] for the exactly solvable case $V'=0$ and $v'=\omega$ (see below). There is $x_i^{(m)} \sim \exp[(1-z)\Omega]$, $\Omega^2 = 2\gamma + \omega^2$, and we found poor agreement between numerical results and analytic solutions whenever $\Omega \geq 5$. However, high computational accuracy is essential in view of the fact the MFP time $\tau(0)$ is defined by Eq. (11) as a difference between two quantities of the same order of magnitude and we therefore propose that the differential equation (10) be first integrated formally and that the resultant integral equation then be solved iteratively.

Equations (10) are given with final conditions at $z=1$, but for purposes of numerical integration it is more convenient to make the change of variables

$$u = 1 - z \quad (12)$$

and to deal with an initial value problem. Taking into account the prescribed initial values $x_i^{(m)}(0)$ at $u=0$ and introducing the notation $dV/du \equiv \dot{V} = -V'$, etc., we obtain

$$x_3^{(m)}(u) = x_3^{(m)}(0) + 2\gamma \int_0^u dt x_1^{(m)}(t), \quad (13)$$

$$x_2^{(m)}(u) = e^{-V(u)} \int_0^u dt e^{V(t)} [x_4^{(m)}(0) - \dot{v}(t)x_1^{(m)}(t)] \quad (14)$$

by directly integrating the last two of the three equations (10). Substituting these two expressions into the first of the three equations (10) and integrating anew, we finally arrive at an integral equation for the unknown function $x_1^{(m)}(u)$:

$$\begin{aligned} x_1^{(m)}(u) = e^{-V(u)} \int_0^u dt \left[x_3^{(m)}(0) e^{V(t)} - x_4^{(m)}(0) \right. \\ \left. \times \dot{v}(t) \int_0^t dt_1 e^{V(t_1)} \right] + e^{-V(u)} \int_0^u dt \int_0^t dt_1 \\ \times [2\gamma e^{V(t)} + \dot{v}(t)\dot{v}(t_1) e^{V(t_1)}] x_1^{(m)}(t_1). \end{aligned} \quad (15)$$

For sample numerical calculations we have chosen the special case of $V'(z)=0$ and $v(z) = \omega z^\rho$ ($\rho \geq 0$) for which Eq. (15) becomes

$$\begin{aligned} x_1^{(m)}(u) = x_3^{(m)}(0)u + x_4^{(m)}(0) \frac{\omega}{1+\rho} [1 - (1-u)^\rho (1+\rho u)] \\ + \int_0^u dt \int_0^t dt_1 [2\gamma + \omega^2 \rho^2 (1-t)^{\rho-1} \\ \times (1-t_1)^{\rho-1}] x_1^{(m)}(t_1). \end{aligned} \quad (16)$$

This equation may formally be written as $x_1^{(m)} = f_0 + \mathcal{O}x_1^{(m)}$, with \mathcal{O} being a bounded linear operator, and we seek its solution iteratively, in the form

$$x_1^{(m)} = \sum_{k=0}^{\infty} \prod_{l=0}^k \mathcal{O}^l f_0. \quad (17)$$

In our numerical calculations the function $x_1^{(m)}(u)$ was represented by the set of $N+1$ value $x_1^{(m)}(u_k)$ at the equidistant points $u_k = k/N, k=0, 1, \dots, N$. These values, which define a piecewise linear approximation, were updated in every iteration step according to the prescription $x_1^{(m)} \rightarrow f_0 + \mathcal{O}x_1^{(m)}$. The iterations were terminated once the relative error in the value of $\int_0^1 du x_1^{(m)}(u)$ was less than 10^{-9} and the optimal value of N was chosen adaptively, so as to yield an N -independent final result. All integrals were done (for $\rho < 1$ after a change of variables) using the trapezoidal rule.

An analytic solution of Eq. (16) is easily derived for the special case of a linear fluctuating potential $\rho=1$ for which, in particular, the MFP time $\tau(0)$ of Eq. (11) becomes

$$\tau(0) = \frac{\gamma}{\Omega^2} + \frac{\omega^2}{\Omega^4} (\cosh \Omega - 1) - \frac{2\gamma\omega^2}{\Omega^4} \frac{(\Omega - \sinh \Omega)^2}{\omega^2 + 2\gamma \cosh \Omega}, \quad (18)$$

