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Multi-dimensional WKB treatment of first passage time

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Abstract. The problem of first passage time is mathematically equivalent to the tunnelling of a particle out of a potential well and hence can be treated by the multi-dimensional WKB technique. In general, the most probable tunnelling path (MPTP) is curved and is difficult to determine. We discuss a model potential for which the curved MPTP can be solved analytically. It is shown that the rate of tunnelling calculated along the straight path as usually assumed is unreliable. Numerical results of the mean switching time for the bistable two-mode laser and comparison with experiments and other theories are also discussed.

1. Introduction

Although the classic problem of first passage time (FPT) has received much attention in many different fields of research (Haken 1979, Arnold and Lefever 1981), there are still very few examples in which quantitative comparison can be made between experiment and theory. The general Fokker-Planck equation is difficult to solve. In most practical cases, the drift coefficients are derivable from a potential and the problem reduces to determining the mean escape time or equivalently the rate at which the system escapes from the metastable state out of the potential well passing through the saddle point of the potential. If one assumes that the quantum effect is negligible and that the motion around the saddle point is nearly simple harmonic, the mean escape time can be derived (see, e.g., Vineyard 1957). The general expression for the mean escape time is a product of the multiplying frequency factor and the dominant exponential factor. Since the problem is mathematically the same as the motion of a particle in a potential well expressed as a function of the generalised coordinate representing the decaying quantity, one can treat it as a tunnelling problem by the WKB technique just like quantum particle dynamics. It has been shown (Bender and Wu 1973) that the mean escape time from the WKB method again contains a multiplying factor which is the normalisation integral and an exponential factor which involves a path integral in the exponent. It is therefore necessary to determine the most probable tunnelling path (MPTP) before any quantitative result can be obtained.

The MPTP is in general a curve rather than a straight line; the latter has been assumed in most of the existing calculations. A general method has already been developed (Banks and Bender 1973) to find the curved MPTP by constructing a multi-dimensional WKB approximation in curved space. The first step is to find the thickness of the tube surrounding the MPTP and then to determine the MPTP by means of a perturbative

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method. Since the method is extremely formal, a system of two coupled anharmonic oscillators of unequal masses is solved in Banks and Bender (1973) as an illustration.

In recent years, more rigorous treatment of the tunnelling problem had been formulated in terms of path integrals (Callan and Coleman 1977) and instantons (Agmon 1979, Simon 1984); it was also recognised (Sethna 1982) that the instanton bounce paths follow the most probable escape path of Banks and Bender (1973) and Bender and Wu (1973) whose method is what we shall use in the present work.

In order to apply the method, we first convert the Fokker-Planck equation into an equation of motion. Because we are only interested in the long-time effect, this is easily done provided the drift coefficients are derivatives of a potential (M-Tehrani and Mandel 1978). The resulting Schrödinger-type equation is then solvable by the multi-dimensional WKB method. When the drift coefficients are not derivable from a potential, an expression for the FPT can be obtained by WKB expansion but in a completely different approach (Matkowsky and Schuss 1981).

In this paper, we discuss the case in which the drift coefficients are derivatives of a potential. We first outline the method (Banks and Bender 1973) of tunnelling along a curved MPTP in § 2. In § 3, we study a model potential for which the problem can be solved analytically. In § 4, we discuss briefly a realistic problem of a bistable two-mode laser for which analytical solutions cannot be found. Numerical integration along the path specified by the minimum potential is carried out to obtain the mean switching time. The validity of this method and comparison with the existing theories are discussed.

2. Tunnelling along curved MPTP

We consider the two-dimensional Schrödinger equation

$$[-(\partial^2/\partial x^2+\partial^2/\partial y^2)+V]\psi=E\psi. \tag{1}$$

The lowest order WKB approximation gives the wavefunction

$$\psi=A\exp\left(-\int(V-E)^{1/2}\,\mathrm{d}s\right) \tag{2}$$

where s is the arc length of the path. Suppose that the vector $\boldsymbol{\phi}=(x,y)$ represents the curved MPTP, we can determine it by minimising the path integral in (2) with the constraint

$$(\mathrm{d}\boldsymbol{\phi}/\mathrm{d}s)^2=1. \tag{3}$$

Following the procedure given by Banks and Bender (1973), we find the Euler-Lagrange equation

$$2(V-E)\frac{\mathrm{d}^2\boldsymbol{\phi}}{\mathrm{d}s^2}+\frac{\mathrm{d}\boldsymbol{\phi}}{\mathrm{d}s}\left(\frac{\mathrm{d}\boldsymbol{\phi}}{\mathrm{d}s}\cdot\nabla V\right)=\nabla V \tag{4}$$

