Decay widths for metastable states. Improved WKB approximation

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(Received 11 December 1981)

We present improved WKB approximations, based on two-turning-point connection formulas, for the decay width of any metastable energy level in a one-dimensional potential.

I. INTRODUCTION

The possibility that the Universe in its evolution may have existed (or now exists) in a metastable configuration[1] ("false vacuum") has stimulated interest in calculations of virtual-state decay widths.[2,3] Functional-integral techniques have been used because simple WKB methods are not available for systems with many degrees of freedom. In order to establish the validity of these saddle-point methods, the authors have typically applied them to a one-dimensional quantum-mechanical potential and demonstrated that they agree with something which is always called the WKB result. However, these WKB approximations are sometimes quite different.

Langer,[4] who was interested in models of first-order phase transitions such as droplet condensation in a vapor, was the first to carefully consider the decay width (of the lowest metastable state) by both WKB and path-integral methods. His approach was generalized and applied by Coleman and Callan[2,3] to the problem of false-vacuum decay in field theory. They sought to dominate the Euclidean functional integral for the generating function by the so-called "bounce" solution and its quadratic fluctuations.

Recently Patrascioiu,[5] motivated by work of Levit, Negele, and Paltiel,[6] has questioned the Callan-Coleman result, arguing that in order to agree with the WKB answer other *complex* paths besides the real "bounce" configuration must be included. Very recent work by Lapedes and Mottola[7] also supports this claim.

As this brief summary makes evident, it is important to have a standard result to which the path-integral techniques can be compared. Ideally, one would like to know which integral approximation corresponds to each of several WKB-type results of increasing accuracy.

As the first step in this program of establishing the relation between WKB and functional-integral approximations, the present paper is devoted to a study of simple and improved WKB calculations for the decay width of a virtual energy level in a one-dimensional potential. For explicitness, we shall consider an unstable potential of the form treated by Langer[4] and shown in Fig. 1, but the techniques can be directly applied to other cases.

Our goal is to derive an expression for the decay width of any level, not just energy states at the bottom of the well. Such a result will also be useful for other applications, such as the decay rate of an unstable system at finite temperatures[8] or the probability of induced (rather than spontaneous) decay of a false vacuum.[9]

The semiclassical techniques which we shall use are not new: nearly all are at least 20 years old. Many physicists, however, seem to be unfamiliar with the powerful method of comparison equations[10] which can produce uniform approximations valid in regions containing one or two turning points. We shall also employ reversible connection formulas, a procedure which though it seems very natural from the point of view of comparison equations is highly controversial and nonrigorous. Past experience with similar problems has shown that the answers derived in this way are likely to be correct and agree with those obtained by methods which maintain a stricter control over the errors. (We discuss the reversibility question further in Sec. II.)

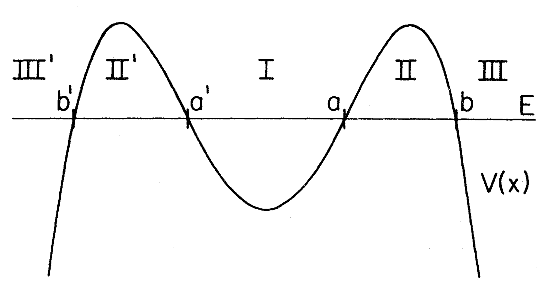

FIG. 1. Quartic potential for a one-dimensional metastable system.

II. SIMPLE WKB APPROXIMATIONS FOR THE DECAY WIDTH

We introduce some definitions which will be useful in all of our work below:

