Two-exponential decay from a double-well potential

S. A. Gurvitz
Department of Physics, The Weizmann Institute of Science, Rehovot 76100, Israel

M. S. Marinov*
The Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem 91904, Israel
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We consider tunneling from a double-well potential to the continuum. Simple expressions are found for the decay rate. For a special configuration of the potential, where the energy levels in two wells are coinciding, the decay time dependence reveals a peculiar quantum-interference behavior. A possibility for observing these effects is discussed.

INTRODUCTION

Considerable attention has been recently paid to quantum-mechanical effects at the macroscopic level.[1] One of such effects, the macroscopic quantum tunneling has been observed.[2] However, a more spectacular effect that violates Bell inequalities may be observed in quantum coherence of *macroscopically distinct* states in a double-well potential. It was proposed to look for such effects in oscillations of a trapped magnetic field in Superconducting quantum interference device (SQUID) rings.[1,3] We will show that similar quantum-coherence effects may also be observable in tunneling from a double-well potential to continuum, and there the quantum-interference results in a peculiar behavior of the two-exponential decay rate.

I. GENERAL ANALYSIS

We discuss here the double-well problem where tunneling to continuum is allowed from the second well [Fig. 1(a)]. [For the sake of simplicity, take $V(R_1)=V(R_2)=V_0$.] Let us assume that each of the wells, taken separately [Figs. 1(b) and 1(c)], has bound states $\Phi_0^{(1)}(r)$ and $\Phi_0^{(2)}(r)$, at energies of $E_0^{(1)}$ and $E_0^{(2)}$, respectively, and that $E_0^{(1)}-E_0^{(2)}$ is much less than the spacing between levels in the wells. We shall start with the system localized in the second well at $t=0$, as a prepared state $|\Phi_0^{(2)}\rangle$, so that $H_0^{(2)}|\Phi_0^{(2)}\rangle=E_0^{(2)}|\Phi_0^{(2)}\rangle$ [where $H_0^{(2)}=-\nabla^2/2m+U_2(r)$]. The potential $U_2(r)$ is shown in Fig. 1(c), and $U_2(r)=V(r)$ for $R_1\le r\le R_2$, while $U_2(r)=V_0$ outside this region. As soon as the distorting potential $W_{10}(r)=V(r)-U_2(r)$ is switched on, the state $|\Phi_0^{(2)}\rangle$ is no longer an eigenstate of the total Hamiltonian $H=H_0^{(2)}+W_{10}$, but is a wave packet $\Psi_0(r,t)$ spreading in time, written as

$$\Psi_0(r,t)=b_0^{(2)}(t)e^{-iE_0^{(2)}t}\Phi_0^{(2)}(r)+\int b_{\mathbf{k}}^{(2)}(t)e^{-iE_k^{(2)}t}\Phi_{\mathbf{k}}^{(2)}(r)(2\pi)^{-3}d^3k \quad (1)$$

in terms of the bound and the continuum eigenfunctions of the Hamiltonian $H_0^{(2)}$. (We take into account only one bound state of $H_0^{(2)}$.) Equation (1) is supplemented with the initial condition $b_0^{(2)}(0)=1$, $b_{\mathbf{k}}^{(2)}(0)=0$. Substituting Eq. (1) into the Schrödinger equation and extracting the singular parts of the noncompact potential $W_{10}(r)$ (cf. Refs. 4 and 5) we obtain a system of coupled equations for $b_0^{(2)}(t), b_{\mathbf{k}}^{(2)}(t)$. Following the same procedure as in Refs. 4 and 5, we obtain for the Laplace transform of $b_0^{(2)}(t)$,

