Coherent and incoherent tunneling in asymmetric double-well potentials

A. Ranfagni,[1] I. Cacciari,[1] M. A. Vitali,[2] G. Viliani,[3] P. Moretti,[4] and R. Ruggeri[4]
[1]*Istituto di Fisica Applicata "Nello Carrara", Consiglio Nazionale delle Ricerche, Via Madonna del Piano 10, 50019 Sesto Fiorentino, Italy*
[2]*Scuola di Specializzazione in Ottica dell'Universita' di Firenze, Firenze, Italy*
[3]*Dipartimento di Fisica, Universitá di Trento, 38050 Povo, Trento, Italy*
[4]*Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, Sezione di Firenze, Firenze, Italy*
(Received 18 April 2006; published 13 July 2006)

The determination of the time scale for coherent and incoherent tunneling in asymmetric double-well potentials is reconsidered according to the instanton-bounce method. In particular, by making use of Feynman's transition elements, a different, relatively simpler approach to this problem, with respect to conventional quantum-mechanical treatments, is obtained.

DOI: 10.1103/PhysRevA.74.014102 PACS number(s): 03.65.Xp

The problem of tunneling processes in the presence of dissipation might have been considered as basically resolved in the 1980s [1], even though new contributions to the subject continued to appear in the literature ([2,3]). However, more recently, this subject has become topical again, especially in relation to the duration of the tunneling process, i.e., a quantity that has been interpreted in a variety of manners [4], and that will be here reconsidered in "closed" systems, such as those consisting of asymmetric double-well potentials. The latter provide a classical picture with applications in a variety of physical cases, ranging from field theory, to solid-state and chemical physics, to biological systems.

The purpose of the present work is to perform a relatively simple analysis of the tunneling-duration scales, based on a path-integral approach and making use, in particular, of the concept of transition elements as introduced by Feynman [5]. The results will be compared to those previously obtained in the framework of conventional quantum mechanics [6,7].

First, let us briefly summarize the results of the latter procedure [7]. For a system consisting of two coupled oscillators, whose energy levels are displaced by an amount σ, the average position $\langle x(t)\rangle$ was evaluated by computing the expectation value:

$$\langle x(t)\rangle = \int \psi^*(x,t)x\psi(x,t)dx. \tag{1}$$

The wave function $\psi(x,t)$ is given by

$$\psi(x,t) = \int G(x,t;x_0,t_0)\psi(x_0,t_0)dx, \tag{2}$$

where $\psi(x_0,t_0)$ is the initial wave function (the system was supposed to be initially prepared in the upper well), and the propagator can be expressed as

$$G(x,t;x_0,t_0) = \sum_{n=0,1,\ldots,} \psi_n(x)\psi_n^*(x_0)\exp\{-iE_nt/\hbar\}. \tag{3}$$

Irreversible decay towards the lower minimum was obtained by including a small imaginary term in the energy eigenvalue, $E_n \to E_n - i\varepsilon_n$. The result of this analysis is given by Eq. (15) in Ref. [7] which, though neglecting the effects of squeezing in the initial state, leads to a rather complex expression [8] that can be qualitatively described as follows [9].

The relaxation trajectories given by Eq. (1) follow on average an irreversible exponential decay (incoherent tunneling) whose decay constant γ can be related to ε_n; superimposed onto the averaged coordinate there is a damped fast oscillation (coherent tunneling) of amplitude $\sim\delta/\sigma$ and period $T=h/(2\delta+\sigma)$; here δ is the energy shift due to tunneling. The period can become comparable to that of oscillations inside the initial well, say $2\pi/\Omega$. Some results are reported in Fig. 3 of Ref. [8] for a two-level system, and show that when $\sigma \gg \delta$, it is natural to assume that the delay time due to tunneling is of the order of ε_1^{-1}. The results obtained in this way are very different (in some real systems, by orders of magnitude) from barrier crossing-time evaluations which, for $\sigma \gtrsim \delta$, can be identified with the half-period $T/2$, and thus are in a time scale comparable to that of fast oscillations. For example, if Ω is of the order of 10^{12} s^{-1}, the relative time unit would be picoseconds, but the time scale of the decay time can be exceedingly longer, and reach in some cases milliseconds [8].