$$p(x)=\{2m[E-V(x)]\}^{1/2}\ , \quad (2.1)$$

$$u(c)=\left|\hbar^{-1}\int_x^c p(x')dx'\right|\ , \quad (2.2)$$

$$v(c)=\left|\hbar^{-1}\int_x^c |p(x')|\,dx'\right|\ , \quad (2.3)$$

$$W_1(c,d)=\hbar^{-1}\int_c^d p(x')dx'\ , \quad (2.4)$$

$$W_2(c,d)=\hbar^{-1}\int_c^d |p(x')|\,dx'\ , \quad (2.5)$$

where the arguments (c,d) refer to classical turning point, i.e., values of x for which $p(x)=0$. Note that u and v are also functions of x. We have defined u and v in order to write the connection formulas [see Eqs. (2.18), (2.19), (3.5), and (3.14)] in the simplest possible form with no need for an explicit description of the analytic structure of $p(x)$ in the complex x plane or E plane. The form of the one- and two-turning-point connection formulas which we shall present are valid when the real scattering energy lies between the bottom and top of the (real analytic) potential well or barrier, and these formulas may be used whether an allowed $(p^2>0)$ or forbidden $(p^2<0)$ region lies to the left or right of a turning point. Note that some case is required in interpreting the resulting expressions. Thus, in an allowed region to the left of a turning point (i.e., $x<c$), we have

$$\exp[iu(c)]=\exp\left[i\int_x^c |p|\,dx\right]\ ,$$

which corresponds to a wave moving to the *left;* whereas for an allowed region to the right of a turning point $(x>c)$, the same

$$\exp[iu(c)]=\exp\left[i\int_c^x |p|\,dx\right]$$

corresponds to a wave moving to the *right.* (In both cases the wave moves away from the turning point.) For the potential pictured in Fig. 1, we define

$$W_1(a',a)=W_1\ , \quad (2.6)$$

$$W_2(a,b)=W_2\ . \quad (2.7)$$

In the symmetric case, $W_2(b',a')=W_2$.

There are several equivalent ways for Γ, the decay width, to be defined. Proceeding from the Schrödinger equation to derive the continuity equation for the probability current density, but allowing the energy eigenvalues to be complex, we find

$$(-2/\hbar)\mathrm{Im}E\rho(x)=\frac{d}{dx}j(x)\ , \quad (2.8)$$

where

$$\rho(x)=\psi^*(x)\psi(x)\ ,$$
$$j(x)=\frac{\hbar}{2mi}\left[\psi^*(x)\frac{d\psi}{dx}-\psi(x)\frac{d\psi^*}{dx}\right]\ . \quad (2.9)$$

Identifying in the usual way, $-\mathrm{Im}E=\frac{1}{2}\Gamma(E)$, and integrating equation (2.8) from x_1 to x_2

$$\Gamma(E)=\hbar[j(x_2)-j(x_1)]\Big/\int_{x_1}^{x_2}\rho(x)dx\ . \quad (2.10)$$

We can use this exact expression to derive a very simple WKB approximation for the decay width. For the symmetric double-hump potential (Fig. 1) centered at $x=0$, we choose $-x_1=x_2>b$. Then, imposing the purely outgoing-wave boundary conditions appropriate for a decaying resonant state, $j(x_1)=-j(x_2)$ and

$$\Gamma=2\hbar j(x_2)\Big/\int_{x_1}^{x_2}\rho(x)dx\ . \quad (2.11)$$

If we now restrict our consideration to a virtual bound state which is deep enough in the well so that the tunneling probability is small, then we can ignore $\rho(x)$ outside of the well, and write

$$\Gamma\simeq 2\hbar j(x_2)\Big/\int_{a'}^{a}\rho(x)dx\ . \quad (2.12)$$

Staring with an outgoing[11] WKB solution in region III $(x>b)$,

$$\psi(\mathrm{III})=Ap^{-1/2}\exp[iu(b)+i\pi/4]\ , \quad (2.13)$$

we determine $\psi(x)$ in region II $(a<x<b)$ from the standard single-turning-point connection formula (as given, for example, by Landau and Lifshitz[12])

$$\psi(\mathrm{II})=A\,|p|^{-1/2}\exp[v(b)] \quad (2.14a)$$

$$=A\,|p|^{-1/2}\exp[W_2-v(a)]\ . \quad (2.14b)$$

Finally, assuming that we are far enough from the bottom of the well that the bound states in the well can be approximated by a "large-n" WKB wave function, we have (from a standard connection formula[12])

$$\psi(\mathrm{I})=2Ap^{-1/2}\exp(W_2)\cos[u(a)-\pi/4]\ . \quad (2.15)$$

Then

$$\int_{a'}^{a}\rho(x)dx=\int_{a'}^{a}|\psi(\mathrm{I})|^2dx$$
$$\simeq 4|A|^2\exp(2W_2)\tfrac{1}{2}\int_{a'}^{a}\frac{dx}{p(x)}$$
$$=|A|^2\exp(2W_2)m^{-1}T(E)\ ,$$

where we replaced $\cos^2\theta$ by its average value and

$$T(E)=2\int_{a'}^{a}\frac{m\,dx}{p(x)}=[\nu(E)]^{-1} \tag{2.16}$$

is the classical period of a particle with energy E in the well, and $\nu(E)$ is the corresponding classical frequency.