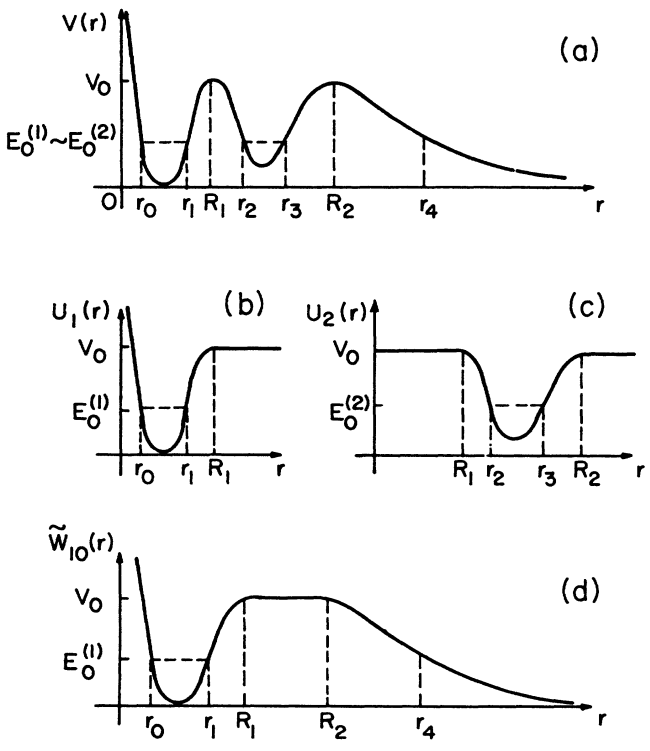

FIG. 1. The potential $V(r)$ and the auxiliary potential functions used in the approximation of Sec. II, r_0, r_1, r_2, r_3, r_4 are the classical turning points.

$$b_0^{(2)}(\epsilon)=i[\epsilon-\langle\Phi_0^{(2)}|W_{10}|\Phi_0^{(2)}\rangle - \langle\Phi_0^{(2)}|W_{10}\tilde{G}(E_0^{(2)}+\epsilon)W_{10}|\Phi_0^{(2)}\rangle]^{-1}, \quad (2)$$

where the Green's function $\tilde{G}(E)$ satisfies the equation

$$\tilde{G}(E)=(1-\Lambda)(E+V_0-H_0)^{-1}(1+\tilde{W}_{10}\tilde{G}). \quad (3)$$

Here $\tilde{W}_{10}(r)=W_{10}(r)+V_0$ [Fig. 1(d)] and $\Lambda=|\Phi_0^{(2)}\rangle\langle\Phi_0^{(2)}|$ is the projection operator onto the state $|\Phi_0^{(2)}\rangle$. Since $b_0^{(2)}(t)$ corresponds to the inverse Laplace transformation of $b_0^{(2)}(\epsilon)$, complex poles of $b_0^{(2)}(\epsilon)$ in the lower half of the ϵ plane would generate an exponential falloff of $b_0^{(2)}(t)$, i.e., $b_0^{(2)}(t)\sim\exp(-\Gamma t/2)$, where $\Gamma=-2\,\mathrm{Im}(\epsilon_0)$ is the decay width. Positions of these poles are obtained directly from Eq. (2) by solving the equation

$$\epsilon_0=\langle\Phi_0^{(2)}|W_{10}|\Phi_0^{(2)}\rangle + \langle\Phi_0^{(2)}|W_{10}\tilde{G}(E_0^{(2)}+\epsilon_0)W_{10}|\Phi_0^{(2)}\rangle. \quad (4)$$

II. APPROXIMATION

Equation (4) might be treated perturbatively by expanding $\tilde{G}(E)$ in power series of the potential $\tilde{W}_{10}$. The first term in such a series for ϵ_0 would correspond to the Weisskopf-Wigner approximation,[6] since it neglects the continuum-to-continuum transitions in the original equations for $b_0^{(2)}$ and $b_k^{(2)}$ (see Ref. 5). However, the potential $\tilde{W}_{10}$ [Fig. 1(d)] is not small and such an expansion would not be practical. Therefore, one has to look for a different series for ϵ_0 with a small expansion parameter. The desired series was found[4,5] by expanding $\tilde{G}(E)$ in powers of

$$G_{\tilde{W}}=(E+\nabla^2/2m-\tilde{W}_{10})^{-1}.$$

The first term in this series [$\tilde{G}=G_{\tilde{W}}$ in Eq. (4)] is the approximation for ϵ_0 to be employed here. Higher-order terms were evaluated[5] and found to be small.