where $\nabla V=\partial V/\partial\boldsymbol{\phi}$. Equation (4) is solved by the perturbation method. The unperturbed MPTP is assumed to be a straight line and is formally represented by the vector $\boldsymbol{\phi}_0$. The derivative of $\boldsymbol{\phi}_0$ is a constant vector parallel to the straight MPTP,

$$\boldsymbol{\phi}_0' = \mathrm{d}\boldsymbol{\phi}_0/\mathrm{d}s. \tag{5}$$

For the purpose of perturbation calculation, we set

$$V = V_0 + \eta V_1$$

and

$$\boldsymbol{\phi} = \boldsymbol{\phi}_0 + \eta\boldsymbol{\phi}_1 + \eta^2\boldsymbol{\phi}_2 + \dots \tag{6}$$

where the perturbation parameter η satisfies $|\eta| < 1$. From (3) and (6) we have

$$\boldsymbol{\phi}_0' \cdot \boldsymbol{\phi}_1' = 0 \tag{7}$$

which implies that

$$\boldsymbol{\phi}_0' \cdot \boldsymbol{\phi}_1 = \text{constant} = 0 \tag{8}$$

where we have taken the constant to be zero without loss of generality. Now we expand the potentials V_0 and V_1 around the unperturbed path $\boldsymbol{\phi}_0$

$$V_{0,1}(\boldsymbol{\phi}) = \sum_{n=0}^{\infty} \frac{1}{n!} \left\{ \left[\left(\sum_{m=1}^{\infty} \eta^m \boldsymbol{\phi}_m \right) \cdot \nabla \right]^n V_{0,1}(\boldsymbol{\phi}_0) \right\}. \tag{9}$$

Substituting (5) and (6) into (4), we obtain an equation for $V_0(\boldsymbol{\phi}_0)$

$$\nabla V_0(\boldsymbol{\phi}_0(s)) = \boldsymbol{\phi}_0' \frac{\mathrm{d}}{\mathrm{d}s} V_0(\boldsymbol{\phi}_0). \tag{10}$$

With the relation (8) we then have

$$\boldsymbol{\phi}_1 \cdot \nabla V_0 = 0. \tag{11}$$

A second-order differential equation for $\boldsymbol{\phi}_1$ then follows from (4):

$$2(V_0 - E)(\boldsymbol{\delta} \cdot \boldsymbol{\phi}_1)'' + \frac{\mathrm{d}V_0}{\mathrm{d}s}(\boldsymbol{\delta} \cdot \boldsymbol{\phi}_1)' = \boldsymbol{\delta} \cdot \nabla V_1 \tag{12}$$

where $\boldsymbol{\delta}$ is a constant vector normal to $\boldsymbol{\phi}_0'$. It may be pointed out here that (12) differs from (3.16) of Banks and Bender (1973) by neglecting one term which should vanish identically because of (11). This vanishing term can be split into four separate terms; one of them is kept in their paper so that their equation (4.6) can be transformed to an inhomogeneous Legendre equation.

The rate of transition is, according to Bender and Wu (1973),

$$\Gamma = \int_{S_V} \boldsymbol{J} \cdot \mathrm{d}\boldsymbol{S} \left(\int \psi^* \psi \, \mathrm{d}V \right)^{-1} \tag{13}$$

where $\boldsymbol{J}$ is the probability current and S is the boundary of volume V. Using the WKB wavefunction (2) with proper normalisation, we can express, apart from the slowly varying normalisation factor,

$$\Gamma \sim \exp\left(-2\int_{s_0}^{s_1} (V-E)^{1/2}\,\mathrm{d}s\right) \tag{14}$$

which dominates the behaviour of the rate expression. The integral is taken along the path of penetration through the barrier region and the integration limits s_0 and s_1 are the nearby and the distant turning points, respectively. We now proceed to calculate (14) up to the second order in η. We have, from (9) and (11),

$$V = V_0 + \eta V_1 + \eta^2[\boldsymbol{\phi}_2 \cdot \nabla V_0 + \tfrac{1}{2}(\boldsymbol{\phi}_1 \cdot \nabla)^2 V_0 + \boldsymbol{\phi}_1 \cdot \nabla V_1]. \tag{15}$$