In spite of its intrinsic complexity, the approach outlined above should be considered as a merely phenomenological one, since the dissipative constants ε_n, the tunneling energy shift δ, and the asymmetry constant σ have all been treated as free parameters. In what follows, we abandon this method, and seek for an alternative solution to the problem. The adoption of the instanton-bounce method [10] in the framework of path integrals allows for a relatively simpler approach, which also supplies detailed expressions for the involved quantities characterizing the process.

In order to derive observable quantities, such as the energy shift δ and the decay rate γ, we need to compare the propagator as given by functional integration, with the corresponding expression of Eq. (3) written for imaginary time $\tau=it$. For a two-level system, this turns out to be

$$G(0,\tau;0,-\tau) = G_0 e^{\sigma\tau/\hbar}\left[\cosh\left(\frac{\sigma+2\delta}{\hbar}\tau\right) - \cos 2\phi \sinh\left(\frac{\sigma+2\delta}{\hbar}\tau\right)\right], \tag{4}$$

where $G_0=(M\Omega/\pi\hbar)^{1/2}e^{-\Omega\tau}$, $\cos 2\phi=\sigma/(2\delta+\sigma)$, and the

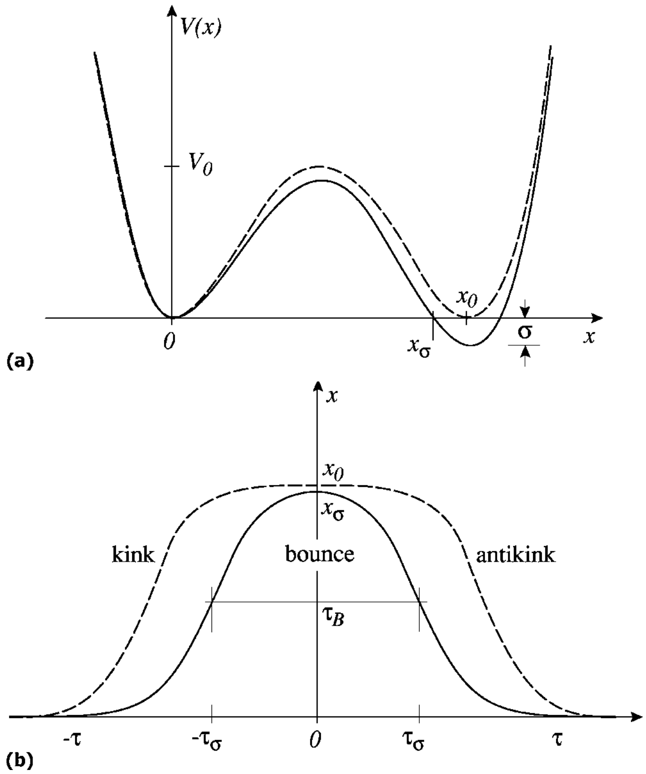

FIG. 1. (a): Potential functions for tunneling processes starting from the upper well at $x=0$. Asymmetric double-well potential, continuous line; perfectly symmetric case, dashed line. (b) Classical trajectories of tunneling events starting from the initial well at $-\tau$ and ending in the same well at $+\tau$. Symmetric kink and antikink, dashed line; bounce path as a sum of an asymmetric kink and antikink, continuous line, with indication of $\pm\tau_\sigma$.

origin of coordinates ($x=0$) is set in the upper minimum. For $2\delta \ll \sigma$, Eq. (4) can be reasonably approximated as

$$G_{0,1} \simeq G_0\left(1+\frac{2\delta\tau}{\hbar} f e^{\sigma\tau/\hbar}\right), \tag{5}$$

where f is a numerical factor of the order of unity ($f \lesssim 1$). The subscript 0,1 means that we are considering contributions relative to zero ($\bar{x}(\tau)=0$) and single bounces, giving the unity and the linear-exponential term within brackets, respectively. In the opposite limit, $2\delta \gg \sigma$, Eq. (4) can be put in the form

$$G_{0,2} = \simeq G_0\left[1+\frac{f}{2}\left(\frac{2\delta\tau}{\hbar}\right)^2\right], \tag{6}$$

where the subscript 0,2 means that we are considering contributions from $\bar{x}(\tau)=0$, and double-tunneling (i.e. kink-plus-antikink) events, with a quadratic time dependence.