Some intuitive reasons in favor of our approximation are the following.[5] It is only the projection operator Λ which makes $\tilde{G}$ different from the total Green's function

$$G=[E+\nabla^2/2m-V(r)]^{-1}.$$

The projection excludes the bound-state wave function $|\Phi_0^{(2)}\rangle$ from the spectral representation of $G(E)$, and only the nonresonant wave functions do appear in the spectral representation of $\tilde{G}(E)$ for $E\sim E_0^{(2)}$. [The resonant wave functions correspond to exponentially *increasing* solution of the Schrödinger equation for $r<r_4$ (Fig. 1) which can be matched only to $|\Phi_0^{(2)}\rangle$ *decreasing* exponentially for $r>r_3$.] Since the nonresonant wave functions are exponentially suppressed in the inner region, the second potential well in $V(r)$ can be filled up, so that $V(r)\to\tilde{W}_{10}(r)$ [Fig. 1(d)] which leads to our approximation, $\tilde{G}\to G_{\tilde{W}}$. Finally the desirable perturbation series for ϵ_0 can be found from iterating the equation

$$\tilde{G}=G_{\tilde{W}}+G_{\tilde{W}}(U_2-V_0)\tilde{G}-G_{\tilde{W}}\Lambda(1+\tilde{W}_{10}\tilde{G}) \quad (5)$$

obtained directly from Eq. (3) (see Ref. 5).

Let us assume that the barrier separating the first well from the continuum in the potential $\tilde{W}_{10}$ [Fig. 1(d)] is so wide, that the tunneling can be discarded and the level $E_0^{(1)}$ can be considered as a stable one. Then $G_{\tilde{W}}(E)$ is given by $G_{U_1}(E)+G_{\tilde{W}_0}(E)$ for $E\sim E_0^{(1)}\sim E_0^{(2)}$, where G_{U_1} and $G_{\tilde{W}_0}$ correspond to potentials $U_1(r)$ and

$$\tilde{W}_0(r)=\tilde{W}_{10}(r)-U_1(r)+V_0,$$

respectively (Fig. 1). [Notice that the potential $\tilde{W}_0(r)$ is obtained from $\tilde{W}_{10}(r)$ by "filling" the first well up.] One can show that the error owing to such an approximation has the order of magnitude

$$\exp[-\sqrt{2m(V_0-E_0)}(r_4-r_1)].$$

Substituting $G_{\tilde{W}}=G_{U_1}+G_{\tilde{W}_0}$ into Eq. (5) and then into Eq. (4), we obtain after some algebra an equation for the energy levels $E=E_0^{(2)}+\epsilon_0$,

$$E=E_0^{(2)}+\langle\Phi_0^{(2)}|W_1|\Phi_0^{(2)}\rangle + \frac{|\langle\Phi_0^{(2)}|W_1|\Phi_0^{(1)}\rangle|^2}{E-E_0^{(1)}-\langle\Phi_0^{(1)}|W_2|\Phi_0^{(1)}\rangle} + \langle\Phi_0^{(2)}|W_0+W_0G_{\tilde{W}_0}W_0|\Phi_0^{(2)}\rangle, \quad (6)$$

where $W_1(r)-V_0$ and $W_2(r)=U_2(r)-V_0$. Apparently, this is the secular equation $\det(E-H_{\mathrm{eff}})=0$ with

$$H_{\mathrm{eff}}=\begin{pmatrix} E_0^{(1)}+d_1 & \frac{1}{2}\delta \\ \frac{1}{2}\delta & E_0^{(2)}+d_2+\Delta_0-i\frac{\Gamma_0}{2}\end{pmatrix}. \quad (7)$$

Here $d_{1,2}=\langle\Phi_0^{(1,2)}|W_{2,1}|\Phi_0^{(1,2)}\rangle$ is the "diagonal" energy shifts of the levels $E_0^{(1,2)}$ and

$$\delta=2\langle\Phi_0^{(2)}|W_1|\Phi_0^{(1)}\rangle=2\langle\Phi_0^{(2)}|W_2|\Phi_0^{(1)}\rangle$$

is the energy splitting due to the tunneling between the two wells. An additional complex energy shift appears as well,

$$\Delta_0-i\Gamma_0/2=\langle\Phi_0^{(2)}|W_0+W_0G_{\tilde{W}_0}W_0|\Phi_0^{(2)}\rangle,$$

