Thermal decay of a metastable state: Exact solution

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Exact solutions are obtained for the thermal decay of a metastable state for two different forms of the potential and for uniform and localized boundary conditions by using the Laplace transform method. The exact inverse Laplace transforms are found for a symmetric case, and the results are compared with other calculations and with the Kramers rate.

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I. INTRODUCTION

Escape from metastable states is an old problem of great importance both in quantum and classical mechanics. The tunneling of quantum particles through a potential barrier is a clearly understood quantum-mechanical problem [1]. We consider here the dynamics of a classical particle. Such a particle with energy less than the barrier height is able to cross the barrier only in the presence of fluctuations. Fluctuation-induced transitions occur in many areas of physics, chemistry, and biology [2]. By definition, these problems include nonlinear potentials which makes their analysis quite difficult. To overcome this impediment, we consider the simplest model of a metastable state formed by piecewise constant barriers (Fig. 1) that allow an exact analytical solution. Many fundamental properties of a particle moving in a nonlinear potential are generic; in particular, they are not very sensitive to the details of the potential. Therefore, it is worthwhile to consider the simplest potential that allows an analytical solution, in addition to numerical simulations for more complicated potentials.

We have previously considered different phenomena involving piecewise constant potentials. Exact solutions have been obtained [3] for the transmission of a classical particle through one barrier of given width and through two barriers with a well between them of the same overall width. An additional periodic force results [4] in the well-known phenomenon of stochastic resonance. The external periodic field [5] as well as the random fluctuations of the barrier height [6] are able to increase the population of metastable states (“stabilization of metastable states”). The latter phenomenon, along with the previously found [7] stabilized action of noise on the escape of a particle subject to a periodic force of large amplitude from a metastable state (“noise enhanced stability”), shows that there are still some interesting features in this “old-fashioned” field.

We consider a particle subject to white noise of intensity $2D$ initially located at a metastable state of two types shown in Figs. 1(a) and 1(b). For the potential shown in Fig. 1(a), the particle has finite probability to remain in the metastable state as $t\rightarrow\infty$, while for the potential shown in Fig. 1(b), this probability vanishes. For simplicity, we consider the symmetric square-well potential shown in Fig. 1(a), although the exact result can be obtained for nonsymmetric case as well. Note that, as one can easily see from Fig. 1, it is sufficient to solve the problem for the potential shown in Fig. 1(a) since the appropriate results for the potential shown in Fig. 1(b) can be obtained by a simple transformations of variables

$$L\rightarrow\frac{A+B}{2},\quad a\rightarrow\frac{B-A}{2},\quad x\rightarrow x-\frac{A+B}{2},\quad U_1\rightarrow\infty. \tag{1}$$

The potentials shown in Fig. 1 belong to the class of simple potentials for which the exact solution to the full dynamic problem can be obtained by using the Laplace transform method or by transferring the Focker-Planck equation into the Schrödinger form [8]. We use the former method which, at the final step, requires the inverse Laplace transform. The latter can be performed exactly only in very special cases, and one such case, $B=2A$, will be considered below. Although one can perform the full analysis for the potentials shown in Figs. 1(a) and 1(b), and we bring here the final formulas for both cases, we perform the analysis only for the potential shown in Fig. 1(b), since the appropriate formulas for the other case are quite cumbersome,

The present paper presents the further development of our previous work as applied to the full dynamic analysis of a metastable state. The outline of this paper is as follows. In Sec. II, we present the general equations with boundary and

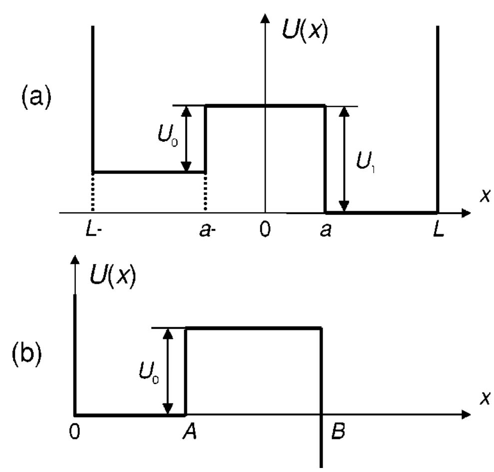

FIG. 1. Square-well potentials descriptive of a metastable state. (a) The metastable and the stable states have the potential barriers U_0 and U_1, respectively. The width of the barrier is $2a$, and the reflecting walls are located at $x=\pm L$. (b) The metastable states are in the well of width A with the potential barrier of height U_0. The trap is located at $x=B$.