For an asymmetric double-well potential, written as [see Fig. 1(a)]

$$V(x) = kx^2\left(1-\frac{x}{x_0}\right)^2 - \sigma\frac{x}{x_0}, \tag{7}$$

where $k=M\Omega^2$, the classical path from $x=0$ to $x_\sigma \lesssim x_0$, and back, for moderate asymmetry can approximately be expressed as [see Fig. 1(b)]

$$\bar{x}(\tau) = \frac{x_0}{2}\left[1 \pm \tanh\frac{\Omega}{2}(\tau \pm \tau_\sigma)\right]. \tag{8}$$

In (8), the plus sign holds for $\tau<0$, and the minus sign for $\sigma>0$, and $\tau_\sigma = 1/2\Omega \ln(16V_0/\sigma)$, with $V_0 = kx_0^2/32$. The propagator for the bounce path of Fig. 1(b), obtained by a classical variational technique [11], is given by

$$G_1 = 2\Omega\tau G_0\left(\frac{6S_0}{\pi\hbar}\right)^{1/2}\left(\frac{16V_0}{\sigma}\right)^{1/2} e^{-2S_\sigma/\hbar}, \tag{9}$$

where

$$S_\sigma = S_0\left\{1-\frac{3\sigma}{16V_0}\left[1+\ln\left(\frac{16V_0}{\sigma}\right)^{1/2}\right]\right\}, \tag{10}$$

with $S_0 = M\Omega x_0^2/6$, is the action for one "kink" in the asymmetric case: for $\sigma=0$ we have $S_\sigma = S_0$. By comparing Eq. (9) with G_1 in Eq. (5) and assuming $f=1$, we obtain the energy shift as

$$\delta \simeq \hbar\Omega\left(\frac{6S_0}{\pi\hbar}\right)^{1/2}\left(\frac{16V_0}{\sigma}\right)^{1/2} e^{-2S_0/\hbar}. \tag{11}$$

since, see below, $2S_\sigma \simeq 2S_0 - \sigma\tau$. By a similar procedure, we find that the propagator for a kink-plus-antikink process, for $\sigma=0$ is given by

$$G_2 = \frac{1}{2}\Omega^2\tau^2 G_0\left(\frac{24S_0}{\pi\hbar}\right)e^{-2S_0/\hbar} \tag{12}$$

and, by comparing with the expression of G_2 in Eq. (6) for $f=1$, we obtain the well-known result for the tunneling splitting $\Delta E = 2\delta$ given by [12]

$$\Delta E = \hbar\Omega\left(\frac{24S_0}{\pi\hbar}\right)^{1/2} e^{-S_0/\hbar}. \tag{13}$$

We are now in the position for evaluating the transition element of the trajectory, namely $\langle x(\tau)\rangle_S$, which is a suitably weighted average where the weighting function is $\exp(-S/\hbar)$. When the action is (or can be reasonably approximated by) a quadratic form, the following relationship worth noting can be used [13]:

$$\langle x(\tau)\rangle_S \simeq \bar{x}(\tau) G(0,\tau;0,-\tau), \tag{14}$$

where $\bar{x}(\tau)$ is the classical trajectory which, for moderate asymmetry, is given by Eq. (8). More precisely, the maximum amplitude is not x_0, but is reduced as

$$x_B \equiv x_\sigma \simeq x_0\left[1-\left(\frac{\sigma}{16V_0}\right)^{1/2}\right]. \tag{15}$$

When Eq. (14) is applied to a bounce process, we have for the maximum bounce amplitude an expression of the type $\langle x_M\rangle_S \propto x_B \exp(-2S_\sigma/\hbar)$. More properly, Eq. (14) can be

TABLE I. Energy shift Eq. (11), half period $\Omega\tau_B$, bounce amplitude Eq. (15), oscillation amplitude Eq. (17), calculated (even beyond the limit of validity) as a function of the asymmetry $\sigma/16V_0=\sigma/(3\pi\hbar\Omega)$, for $S_0=\pi\hbar$. For $\sigma=0$ the energy shift (tunneling splitting) is given by Eq. (13). The data of the last column refer to the amplitude as given by the quantum-mechanical approach of Ref. [8].