due to tunneling to continuum from second well [cf. Eq. (3)]. In the quasiclassical limit[4,5] $\delta=(N_1N_2P_{12})^{1/2}/2m$, $\Gamma_0=N_2P_{34}/4m$, where

$$P_{jl}=\exp(-2\int_{r_j}^{r_l}|p(r)|dr)$$

is the barrier penetration probability, N_1 and N_2 are quasiclassical normalization factors of the bound-state wave functions $\Phi_0^{(1)}$ and $\Phi_0^{(2)}$, respectively. It is noteworthy that in the case of overlapping levels the quasiclassical approximation cannot be applied straightforwardly to calculations of the level widths, but it is valid for matrix elements in the secular equation (7) (cf. Sec. V).

Solving Eq. (7), we obtain the energy levels

$$E_\pm=\tfrac{1}{2}(E_1+E_2-\tfrac{1}{2}i\Gamma_0) \pm\tfrac{1}{2}[(E_1-E_2+\tfrac{1}{2}i\Gamma_0)^2+\delta^2]^{1/2}, \quad (8)$$

where $E_1=E_0^{(1)}+d_1$ and $E_2=E_0^{(2)}+d_2+\Delta_0$. For degenerate levels ($E_1=E_2$), one has a peculiar physical behavior resulting from an interplay of the "coherent" tunneling between two wells and a tunneling from the second well to the continuum. We find that if $2\delta>\Gamma_0$ then

$$E_\pm=E_1-\tfrac{1}{4}i\Gamma_0\pm\tfrac{1}{4}(4\delta^2-\Gamma_0^2)^{1/2} ,$$

i.e., the system has two different levels with the same width, ($\Gamma_0/2$). In the opposite case, $2\delta<\Gamma_0$, and

$$E_\pm=E_1-i\tfrac{1}{4}[\Gamma_0\pm(\Gamma_0^2-4\delta^2)^{1/2}] ,$$

the system has the same level with two different widths.

III. TIME DEVELOPMENT

In order to get the time dependence of the wave function, Eq. (1), let us perform the inverse Laplace transform of $b_0^{(2)}(\epsilon)$ [Eq. (2)] by closing the integration contour around the poles in the complex ϵ plane. Using Eq. (8) and $\epsilon=E-E_0^{(2)}$ we obtain

$$b_0^{(2)}(t)=[\Gamma_+\exp(-\Gamma_+t/2) -\Gamma_-\exp(-\Gamma_-t/2)]/(\Gamma_+-\Gamma_-) , \quad (9)$$

where $\Gamma_\pm=[\Gamma_0\pm(\Gamma_0^2-4\delta^2)^{1/2}]/2$. In Eq. (1), the wave function is given as a sum of two terms,

$$\Psi_0(r,t)=\psi_2(r,t)+\tilde{\psi}_2(r,t) ,$$

so that $|\psi_2(r,t)|^2$ is the probability to find the system in the second well, and $|\tilde{\psi}_2(r,t)|^2$—outside the second well. One can derive from the original equations for $b_0^{(2)}$ and $b_k^{(2)}$ (Ref. 5) that $\tilde{\psi}_2=\tilde{G}\tilde{W}_{10}\psi_2$, where the potential $\tilde{W}_{10}$ is shown in Fig. 1(d). In the present approximation, $\tilde{G}\simeq G_{\tilde{W}}\simeq G_{U_1}+G_{\tilde{W}_0}$, and $\tilde{\psi}_2$ is represented, in turn, as a sum of two terms: the first one would give the probability to find the system in the first well, and the second one—to find it in the continuum. Using the spectral representation of the Green's function G_{U_1} one obtains after some algebra that the first term is $G_{U_1}\tilde{W}_{10}\psi_2=b_0^{(1)}\Phi_0^{(1)}$, where

$$b_0^{(1)}(E-E_0^{(1)}) =\frac{\langle\Phi_0^{(2)}|W_1|\Phi_0^{(1)}\rangle}{E-E_0^{(1)}-\langle\Phi_0^{(1)}|W_2|\Phi_0^{(1)}\rangle}b_0^{(2)}(E-E_0^{(2)}) , \quad (10)$$

is the probability amplitude for finding the system in the first well. One can see that the two-vector $B(t)=(b_0^{(1)}(t),b_0^{(2)}(t))$ satisfies the equation

$$i\frac{dB(t)}{dt}=H_{\rm eff}B(t) , \quad (11)$$

where the nonHermitean 2×2 matrix $H_{\rm eff}$ is given in (7). If the system starts from the second well, the initial condition is $B(0)=(0,1)$, if it starts from the first well, $B(0)=(1,0)$.