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matching conditions, which are solved afterward for the uniform initial conditions. The slightly more complicated case of localized initial conditions is considered in Sec. III. The inverse Laplace transform is performed in Sec. IV for the special case of the potential shown in 1(b) with equal widths of the well and the barrier. Section V contains some conclusions.

II. BASIC EQUATIONS

The Fokker-Planck equation for the probability density function $P(x,t)$ for the position x of a diffusing particle at time t has a following form:

$$\frac{\partial P}{\partial t}=\frac{\partial}{\partial x}\left(\frac{dU}{dx}P\right)+D\frac{\partial^2 P}{\partial x^2}\equiv-\frac{\partial J}{\partial x}, \tag{2}$$

where $J\equiv-D\exp(-U/D)\partial/\partial x[\exp(U/D)P]$ is the probability current.

For the potential shown in Fig. 1, $dU/dx=0$, and Eq. (2) reduces to the simple diffusion equation with $J=-D(\partial P/\partial x)$:

$$\frac{\partial P}{\partial t}=D\frac{\partial^2 P}{\partial x^2}. \tag{3}$$

The boundary conditions are different for potentials shown in Figs. 1(a) and 1(b). We assume reflecting boundary condition at both boundaries $x=-L$ and $x=L$ of the potential shown in Fig. 1(a), which means that the probability current vanishes at these points,

$$\frac{\partial P}{\partial x}(x=-L,t)=\frac{\partial P}{\partial x}(x=L,t)=0 \quad \text{for the potential shown in Fig. 1(a)}, \tag{4}$$

while for the potential shown in Fig. 1(b), we assume the reflecting boundary condition at $x=0$ and absorbing boundary conditions at $x=B$,

$$\frac{\partial P}{\partial x}(x=0,t)=0: \quad P(x=B,t)=0 \quad \text{for the potential shown in Fig 1(b)}. \tag{5}$$

The latter condition means that a particle escapes from a metastable state through the barrier once it has reached the boundary at $x=B$.

One has to find the solutions $P_1(x,t)$ and $P_2(x,t)$ of Eq. (3) in each of two regions, $(0,A)$ and (A,B), for the potential shown in Fig. 1(b), and $P_1(x,t)$, $P_2(x,t)$ and $P_3(x,t)$ for three regions, $(-L,-a)$, $(-a,a)$, and (a,L) for the potential shown in Fig. 1(a). Continuity of J at the boundaries of the two adjusted regions means that at the points z of the finite jumps of potentials, one gets [9]

$$\frac{\partial P_i(z,t)}{\partial x}=\frac{\partial P_{i+1}(z,t)}{\partial x},$$

$$P_i(z-0,t)\exp\left(\frac{U(z-0)}{D}\right)=P_{i+1}(z+0,t)\exp\left(\frac{U(z+0)}{D}\right). \tag{6}$$

Initially, a particle is located in a metastable state, being either uniformly distributed,

$$P_1(x,t=0)=\frac{1}{c}, \tag{7}$$

where $c=a$ and $c=A$ for the potentials shown in Figs. 1(a) and 1(b), respectively, or localized at some point x_0 of a metastable region

$$P_1(x,t=0)=\delta(x-x_0). \tag{8}$$

It is convenient to use the Laplace transform

$$W(x,s)=\int_0^\infty P(x,t)\exp(-st)dt, \tag{9}$$

which, after substitution into Eq. (3), gives

$$\frac{\partial^2 W}{\partial x^2}=r^2W-\frac{P(x,t=0)}{D}, \quad r^2\equiv\frac{s}{D}. \tag{10}$$

Let us start from the uniformly distributed initial condition (7), leaving the slightly more complicate case of the localized initial conditions (8) for the following section.