It can then be shown, after some manipulation of integrals, that

$$\begin{aligned}\ln\Gamma &= -2\int_{s_0}^{s_1} \{V_0 + \eta V_1 - E \\ &\quad + \eta^2[\boldsymbol{\phi}_2 \cdot \nabla V_0 + \tfrac{1}{2}(\boldsymbol{\phi}_1 \cdot \nabla)^2 V_0 + \boldsymbol{\phi}_1 \cdot \nabla V_1]\}^{1/2}\,\mathrm{d}s \\ &\approx -2\int_{s_0}^{s_1} (V_0 + \eta V_1 - E)^{1/2}\,\mathrm{d}s - \eta^2 \int_{\bar{s}_0}^{\bar{s}_1} \frac{\mathrm{d}s}{2}\,\frac{\boldsymbol{\phi}_1 \cdot \nabla V_1}{(V_0 - E)^{1/2}}\end{aligned} \tag{16}$$

where the integration limits $\bar{s}_0$ and $\bar{s}_1$ are the zeros of $V_0 - E$.

3. Switching between double potential wells

Consider the model potential written in dimensionless form

$$V = -\tfrac{1}{4}(x^2+y^2) + (1/16a^2)(x^4+y^4+6x^2y^2) + (\eta/4a^2)x^2y^2 = V_0 + \eta V_1 \tag{17}$$

where a is a parameter and $|\eta| < 1$. As shown in figure 1, this potential has two minima at $(x, y) = (\sqrt{2}a, 0)$ and $(x, y) = (0, \sqrt{2}a)$ and one saddle point at $(x, y) = (a/(2+\eta)^{1/2}, a/(2+\eta)^{1/2})$. Examples of such a double well potential can be found, for instance, in the movement of defects in solids (Vineyard 1957), the thermally activated random processes (Landauer and Swanson 1961), the optical bistability

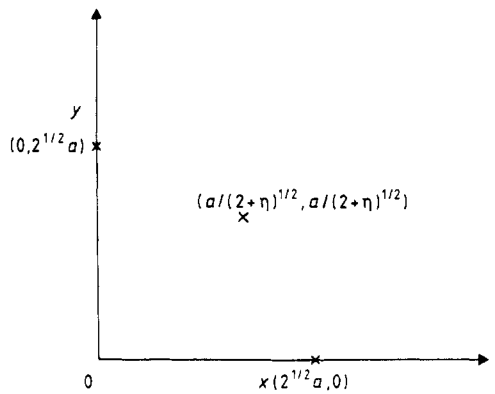

Figure 1. Positions of the potential extrema in the xy plane.

(Bonifacio *et al* 1981) and the bistable two-mode laser (M-Tehrani and Mandel 1978). When the perturbation parameter $\eta = 0$, the MPTP is a straight line joining the two minima and is represented by

$$\boldsymbol{\phi}_0 = (2a - s, s)/\sqrt{2} = (a/\sqrt{2})(2 - r, r) \tag{18}$$

where we have introduced the new variable $r = s/a$ for convenience. Thus

$$\boldsymbol{\phi}_0' = \mathrm{d}\boldsymbol{\phi}_0/\mathrm{d}s = (-1, 1)/\sqrt{2} \tag{19}$$

it then follows from (8) and (19) that

$$\boldsymbol{\phi}_1 = a(\varphi_1, \varphi_1)/\sqrt{2} \tag{20}$$

and the constant vector $\boldsymbol{\delta} = (1, 1)/\sqrt{2}$. Hence

$$(\boldsymbol{\delta} \cdot \boldsymbol{\phi}_1)' = \mathrm{d}\varphi_1/\mathrm{d}r \tag{21}$$

$$(\boldsymbol{\delta} \cdot \boldsymbol{\phi}_1)'' = a^{-1}\, \mathrm{d}^2\varphi_1/\mathrm{d}r^2. \tag{22}$$

We need the potential V_0 and ∇V_1 along the path and they are given by

$$V_0 = -\tfrac{1}{4}a^2 - \tfrac{1}{8}a^{-2}(-4a^2s^2 + 4as^3 - s^4) = -\tfrac{1}{4}a^2 + \tfrac{1}{8}a^2r^2(r-2)^2 \tag{23}$$

and

$$\boldsymbol{\delta} \cdot \nabla V_1 = \frac{1}{\sqrt{2}}(1, 1) \cdot \frac{s(2a-s)}{4\sqrt{2}a^2}(s, 2a - s) = ar(2-r)/4. \tag{24}$$