Now (2.9) and (2.13) imply

$$j(\text{III})=(p/m)\,|Ap^{-1/2}|^2 ,$$

and hence, from Eq. (2.12),

$$\Gamma(E)\simeq 2\hbar\nu(E)\exp(-2W_2) . \tag{2.17}$$

For the case of the quartic potential of Fig. 1 the quantities $\nu(E)$, $\text{Re}W_1$, and W_2 can each be expressed in terms of complete elliptic integrals. We give these results in Appendix A.

The simple result of Eq. (2.17) is intuitively very appealing: $\exp(-2W_2)$ is the familiar tunneling probability, $\nu(E)$ is the frequency at which a classical particle strikes the barrier, and the factor of 2 is due to the double-hump structure of the potential. Recall also that the derivation of (2.17) depended on assuming that the energy level was not too near either the top or bottom of the well.

We next calculate $\Gamma(E)$ by a scattering method[13] which will be employed (in Sec. III) when we consider improvements in the basic WKB result. Again, it will be assumed that we are not too near the extremes of the well so that we can use single-turning-point connection formulas and simple WKB solutions away from the turning points.

The only new ingredients which we add at this time are *reversible* connection formulas. The first uniform approximation, i.e., a single solution valid for a range of x which included a turning point, was given by Langer.[14] Murphy and Good[15] and Miller and Good[10] derive the "reversible" connection formulas which we shall use below by finding an exact solution to the differential equation in the neighborhood of the turning points and then regarding the asymptotic behaviors, which follow from expanding this exact solution on opposite sides of the transition region, as being reversibly connected. From this point of view, the decreasing exponential term in a connection formula has meaning, even in the presence of an increasing exponential term, in order to maintain a one-to-one correspondence with the exact solutions and any linear combination of exact solutions. Those who vehemently oppose the notion of reversibility[16] properly emphasize the irrefutable fact that just knowing the leading asymptotic behavior in one region does not in general allow us to pass in a unique way to the asymptotic behavior of the solution on the opposite side of a turning point, since the precise identity of the exact solution in question cannot be fixed by the incomplete asymptotic information available. Sometimes a precise specification of the boundary conditions removes the nonuniqueness. Nevertheless, even in cases where the errors are not strictly controlled (which can be done using methods such as those of Fröman and Fröman[16] or Olver[17]), the use of reversible connection formulas leads to generally reliable results. Further study is necessary before the long-standing controversy over reversibility will finally be settled.[18]

Murphy and Good's linear (one-turning-point) connection formulas[15] (using our notation) are

$$2p^{-1/2}\sin[u(c)+\pi/4]\leftrightarrow |p|^{-1/2}\exp[-v(c)] , \tag{2.18}$$

$$p^{-1/2}\cos[u(c)+\pi/4]\leftrightarrow |p|^{-1/2}\exp[v(c)] . \tag{2.19}$$

In what follows we shall freely use these relations (and any linear combination of them) without regard to direction.

We now shall calculate $\Gamma(E)$ by looking for resonances when a wave is incident from the left (region III′) on the potential well of Fig. 1. Using a linear combination of (2.18) and (2.19), an outgoing wave in region III,

$$\psi(\text{III})=Ap^{-1/2}\exp[iu(b)+i\pi/4] , \tag{2.20}$$

connects to

$$\psi(\text{II})=A\,|p|^{-1/2}\left\{\exp[v(b)]+\frac{i}{2}\exp[-v(b)]\right\} . \tag{2.21a}$$

Rewriting this as

$$\psi(\text{II})=A\,|p|^{-1/2}\{\exp(W_2)\exp[-v(a)]+(i/2)\exp(-W_2)\exp[v(a)]\} , \tag{2.21b}$$

we use (2.18) and (2.19) to obtain

$$\psi(\text{I})=Ap^{-1/2}\{2\exp(W_2)\sin[u(a)+\pi/4]+(i/2)\exp(-W_2)\cos[u(a)+\pi/4]\} . \tag{2.22}$$