For the initial condition $P_1(x,t=0)=1/c$, one gets $W_1=1/cs$, and the solution of the inhomogeneous differential equation (10) in the region $(-L,-a)$ has the following form:

$$W_1(x,s)=\frac{1}{as}+C_1\exp(rx)+C_2\exp(-rx), \tag{11}$$

while for the regions $(-a,a)$ and (a,L), where at $t=0$, $P_2=W_2=0$ and $P_3=W_3=0$, the solutions of Eq. (10) are given by

$$W_2(x,s)=C_3\exp(rx)+C_4\exp(-rx),$$

$$W_2(x,s)=C_5\exp(rx)+C_6\exp(-rx). \tag{12}$$

The coefficients C_i are determined from the boundary conditions (4), the initial condition (7), and the matching conditions (6), where in Eqs. (4) and (6), P is replaced by W.

Omitting the routine algebra, we write down the solutions of Eq. (10) subject to boundary conditions (4), initial condition (7), and the matching conditions (6),

$$W_1=\frac{1}{as}-\frac{\exp\left(-\frac{U_0}{D}\right)\cosh[r(L+x)][A_+\exp(2ra)-A_-\exp(-2ra)]}{as[A_+B_+\exp(2ra)-A_-B_-\exp(-2ra)]}\quad\text{for}\quad x\epsilon(-L,-a),$$

$$W_2=\frac{\exp\left(-\frac{U_0}{D}\right)\sinh[r(L-a)]\{(A_++A_-)\cosh[r(x-a)]-(A_+-A_-)\sinh[r(x-a)]\}}{as[A_+B_+\exp(2ra)-A_-B_-\exp(-2ra)]}\quad\text{for}\quad x\epsilon(-a,a),$$

$$W_3=\frac{2\exp\left(-\frac{U_0}{D}\right)\sinh[r(L-a)]\cosh[r(L-x)]}{as[A_+B_+\exp(2ra)-A_-B_-\exp(-2ra)]}\quad\text{for}\quad x\epsilon(a,L), \tag{13}$$

where

$$A_\pm=\exp\left(-\frac{U_1}{D}\right)\cosh[r(L-a)]\pm\sinh[r(L-a)],$$

$$B_\pm=\exp\left(-\frac{U_0}{D}\right)\cosh[r(L-a)]\pm\sinh[r(L-a)]. \tag{14}$$

Equations similar to Eq. (13) had been obtained earlier [3] for different boundary conditions and the bistable potential with $U_0=U_1$.

The inverse Laplace transform of Eqs. (13) is a challenging task, but the asymptotic behavior ($t\to\infty$ or $s\to 0$) can be easily found from Eq. (13) which gives,

$$\frac{P_1(t\to\infty)}{P_3(t\to\infty)}=\frac{\exp\left(-\frac{U_1}{D}\right)}{\exp\left(-\frac{U_0}{D}\right)}, \tag{15}$$

as expected.

According to Eq. (1), one can easily get from Eq. (13) the full solution for the potential shown in Fig. 1(b),

$$W_1(x,s)=\frac{1}{as}-\frac{\cosh\left[\sqrt{\frac{s}{D}}(B-A)\right]\cosh\left(\sqrt{\frac{s}{D}}x\right)}{as\left\{\cosh\left(\sqrt{\frac{s}{D}}A\right)\cosh\left[\sqrt{\frac{s}{D}}(B-A)\right]+\left[\sinh\left(\sqrt{\frac{s}{D}}A\right)\right]\sinh\left[\sqrt{\frac{s}{D}}(B-A)\right]\exp\left(\frac{U_0}{D}\right)\right\}}\quad\text{for}\quad x\,\epsilon(0,A),$$

$$W_2(x,s)=\frac{\sinh\left(\sqrt{\frac{s}{D}}A\right)\sinh\left[\sqrt{\frac{s}{D}}(B-x)\right]}{as\left\{\cosh\left(\sqrt{\frac{s}{D}}A\right)\cosh\left[\sqrt{\frac{s}{D}}(B-A)\right]+\left[\sinh\left(\sqrt{\frac{s}{D}}A\right)\right]\sinh\left[\sqrt{\frac{s}{D}}(B-A)\right]\exp\left(\frac{U_0}{D}\right)\right\}}\quad\text{for}\quad x\,\epsilon(A,B). \tag{16}$$

Before the analysis of Eqs. (13) and (16), we consider in the following section the localized initial condition (8), which is different from the uniform condition (7).