Plugging (21)-(24) into (13), we find

$$\frac{\mathrm{d}^2\varphi_1}{\mathrm{d}r^2} + Q\frac{\mathrm{d}\varphi_1}{\mathrm{d}r} = R \tag{25}$$

where we have defined

$$Q = \frac{1}{2(V_0 - E)}\frac{\mathrm{d}V_0}{\mathrm{d}r} \tag{26}$$

$$R = a^2r(2-r)/8(V_0 - E). \tag{27}$$

Since the MPTP is symmetric with respect to the line joining the origin and the saddle point, we have

$$\mathrm{d}\varphi_1/\mathrm{d}r|_{r=1} = 0. \tag{28}$$

Furthermore, since the MPTP passes through the saddle point, we have

$$\varphi_1|_{r=1} = \left[\left(\frac{2}{2+\eta}\right)^{1/2} - 1\right]\eta^{-1}. \tag{29}$$

Integrating (25) once we obtain

$$\frac{\mathrm{d}\varphi_1}{\mathrm{d}r} = \exp\left(-\int_1^r Q\,\mathrm{d}r\right)\int_1^r R\left[\exp\left(\int_1^r Q\,\mathrm{d}r'\right)\right]\mathrm{d}r. \tag{30}$$

With the boundary condition (29), we can write

$$\varphi_1 = \int_1^r \frac{\mathrm{d}\varphi_1}{\mathrm{d}r}\mathrm{d}r + \frac{1}{\eta}\left[\left(\frac{2}{2+\eta}\right)^{1/2} - 1\right]. \tag{31}$$

If the energy is very close to the well minimum, namely $E \approx -a^2/4$, then the rate equation (14) can be derived analytically. Since $\int Q\,\mathrm{d}r = \ln(V_0 - E)^{1/2}$, we find from

(26), (30) and (31), after a little algebra, that

$$\varphi_1 = -\tfrac{1}{2}\ln[r(2-r)] + \frac{1}{\eta}\left[\left(\frac{2}{\eta+2}\right)^{1/2} - 1\right]. \tag{32}$$

To calculate Γ, we first note that

$$\boldsymbol{\phi}_1 \cdot \nabla V_1 = \tfrac{1}{4}a^2 r(2-r)\varphi_1. \tag{33}$$

Combining (32) and (33), and substituting in (16), we obtain by direct integration

$$\ln\Gamma \sim -a^2\left\{\tfrac{2}{3}(2+\eta)^{1/2} + \eta\left[\left(\frac{1}{2+\eta}\right)^{1/2} - \frac{1}{\sqrt{2}}\right]\right\}. \tag{34}$$

It has been found (Wang *et al* 1985) that the most probable path is practically the same as that characterised by the minimum potential as we shall discuss in § 4. It is therefore possible to carry out the integral in (14) numerically by taking the minimum of the potential at every point along the path. In figure 2, we plot $\ln\Gamma$ as a function of η calculated by different methods. It is observed that the assumption of a straight path is not at all reliable, but (34) yields quite accurate results. The deviation occurring near $|\eta| \sim 1$ is understandable and can be corrected by higher-order corrections.

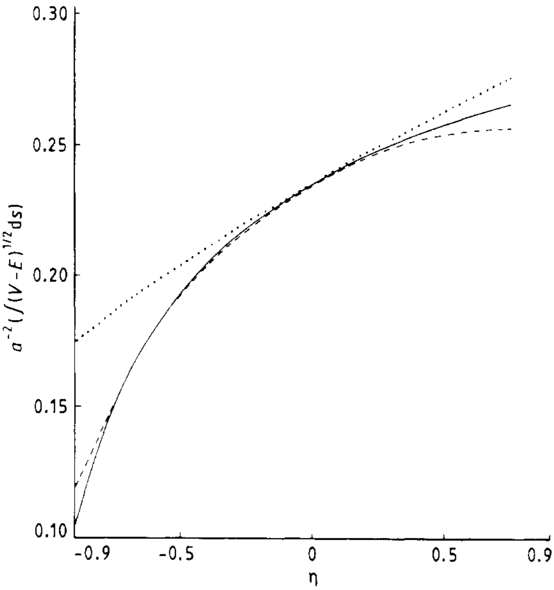

Figure 2. Comparison of the rate calculated along different paths. The full curve is along the path corresponding to minimum potential, the broken curve is from (34) and the dotted curve is along the straight path.

4. Bistability switching of a two-mode laser

The measured mean switching time of the spontaneous mode switching in a two-mode laser seems to be qualitatively accounted for by the one-dimensional FPT calculation (Roy *et al* 1980) based on the approximation that is valid for large pump parameter a. In the large a region, however, the theoretical curve grows too fast as a increases. This may be understandable because a is not large under the experimental conditions.