$\sigma/16V_0$	$2\delta/\hbar\Omega$ $(S_0=\pi\hbar)$	$\Omega\tau_B$	$2\delta\tau/\hbar$ $(\tau=2\tau_B)$	x_B/x_0	$1-\langle x_M\rangle/x_0$	δ/σ
0	0.213			1	1	
0.005	0.129	5.3	0.69	0.93	0.64	1.37
0.01	0.091	4.6	0.42	0.90	0.38	0.48
0.015	0.075	4.2	0.31	0.88	0.27	0.26
0.02	0.065	3.9	0.25	0.86	0.22	0.17
0.025	0.058	3.7	0.21	0.84	0.18	0.12
0.03	0.053	3.5	0.18	0.83	0.15	0.09

adapted to a bounce process by taking into account, besides the bounce trajectory $\bar{x}_1(\tau)$, also the other solution of the classical motion, that is the path of permanence in the initial minimum $\bar{x}_0(\tau)\equiv 0$. By applying Eq. (14) to each classical path, for $2\delta\ll\sigma$ we have

$$\langle x(\tau)\rangle_S = N[\bar{x}_1(\tau)G_1+\bar{x}_0(\tau)G_0], \tag{16}$$

where N is a suitable normalization constant, and G_0 and G_1 are the relative propagators. By changing the origin of the spatial coordinate, i.e., $x\to x_0-x$, $\bar{x}_0(\tau=0)/x_0=1$, the relative averaged value must be conserved equal to 1. This means that $N=G_0^{-1}$; therefore, Eq. (16) for the averaged maximum amplitude becomes

$$\langle x_M\rangle_S/x_0 = 1-\frac{x_B}{x_0}\frac{G_1}{G_0}\simeq 1-\frac{x_B}{x_0}\left(\frac{2\delta\tau}{\hbar}\right), \tag{17}$$

where in the second member we have assumed $\exp(\sigma\tau/\hbar)\gtrsim 1$; δ is given by Eq. (11) and τ can be reasonably identified with $2\tau_\sigma$ [see Fig. 1(b)]. Likewise, for the case $\sigma\ll 2\delta$, we find that Eq. (17) is modified as follows:

$$\langle x_M\rangle_S/x_0 \simeq 1-\frac{x_B}{2x_0}\left(\frac{2\delta\tau}{\hbar}\right)^2, \tag{18}$$

where δ as given by Eq. (11) in this case can be considered only as a rough estimate.

The results of Eqs. (17) and (18) can be interpreted as representing an oscillating, persisting behavior whose amplitude (given by $1-\langle x_M\rangle_S/x_0$) decreases with increasing σ. Its half period is approximately given by $2\tau_\sigma$ [actually, $2\sigma\tau_\sigma=\ln(16V_0/\sigma)$, for $16V_0/\sigma=20\div 50$ turns out to be $3.0\div 3.9$, thus comparable with π]; this oscillation takes place below a constant value equal to x_0 (see Table I).

The remaining problem we are faced with is the evaluation of the damping constant resulting from dissipative effects due to the coupling with a thermal bath. In order to perform this evaluation, we need to consider two concomitant and opposite effects: one is the *decrease* of the action due to the bias σ, while the other is the *increment* of the action properly due to dissipation. It is just the combination of these two effects which causes the irreversibility of the process [14]. According to Eq. (10), for moderate asymmetry such that we can assume $\ln(16V_0/\sigma)\gg 1$, the decrease of the action for a bounce path turns out to be $\Delta S_\sigma=2(S_0-S_\sigma)\simeq\sigma\tau_B$, where τ_B can be identified with $2\tau_\sigma$ [see Fig. 1(b)].