III. LOCALIZED INITIAL CONDITIONS

Although it is physically obvious that the qualitative results do not depend on the precise initial position of a particle in a metastable state, we consider in addition to the uniform initial condition (7), the localized initial condition (8). For brevity, we bring here the results only for potential shown in Fig. 1(b).

We seek the solution of Eq. (10) in region $(0,A)$ as $P=R+S$ where R is the solution of Eq. (10) for $-\infty<x<\infty$ such that at $t=0$, $R(x,t=0)=\delta(x-x_0)$, and S is the solution of Eq. (10) which is equal to zero at $t=0$. It is well known [10] that

$$R(x,t)=\frac{1}{\sqrt{\pi Dt}}\exp\left[-\frac{(x-x_0)^2}{4Dt}\right], \tag{17}$$

while $S(x,s)$ satisfies Eq. (10) with $P(x,t=0)=0$,

$$S(x,s)=C_1\exp(rx)+C_2\exp(-rx). \tag{18}$$

The Laplace transform of Eq. (17) is [11]

$$R(x,s)=\frac{\exp(-r|x-x_0|)}{2Dr}. \tag{19}$$

Therefore, the Laplace transform of $P(x,t)$ in the region $(0,A)$ has the following form:

$$W(x,s)=\frac{\exp(-r|x-x_0|)}{2Dr}+C_5\sinh rx+C_6\cosh rx, \tag{20}$$

while for $x\,\epsilon(A,B)$, $W_2(x,s)$ is given, as before, by Eq. (12). Analogously to Eqs. (11) and (12), the four constants of integration can be found from the boundary conditions (5), initial condition (8), and matching conditions (6). Finally, one gets for the localized initial condition, $P(x,t=0)=\delta(x-x_0)$, when $x<x_0$,

$$W_1(x,s)=\frac{\cosh(rx)\cosh(rx_0)\left\{\cosh\left[\sqrt{\frac{s}{D}}(B-A)\right]\sinh\left(\sqrt{\frac{s}{D}}A\right)+\sinh\left[\sqrt{\frac{s}{D}}(B-A)\right]\cosh\left(\sqrt{\frac{s}{D}}A\right)\exp\left(\frac{U_0}{D}\right)\right\}}{\sqrt{sD}\left\{\cosh\left(\sqrt{\frac{s}{D}}A\right)\cosh\left[\sqrt{\frac{s}{D}}(B-A)\right]+\left[\sinh\left(\sqrt{\frac{s}{D}}A\right)\right]\sinh\left[\sqrt{\frac{s}{D}}(B-A)\right]\exp\left(\frac{U_0}{D}\right)\right\}}$$
$$-\frac{\cosh(rx)\sinh(rx_0)}{\sqrt{sD}}\ \text{for } x\,\epsilon(0,A) \tag{21}$$

and for $x_0<x<A$, the result is the same with x and x_0 interchanged.

Above the barrier,

$$W_2(x,s)=\frac{\cosh\left(\sqrt{\frac{s}{D}}x_0\right)\sinh\left[\sqrt{\frac{S}{D}}(B-x)\right]}{\sqrt{sD}\left\{\cosh\left(\sqrt{\frac{s}{D}}A\right)\cosh\left[\sqrt{\frac{s}{D}}(B-A)\right]+\left[\sinh\left(\sqrt{\frac{s}{D}}A\right)\right]\sinh\left[\sqrt{\frac{s}{D}}(B-A)\right]\exp\left(\frac{U_0}{D}\right)\right\}}\quad\text{for}\ \ x\,\epsilon(a,b). \tag{22}$$

Equations (21) and (22) reduce to Eq. (16) if one performs in the former the additional average over x_0. Since the inverse Laplace transform of Eq. (16) and Eqs. (21) and (22) is not trivial, we consider in the following section the special case of equal widths of the well and the barrier, $B=2A$. For brevity, we omit other exactly soluble cases such as $B=3A/2$ or $B=4A/3$.