It has been shown (M-Tehrani and Mandel 1978) that the Fokker–Planck equation describing a two-mode laser can be transformed to a four-dimensional Schrödinger-type equation in which the potential energy is

$$V=\sum_{i=1}^{2}\left\{-\tfrac{1}{2}\left(\frac{\partial^2 U}{\partial x_i^2}+\frac{\partial^2 U}{\partial y_i^2}\right)\right\}+\tfrac{1}{4}\left[\left(\frac{\partial U}{\partial x_i}\right)^2+\left(\frac{\partial U}{\partial y_i}\right)^2\right] \tag{35}$$

where

$$U=-\tfrac{1}{2}a_1(x_1^2+y_1^2)-\tfrac{1}{2}a_2(x_2^2+y_2^2)+\tfrac{1}{4}[(x_1^2+y_1^2)^2+(x_2^2+y_2^2)^2+2\xi(x_1^2+y_1^2)(x_2^2+y_2^2)]. \tag{36}$$

In equation (36), a_1 and a_2 stand for the pump parameters of the two modes and ξ denotes the coupling constant between the two modes. This potential is much more complicated than the model potential studied above. An attempt has been made to solve the MPTP analytically for this potential (Wang *et al* 1986). It turns out that ϕ_1 is expressed as an integral with integrand involving various kinds of incomplete elliptic integrals and Jacobi elliptic integrals. A detailed account of this investigation will be published elsewhere and here we shall report some of the findings.

In our numerical study we find that the MPTP, to a good degree of accuracy, is the same as the path characterised by the minimum of the function $(V-E)^{1/2}$ for $1 \leqslant \xi \leqslant 5$ and in the actual experiment $\xi \approx 2$. This discovery makes it possible for the first time to calculate the mean switching time that is valid throughout the whole range of the pump parameter. Thus the mean switching time is, according to (13) and (14),

$$T=\left(\int \psi^*\psi \,\mathrm{d}x\right)\exp\left(2\int (V-E)_{\min}^{1/2}\,\mathrm{d}s\right) \tag{37}$$

where the normalisation integral serves as the multiplying frequency factor and the dominant exponential factor is the inverse of the barrier penetration integral. It is

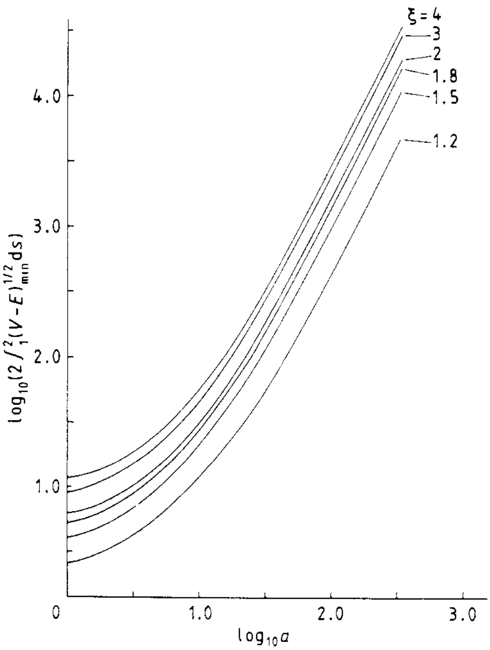

Figure 3. a dependence of the exponent from WKB method with curved MPTP.

found that in the large a limit our numerical results agree completely with the analytical large a formula mentioned before. To study the behaviour of T more carefully we plot in figure 3 the numerical results of $\log_{10}[2(V-E)^{1/2}_{\min}\,ds]$ against $\log_{10} a$ for several values of ξ. It is observed that the slope starts with ~0.4, increases gradually with increasing a, and becomes about unity around $a \sim 10$ where measurements are performed. It does not reach the limiting value of 2 until $a \gtrsim 150$ according to our computation. Therefore extrapolation of the large a formula to the experimental range tends to overestimate the mean switching time.

To check the method of calculation, we have also computed (Wang *et al* 1986) the FPT from the generalised Kramer method (Vineyard 1957, Landauer and Swanson 1961) by integrating along the path specified by minimum potential. The results are completely consistent with the WKB calculation. Finally, we remark that numerical integrations along the straight path have also been carried out for both the WKB and generalised Kramer method. In both cases the resulting mean switching time grows much faster than those from the curved MPTP corresponding to minimum potential.

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