Writing

$$\sin[u(a)+\pi/4]=\cos[u(a)-\pi/4]=\cos[W_1-u(a')-\pi/4]$$
$$=\cos W_1\cos[u(a')+\pi/4]+\sin W_1\sin[u(a')+\pi/4]$$

and making a similar manipulation of $\cos[u(a)+\pi/4]$, we have

$$\psi(\mathrm{I})=Ap^{-1/2}\{B(E)\cos[u(a')+\pi/4]+C(E)\sin[u(a')+\pi/4]\}\ , \tag{2.23a}$$

where

$$B(E)=2\cos W_1\exp(W_2)-(i/2)\sin W_1\exp(-W_2)\ ,$$
$$C(E)=2\sin W_1\exp(W_2)+(i/2)\cos W_1\exp(-W_2)\ . \tag{2.23b}$$

Again we use (2.18) and (2.19) and find

$$\psi(\mathrm{II}')=A\,|\,p\,|^{-1/2}\{B(E)\exp[v(a')]+\tfrac{1}{2}C(E)\exp[-v(a')]\} \tag{2.24a}$$

$$=A\,|\,p\,|^{-1/2}\{B(E)\exp(W_2)\exp[-v(b')]+\tfrac{1}{2}C(E)\exp(-W_2)\exp[v(b')]\}\ . \tag{2.24b}$$

Connecting to region III′, we have finally

$$\psi(\mathrm{III}')=Ap^{-1/2}\{2B(E)\exp(W_2)\sin[u(b')+\pi/4]+\tfrac{1}{2}C(E)\exp(-W_2)\cos[u(b')+\pi/4]\}\ . \tag{2.25}$$

At resonance we require purely outgoing waves and thus set the coefficient of the incident wave to zero. From (2.25) this implies

$$\tfrac{1}{2}C(E)\exp(-W_2)+2iB(E)\exp(W_2)=0\ . \tag{2.26a}$$

Using (2.23b) and rearranging, this becomes

$$\exp(2iW_1)=-[1+\tfrac{1}{2}\exp(-2W_2)+\tfrac{1}{16}\exp(-4W_2)][1-\tfrac{1}{2}\exp(-2W_2)+\tfrac{1}{16}\exp(-4W_2)]^{-1}\ . \tag{2.26b}$$

Recall

$$W_1=\hbar^{-1}\int_{a'}^{a}p(x)dx=\hbar^{-1}\int_{a'}^{a}\left[2m\left[E_n-\frac{i}{2}\Gamma(E_n)-V(x)\right]\right]^{1/2}dx\ .$$

Expanding for $\Gamma \ll E_n$, we have

$$W_1\simeq\hbar^{-1}\int_{a'}^{a}\{2m[E_n-V(x)]\}^{1/2}dx-(i/4\hbar)\Gamma(E_n)T(E_n)=W_1(E_n)-(i/4)\Gamma(E_n)/\hbar\nu(E_n)\ , \tag{2.27}$$

where we have introduced the complex resonance energy

$$E=E_n-i\Gamma(E)/2$$

and

$$T(E)=1/\nu(E)$$

is defined by Eq. (2.16). Using (2.27), the real and imaginary parts of (2.26b) imply

$$W_1(E_n)=(n+\tfrac{1}{2})\pi \tag{2.28a}$$

and

$$\Gamma(E_n)=2\hbar\nu(E_n)\ln[1+\exp(-2W_2)+\tfrac{1}{2}\exp(-4W_2)]\ , \tag{2.28b}$$

where terms of order $\exp(-6W_2)$ have been ignored in the argument of the logarithm. For $\exp(-2W_2)\ll 1$, this reduces to Eq. (2.17),

$$\Gamma(E_n)\simeq 2\hbar\nu(E_n)\exp(-2W_2)\ .$$

Equation (2.28a) is the usual Bohr-Sommerfeld quantization condition for energy levels in a potential well.