IV. SYMMETRIC POTENTIAL

The inverse Laplace transform of Eq. (16) for uniform initial condition, $P(x,t=0)=1/A$, and the symmetric potential, $B=2A$, has the following form:

$$W_1(x,t)=\frac{1}{2\pi iA}\int_C\frac{\exp(st)ds}{s}\left[1-\frac{\cosh\left(\sqrt{\frac{s}{D}}A\right)\cosh\left(\sqrt{\frac{s}{D}}x\right)}{\cosh^2\left(\sqrt{\frac{s}{D}}A\right)+\sinh^2\left(\sqrt{\frac{s}{D}}A\right)\exp\left(\frac{U_0}{D}\right)}\right]\ \text{for } x\,\epsilon(0,A),$$

$$W_2(x,t)=\frac{P_0}{2\pi iA}\int_C\frac{\exp(st)ds}{s}\frac{\sinh\left(\sqrt{\frac{s}{D}}A\right)\sinh\left[\sqrt{\frac{s}{D}}(2A-x)\right]}{\cosh^2\left(\sqrt{\frac{s}{D}}A\right)+\sinh^2\left(\sqrt{\frac{s}{D}}A\right)\exp\left(\frac{U_0}{D}\right)}\ \ \text{for}\ \ x\,\epsilon(A,2A), \tag{23}$$

where C is the usual integration contour of the inverse Laplace transform.

The poles of the integrand in Eq. (23) occur at $s=0$ and at

$$s=-\frac{D(\alpha+2n\pi)^2}{A^2},\quad n=1,2,3,\ldots, \tag{24}$$

where α is the root of the equation

$$\tan(\alpha)=\exp\left(-\frac{U_0}{2D}\right). \tag{25}$$

One finds the residue at these poles from

$$s\frac{d}{ds}\left[\cosh^2\left(\sqrt{\frac{s}{D}}A\right)+\sinh^2\left(\sqrt{\frac{s}{D}}A\right)\exp\left(\frac{U_0}{D}\right)\right]_{s=-D(\alpha+2n\pi)^2/A^2}=-(\alpha+2n\pi)\exp\left(\frac{U_0}{2D}\right). \tag{26}$$

Equation (25) has been used in Eq. (26).

The time variations of the probability distributions from the initial homogeneous distribution in the wall are

$$P_1(x,t)=\frac{1}{\sqrt{1+\exp\left(\frac{U_0}{D}\right)}}\sum_{n=-\infty}^{\infty}\cos\left(\frac{\alpha+2n\pi}{A}x\right)\frac{\exp\left[-\frac{D(\alpha+2n\pi)^2}{A^2}t\right]}{A(\alpha+2n\pi)}\quad\text{for}\quad x\,\epsilon(0,A),$$

$$P_2(x,t)=\frac{\exp\left(-\frac{U_0}{2D}\right)}{\sqrt{1+\exp\left(\frac{U_0}{D}\right)}}\sum_{n=-\infty}^{\infty}\sin\left[\frac{\alpha+2n\pi}{A}(2A-x)\right]\frac{\exp\left[-\frac{D(\alpha+2n\pi)^2}{A^2}t\right]}{A(\alpha+2n\pi)}\quad\text{for}\quad x\,\epsilon(A,2A). \tag{27}$$

The survival probability $S(t)$ for $P(x,t=0)=1/c$, can be found from Eq. (27),

$$S_1(t)=\int_0^a P_1(x,t)dx=\frac{1}{1+\exp\left(\frac{U_0}{D}\right)}\sum_{n=-\infty}^{\infty}\frac{\exp\left[-\frac{D(\alpha+2n\pi)^2}{A^2}t\right]}{(\alpha+2n\pi)^2},$$

$$S_2(t)=\int_a^{2a} P_2(x,t)dx=\left(\frac{\exp\left(-\frac{U_0}{2D}\right)}{\sqrt{1+\exp\left(\frac{U_0}{D}\right)}}-\frac{1}{1+\exp\left(\frac{U_0}{D}\right)}\right)\sum_{n=-\infty}^{\infty}\frac{\exp\left[-\frac{D(\alpha+2n\pi)^2}{A^2}t\right]}{(\alpha+2n\pi)^2}. \tag{28}$$

The expression for $S_1(t)$ coincides with the result of the calculation in Ref. [8] performed by a different method.