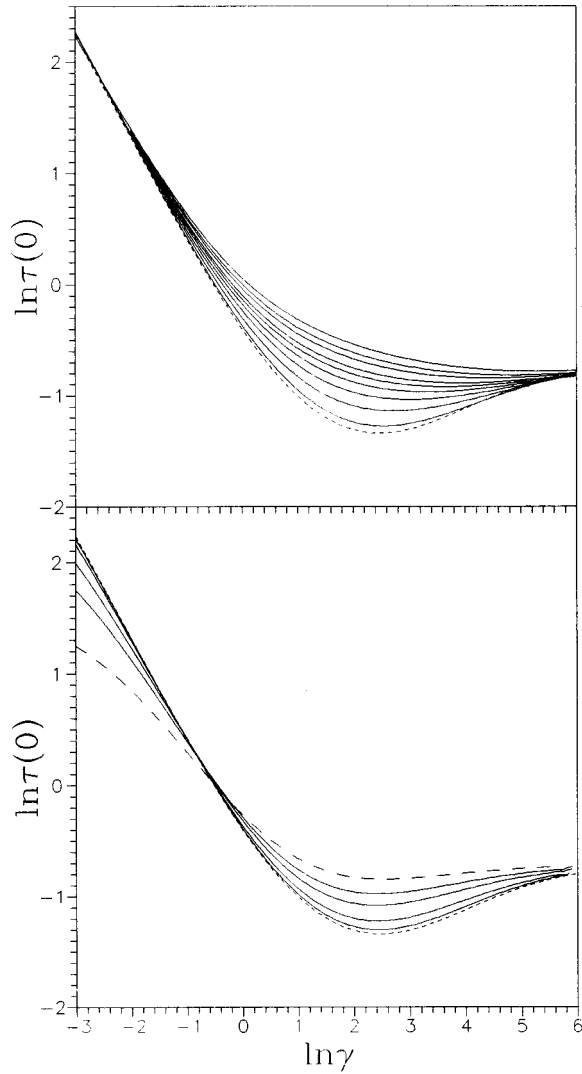


FIG. 1. Mean first passage time $\tau(0)$ versus γ for the potential $v(z) = \omega z^\rho$ and the boundary conditions (2) and (3). Top: $\rho=1$ (short dash) and, in ascending order, 2, 3, 4, 5, 6, 7, 9, 11, and 15 (topmost curve). Bottom: $\rho=1$ (short dash) and, in ascending order, 0.8, 0.6, 0.4, 0.3, and 0.2 (long-dashed curve). The apparent common intercept of the curves is only approximate for ρ close to 1 and in the limit $\rho \rightarrow 0$ there is $\tau(0) \equiv 1/2$.

where $\Omega^2 = 2\gamma + \omega^2$ was already defined above. For $\omega = 10$ we found excellent agreement between this equation and numerical data at the optimal value of $N = 5000$. For selected values of $\rho > 0$ we plot the MFP time values $\tau(0)$ versus γ in Fig. 1. A striking feature of these plots is the fact that the strongest resonance of the activation rate takes place for $\rho = 1$, i.e., in the field of a fluctuating linear potential. The physical origin of this phenomenon is not clear to us and we offer here only two comments on the attenuation of the resonance at small and large ρ : The limit $\rho \rightarrow 0$ corresponds to a free Brownian particle for which, according to the above equation with $\omega = 0$, there is $\tau(0) \equiv 1/2$ and no resonance takes place. Similarly, the potential $v(z)$ goes over to a step

function $v(z) \rightarrow \omega \theta(z - 1)$ as $\rho \rightarrow \infty$ and the particle is again free, with a wall of height ω at the right edge of the integration domain. This approximation is not compatible with the boundary conditions (2) and (3), but we found no resonance [2] for the closely related shifted potential $v(z) = \omega \theta(z - \varepsilon)$, $\varepsilon \in (0, 1)$, for which Eq. (1) is solvable analytically up to the matching conditions at $z = \varepsilon$.

IV. CONCLUDING REMARKS

Using the method of adjoints we have transformed the boundary value problem for the MFP time into an initial value problem and, assuming the symmetric boundary conditions (2) and (3), found particularly simple expressions for the resonant activation rate. In this concluding section we outline an algorithm for the numerical integration of Eq. (1) with general boundary conditions $\tau_i(z_0) = \tau_i(z_1) = 0$, corresponding, by virtue of Eq. (7), to the conditions $y_3(z_0) = y_4(z_0) = 0$ and $y_3(z_1) = y_4(z_1) = 0$ imposed on Eq. (4).

As in the previous case we require first the missing initial values $\tau'_i(z_0)$ and to this end we again rewrite Eq. (1) in the form (4) and solve, exactly as in the previous case, the adjoint equation (10) with the final conditions $x^{(1)}(z_1) = (0, 0, 1, 0)$ and $x^{(2)}(z_1) = (0, 0, 0, 1)$. By virtue of Eq. (5) the missing initial conditions $y_1(z_0)$ and $y_2(z_0)$ satisfy the 2×2 linear system

$$y_1(z_0)x_1^{(m)}(z_0) + y_2(z_0)x_2^{(m)}(z_0) = \int_{z_0}^{z_1} dz x_2^{(m)}(z), \quad (19)$$

$m = 1$ and 2, and given its solutions we integrate the differential system (4) and obtain

$$\begin{aligned} y_1(z) &= y_1(z_0)e^{V(z)-V(z_0)} + e^{V(z)} \int_{z_0}^z dt e^{-V(t)} \left[v'(t)y_2(t) \right. \\ &\quad \left. + 2\gamma \int_{z_0}^t dt' y_1(t') \right], \quad (20) \\ y_2(z) &= y_2(z_0)e^{V(z)-V(z_0)} + e^{V(z)} \int_{z_0}^z dt e^{-V(t)} \\ &\quad \times [v'(t)y_1(t) - 1]. \quad (21) \end{aligned}$$

Substitution of Eq. (21) into Eq. (20) yields an integral equation for the unknown function $y_1(z)$ and we propose that this equation be solved iteratively by the method used above to solve Eq. (16). The MFP time function, finally, is given by the equation

$$\tau(z) = y_4(z) = \int_{z_0}^z dt y_2(t), \quad (22)$$

where $y_2(z) = y_2[z, y_1(z)]$ is defined by Eq. (21). The initial conditions $y_1(z_0)$ and $y_2(z_0)$ given by Eq. (19) correspond to $y_4(z_1) = 0$ and this final condition provides here a test of computational accuracy.

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