The increase of the bounce action due to dissipation is given by [15]

$$\Delta S_\alpha = 2\alpha\hbar\ln|\Omega\tau_B| + \text{const}, \tag{19}$$

where $2\alpha\hbar=\eta x_0^2/\pi$, and η is the usual notation for the damping coefficient [11]. Therefore, neglecting the constant term in (19), we have that the total bounce-action variation with respect to the case $\sigma=0$ is given by

$$-\Delta S/\hbar = -2\alpha\ln|\Omega\tau_B| + \sigma\tau_B/\hbar; \tag{20}$$

a result, this latter, which holds for weakly damped systems. In order to obtain the decay rate γ, we must consider the contribution to the free energy of the quantum fluctuations around the bounce path; these are determined by the integral [7]

$$I(\sigma,\alpha) = \int \exp(-\Delta S/\hbar)d\Omega\tau_B. \tag{21}$$

From the stationarity condition, we have that the main contribution to this integral arises from $\tau_B=2\alpha/\sigma$, which is a minimum of Eq. (20), and the integral might be evaluated according to the saddle-point method by properly selecting the steepest-descent path: in this case, along the imaginary axis of the complex variable $\Omega\tau_B$. However, for the action variation (20), the integral can be evaluated exactly by changing the variable to $z=\sigma\tau_B$, and the result is

$$I(\sigma,\alpha) = \frac{2\pi i}{\Gamma(2\alpha)}\left(\frac{\sigma}{\hbar\Omega}\right)^{2\alpha-1}. \tag{22}$$

Now, recovering the form of the propagator for the symmetric case, Eq. (12), we have that the decay rate γ is given by [1,16]

$$\gamma = \left(\frac{\Delta\omega_0}{2}\right)^2\left|\frac{\text{Im}\, I}{\Omega}\right| = \frac{\pi}{2}\frac{\Delta\omega_0^2}{\Omega}\frac{1}{\Gamma(2\alpha)}\left(\frac{\sigma}{\hbar\Omega}\right)^{2\alpha-1}, \tag{23}$$

where $\Delta\omega_0=\Delta E/\hbar$ is the tunneling frequency relative to the symmetric case. Making use of the Γ-function property

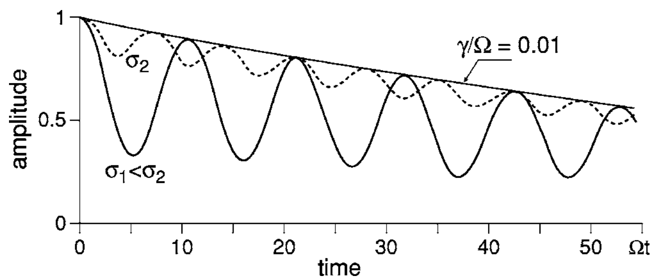

FIG. 2. Two examples of relaxation trajectory represented by a sequence of attenuated bounces, the duration of each one being $2\Omega\tau_B$. The normalized amplitude is computed through Eq. (26), for values of the involved (dimensionless) parameters as $\sigma/16V_0=0.005$, $2\delta/\hbar\Omega=0.13$, continuous curve; $\sigma/16V_0=0.03$, $2\delta/\hbar\Omega=0.053$, dotted curve; and indicated value of γ/Ω.

$\Gamma(z+1)=z\Gamma(z)$, in the case $2\alpha\ll 1$ we obtain the following approximate result:

$$\gamma \simeq \Delta\omega_0^2 \frac{\pi\alpha\hbar}{\sigma} = \Delta\omega_0^2 \eta x_0^2/2\sigma. \tag{24}$$