Another characteristic of the decay of the metastable state is the mean free passage time τ, the time elapsing before reaching the absorbing boundary at $x=B$. This time is defined through the survival probability $S_1(t)$ as $\tau=\int_0^\infty S_1(t)dt$ and can be found from Eq. (28),

$$\tau=\frac{A^2}{D\left[1+\exp\left(\frac{U_0}{D}\right)\right]}\sum_{n=-\infty}^{\infty}\frac{1}{(\alpha+2n\pi)^4}$$

$$\simeq\frac{A^2}{16D}\left[\exp\left(\frac{U_0}{D}\right)+\frac{1}{3}\right], \tag{29}$$

which, for $\exp(U_0/D)>\frac{1}{3}$, i.e., according to Eq. (25), for $\tan\alpha<\sqrt{3}$, coincides—to within a numerical factor—with the well-known Kramers formula [12]. The third derivative of the summation formula [13] $\cot(\alpha/2)=2\Sigma_{n=-\infty}^{\infty}1/(\alpha+2n\pi)$ has been used in Eq. (29).

Turning now to the case of a localized boundary condition, $P(x,t=0)=\delta(x-x_0)$, and symmetric potential, $B=2A$, one can find, in complete analogy to the preceding calculation,

$$P_1(x,t)=\frac{1}{A}\sum_{n=-\infty}^{\infty}\cos\left(\frac{\alpha+2n\pi}{A}x\right)\cos\left[\frac{\alpha+2n\pi}{A}x_0\right]\exp\left[-\frac{D(\alpha+2n\pi)^2}{A^2}t\right]\ \text{for}\ x\ \epsilon(0,A),$$

$$P_2(x,t)=\frac{1}{A}\exp\left(-\frac{U_0}{2D}\right)\sum_{n=-\infty}^{\infty}\sin\left[\frac{\alpha+2n\pi}{A}(2A-x)\right]\cos\left[\frac{\alpha+2n\pi}{A}x_0\right]\exp\left[-\frac{D(\alpha+2n\pi)^2}{A^2}t\right]\ \text{for}\ x\ \epsilon(A,2A). \tag{30}$$

Again, after averaging over x_0, Eq. (30) reduces to Eq. (27).

V. CONCLUSIONS

Within the past years, nonlinear phenomena have been extended into different fields of modern science. At the same time, it is the nonlinearity that severely complicates the qualitative analysis leading, as a rule, to the use of numerical simulations. Therefore, the analysis of simple nonlinear models that allow an exact solution is of considerable importance.

The piecewise constant potential (along with the piecewise linear potential) is one of such models. In the framework of this model, we have performed a comprehensive analysis of the one-dimensional decay of a metastable state. The Focker-Planck equation has been solved exactly for two types of metastable states, characterized by asymptotic partial [Fig. 1(a)] or full [Fig. 1(b)] decay. The Laplace transform method has been used in two slightly different forms for uniform and localized initial conditions. The final answers have been found in terms of Laplace transforms, which allows one to analyze the asymptotic properties, and—for certain symmetric potentials—to perform the inverse Laplace transform explicitly, or to calculate the inverse Laplace transform numerically.

The probability distribution functions found in all these cases allow one to describe all statistical properties of systems considered. Here, we used them to find the survival probabilities as well as the escape time that was compared with the Kramers rate. The next step will be the analysis of the same systems with additional periodic forces that will allow one to describe the peculiar forms of interactions between periodic and random forces in nonlinear systems (stochastic resonance, noise enhanced stability, and others), implying that order and chaos are complementary rather than contradictory phenomena [14].

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