Equations like (11) have been used for describing decays of two-state systems. They are usually derived by neglecting the continuum-to-continuum transitions.[6] A similar equation can be derived for an n-well potential. There the effective Hamiltonian is a $n\times n$ matrix with all elements zero except for diagonal $H_{i,i}$, and off-diagonal $H_{i,i\pm1}$ matrix elements describing transitions between adjacent wells. When a well i is coupled to the continuum, $H_{i,i}$ acquires an imaginary part $-\Gamma_i/2$.

IV. DECAY RATE AND A COMPARSION WITH CLASSICAL MACROSCOPIC THEORIES

The time dependence of the decay rate

$$R(t)=-(d/dt)[|b_0^{(1)}(t)|^2+|b_0^{(2)}(t)|^2]$$

is obtained from Eq. (11). If the system was initially in the second well,

$$R(t)=(\Gamma_++\Gamma_-)[\Gamma_+\exp(-\tfrac{1}{2}\Gamma_+t) -\Gamma_-\exp(-\tfrac{1}{2}\Gamma_-t)]^2/(\Gamma_+-\Gamma_-)^2 , \quad (12)$$

$R(t)$ has a maximum at $t=0$, then it goes to zero at

$$t=t_0=[2/(\Gamma_+-\Gamma_-)]\ln(\Gamma_+/\Gamma_-) ,$$

and reaches the second maximum at $t=2t_0$. However, if the system was localized initially in the first well, the decay rate is quite different,

$$R(t)=\Gamma_+\Gamma_-(\Gamma_++\Gamma_-)[\exp(-\tfrac{1}{2}\Gamma_+t) -\exp(-\tfrac{1}{2}\Gamma_-t)]^2/(\Gamma_+-\Gamma_-)^2 . \quad (13)$$

It is zero at $t=0$ and reaches a maximum at $t=t_0$. Equations (12) and (13) describe the extreme cases of the localized initial states. Unlike the one-level decay, the time dependence of the decay rate depends essentially on the state preparation. Practically, the initial state may be not even pure. The general case will be considered in a forthcoming work.

The results for the decay rate obtained in the framework of quantum-mechanical description, Eqs. (12) and (13), in particular, the dip due to *destructive* interference with the flux from the first well, Eq. (12), apparently, contradicts the classical probabilistic approach. According to that approach,[1,3] the macroscopic system at a given time t must be in one of the wells [with respective probabilities $n^{(1)}(t)$ and $n^{(2)}(t)$], or in the continuum. Using the standard arguments of the probability conservation one gets a system of master equations for $n^{(i)}(t)$

$$\dot{n}^{(1)}(t)=-\gamma_{12}n^{(1)}(t)+\gamma_{12}n^{(2)}(t) ,$$
$$\dot{n}^{(2)}(t)=\gamma_{12}n^{(1)}(t)-(\gamma_{12}+\gamma_{20})n^{(2)}(t) , \quad (14)$$

where γ_{12} stands for the probability of nonradiative transitions between the wells, and γ_{20} is for the probability to escape from the second well to the continuum [corresponding to δ and Γ_0 in Eq. (11)]. (Equations of this type were used for description of the nuclear fission in presence of a double-humped barrier.[7]) In contrast to Eq. (11), all the matrix elements were *real* there. This would destroy the interference effects in quantum-mechanical descriptions. Actually, if the system was initially in the second well, i.e., $n^{(1)}(0)=0$, $n^{(2)}(0)=1$, the decay rate

$$R(t)=-[\dot{n}^{(1)}(t)+\dot{n}^{(2)}(t)] ,$$

as given by Eq. (14), would be

$$R(t)=\tfrac{1}{2}\gamma_{20}[(1-\beta)e^{-\gamma_- t}+(1+\beta)e^{-\gamma_+ t}] . \quad (15)$$

Here $\beta=(1+4\gamma_{12}^2/\gamma_{20}^2)^{-1/2}$,

$$\gamma_\pm=\gamma_{12}+\gamma_{20}(1\pm\beta^{-1})/2 .$$

Unlike the quantum expression in Eq. (12), this result shows no dip in the decay rate.