In order to obtain the damped behavior of the averaged trajectory, we need to go back to a real-time dependence of the propagator like in Eq. (3). Taking into account the imaginary-energy correction to the energy shift, given by $\mathrm{Im}\,\delta=\gamma\hbar/2$, so that $\delta\to\delta+i\gamma\hbar/2$, and remembering that $\tau=it$, the $G_{0,1}$ propagator [still for $f\exp(\sigma\tau/\hbar)\approx 1$] becomes

$$G_{0,1} \simeq G_0\left(1+\frac{2\delta\tau}{\hbar}\right)e^{-\gamma t}. \tag{25}$$

In a similar way, for the propagator $G_{0,2}$ we can proceed by including the imaginary correction to δ, but we obtain a more complex expression which only in a selected range of values of $2\delta\tau$ can be put in a form similar to (25). By adopting these results, we can modify Eqs. (17) and (18), with $\tau=\tau_B$, as follows, for $\delta\ll\sigma$:

$$\langle x_M\rangle_S/x_0 \simeq \left[1-\frac{x_B}{x_0}\frac{2\delta\tau_B}{\hbar}\right]e^{-\gamma t}, \tag{26}$$

and (but less properly) for $\sigma\ll\delta$:

$$\langle x_M\rangle_S/x_0 \simeq \left[1-\frac{x_B}{2x_0}\left(\frac{2\delta\tau_B}{\hbar}\right)^2\right]e^{-\gamma t}. \tag{27}$$

Some examples of computed relaxation trajectories, obtained as a sequence of attenuated bounce paths (considered not merely as mathematical artifices but rather as real physical processes [17]), are reported in Fig. 2. They clearly show both behaviors, namely the oscillating part (coherent tunneling) and the irreversible decay (incoherent tunneling), whose relative importance strongly depends on the asymmetry of the potential. In this way, we recover an overall behavior similar to the one already obtained by conventional quantum-mechanical approaches [7–9], see Table I. In particular, it is quite evident that, with increasing σ, the fast oscillation tends to become less important and the exponential decay, with time constant γ^{-1}, becomes dominant for characterizing the tunneling time scale.

[1] See, for example, the exhaustive review by A. J. Leggett *et al.*, Rev. Mod. Phys. **59**, 1 (1987).
[2] K. Fujikawa, S. Iso, M. Sasaki, and H. Suzuki, Phys. Rev. Lett. **68**, 1093 (1992).
[3] A. Agresti, M. Barilli, A. Ranfagni, R. Ruggeri, and C. Susini, Phys. Rev. E **65**, 066616 (2002).
[4] N. Yamada, Phys. Rev. Lett. **93**, 170401 (2004), and references therein, for the cases of tunneling in "pen" systems.
[5] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), Chap. 7.
[6] D. Mugnai, A. Ranfagni, M. Montagna, O. Pilla, G. Viliani, and M. Cetica, Phys. Rev. A **38**, 2182 (1988).
[7] D. Mugnai, A. Ranfagni, M. Montagna, O. Pilla, and G. Viliani, Phys. Rev. A **40**, 3397 (1989).
[8] A. Ranfagni *et al.*, Phys. Rev. B **72**, 012101 (2005).
[9] I. Cacciari and P. Moretti Phys. Lett. A (to be published).
[10] S. Coleman, in *The Whys of Subnuclear Physics*, edited by A. Zichichi (Plenum, New York, 1979).
[11] A. Ranfagni, D. Mugnai, P. Moretti, and M. Cetica, *Trajectories and Rays: The Path-summation in Quantum Mechnanics and Optics* (World Scientific, Singapore, 1990).
[12] E. Gildener and A. Patrascioiu, Phys. Rev. D **16**, 423 (1977).
[13] See *Quantum Mechanics and Path Integrals* (Ref. [5]), p. 179, Problem 7-7.
[14] J. P. Sethna, Phys. Rev. B **25**, 5050 (1982).
[15] See *Trajectories and Rays: The Path-summation in Quantum Mechnanics and Optics* (Ref. [11]), p. 144.
[16] U. Weiss, H. Grabert, P. Hanggy, and P. Riseborough, Phys. Rev. B **35**, 9535 (1987).
[17] D. Mugnai and A. Ranfagni, Europhys. Lett. **6**, 1 (1988); Nuovo Cimento D **14D**, 541 (1992).