V. NONOVERLAPPING LEVELS

Equations (7) and (11), which are fundamental for the present work, have been derived for close levels, $|E_0^{(1)}-E_0^{(2)}|\lesssim\delta,\Gamma_0$. The method is valid, however, also in the case of nonoverlapping levels, $|E_1-E_2|\gg\delta,\Gamma_0$, as soon as these levels can be considered as isolated from other discrete states. We will show it by the comparison of $E_\pm$ given by Eq. (8) with the result of the semiclassical approach which can be applied for nonoverlapping levels.

First of all, if $\delta\ll|E_1-E_2|$ in Eq. (8), the width of the state localized in the outer well is just $-2\,\mathrm{Im}E_-=\Gamma_0$. The width of the state localized in the inner well is given by expanding the square root in Eq. (8),

$$-2\,\mathrm{Im}E_+=\Gamma_0\delta^2/4(E_1-E_2)^2 . \quad (16)$$

On the other hand, the width can be calculated by means of the semiclassical approximation, which stems from a simple formula of Ref. 5,

$$\Gamma_+=(4\alpha^2/mk)|\varphi(R_1)\chi_k(R_1)|^2 . \quad (17)$$

Here $\alpha^2=2m[V(R_1)-E_1]$, R_1 is shown in Fig. 1, $k^2=2mE_1$, $\varphi(r)\equiv\Phi_0^{(1)}(r)$ is the bound-state wave function, and $\chi_k(r)$ is the wave function of the continuous spectrum (with the first well filled up), normalized to $\chi_k(r)=\cos(kr+\delta_k)$ as $r\to\infty$. The semiclassical expression for $\varphi(r)$ under the barrier is

$$\varphi(r)=[N_1/4|p(r)|]^{1/2}\exp\left[-\int_{r_1}^{r}|p(r')|dr'\right] .$$

Matching the semiclassical expressions for χ_k at the turning points r_2,r_3,r_4, we get finally

$$\Gamma_+=N_1P_{12}P_{34}/16m\cos^2\eta , \quad (18)$$

where $\eta=\int_{r_2}^{r_3}p(r')dr'$, and P_{12},P_{34} are the penetration probabilities for the barriers.

The width is increasing sharply, if η is close to $\pi(n+\frac{1}{2})$, which corresponds to the quantization condition for the state bound in the second well. For E_1 close to E_2, $\cos\eta\approx\frac{1}{2}(E_1-E_2)T_2$, where

$$T_2=2\int_{r_2}^{r_3}dr\,(dp/dE)|_{E=E_2}$$

is the classical period of motion in the well. The resulting expression

$$\Gamma_+=N_1P_{12}P_{34}/4mT_2^2(E_1-E_2)^2$$

coincides with (16), as $\Gamma_0=P_{34}/T_2$, $\delta^2=N_1P_{12}/mT_2$, and $N_2=4m/T_2$ in the semiclassical limit.

CONCLUSION

If the shape of a two-well potential can be controlled, it is possible to detect a sort of resonance in the decay of two close levels. (A similar resonance in the penetration probability was considered by Ricco and Azbel.[8]) When the levels are not overlapping, each corresponds to a state localized mainly in one well, and their widths are quite different. Yet as soon as the potential parameters are tuned to make the levels coinciding, the states are rearranged drastically, and the widths become comparable. In this situation the quantum interference makes the time dependence more complicated than just the sum of two exponents. The preparation of the initial state is also important now, as the level population number is no longer sufficient for its complete description. Probably, the effect which manifests itself as a dip in the time dependence of the decay can be observed experimentally. This can be realized for a particle moving in a "washboard potential" with small tilt. Such a potential is obtained in the current-biased Josephson junction[2] in experiments for observation of macroscopic quantum tunneling. For observation of two-exponential decay one has to choose the potential tilt in such a way that some level in the inner well would coincide with an initially higher level in the outer well.

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*Present address: Faculty of Physics, Technion–Israel Institute of Technology, Haifa 32000, Israel.

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