III. IMPROVED WKB APPROXIMATIONS

The derivations of Γ in Sec. II assume that the simple WKB solution is valid between turning points. This is true when the potential does not change rapidly. We also assumed that the turning points are well separated. Obviously, both of these conditions fail for energies near the top or bottom of the well. To derive improved WKB results which will be valid even for these extreme cases, we shall use the two-turning-point uniform approximations of Miller and Good[10] which allow us to connect solutions on both sides of a region containing two turning points.

A. Method of comparison equations[10,18]

The idea is to obtain an approximate solution of the differential equation

$$\frac{d^2\psi(x)}{dx^2}+f(x)\psi(x)=0 \qquad (3.1)$$

in terms of known solutions of

$$\frac{d^2\phi(\sigma)}{d\sigma^2}+G(\sigma)\phi(\sigma)=0\ . \qquad (3.2)$$

$G(\sigma)$ is chosen to be similar to $f(x)$ in basic properties (e.g., shape) but simpler so that the solutions of (3.2) are known functions. Substituting

$$\psi(x)=\left[\frac{d\sigma}{dx}\right]^{-1/2}\phi[\sigma(x)]$$

in Eq. (3.1), if $G(\sigma)$ has been chosen appropriately, then $\sigma(x)$ will be a slowly varying function. This implies

$$\frac{d\sigma}{dx}\simeq[f(x)/G(\sigma)]^{1/2}$$

which gives us the relation between the new and old independent variables, and thus $\psi(x)$.

B. Decay width for E_n near the bottom of the well

To find improved solutions which will also be valid for low-lying states in the potential well, the appropriate comparison equation[10] is

$$\frac{d^2\phi(\sigma)}{d\sigma^2}+(t-\sigma^2)\phi(\sigma)=0\ . \qquad (3.3)$$

With t chosen so that

$$\tfrac{1}{2}\pi t=\hbar^{-1}\int_{a'}^{a}p(x)dx=W_1=\int_{-\sqrt{t}}^{+\sqrt{t}}(t-\sigma^2)^{1/2}d\sigma\ , \qquad (3.4)$$

the independent solutions of (3.3) are the parabolic cylinder functions

$$\phi(\sigma)=D_{(t-1)/2}(\pm\sqrt{2}\sigma)\ .$$

Miller and Good[10] use the asymptotic expansions of the resulting uniform approximations for $\psi(x)$ to arrive at the two-turning-point (or parabolic) connection formulas which can be expressed in our notation as

$$\{a_1|p|^{-1/2}\exp[v(a')]+\sin W_1|p|^{-1/2}\exp[-v(a')]\}\underset{x\to-\infty}{\longleftarrow}\gamma_B(W_1)(\sigma')^{-1/2}D_{(t-1)/2}(\sqrt{2}\sigma)$$
$$\underset{x\to+\infty}{\longrightarrow}|p|^{-1/2}\exp[-v(a)] \qquad (3.5a)$$

and

$$|p|^{-1/2}\exp[-v(a')]\underset{x\to-\infty}{\longleftarrow}\gamma_B(W_1)(\sigma')^{-1/2}D_{(t-1)/2}(-\sqrt{2}\sigma)$$
$$\underset{x\to+\infty}{\longrightarrow}\{a_1|p|^{-1/2}\exp[v(a)]+\sin W_1|p|^{-1/2}\exp[-v(a)]\}\ , \qquad (3.5b)$$

where

$$a_1=2\alpha_B(W_1)\cos W_1\ , \qquad (3.6a)$$

$$\alpha_B(W_1)=(2\pi)^{-1/2}(e\pi/W_1)^{W_1/\pi}\Gamma(\tfrac{1}{2}+W_1/\pi)\ , \qquad (3.6b)$$

and

$$\gamma_B(W_1)=2^{1/4}(e\pi/W_1)^{W_1/2\pi}\ . \qquad (3.6c)$$

(See Appendix B for a discussion and evaluation of α_B.) We shall use these parabolic connection formulas to join solutions in region II to region II′. We connect II (II′) to III (III′) using the linear connection formulas, Eqs. (2.18) and (2.19).

The outgoing wave in region III, Eq. (2.20), thus connects to ψ(II) given by Eq. (2.21a) and (2.21b). We now must match this to the appropriate linear combination of (3.5a) and (3.5b) which, for large positive x, equals ψ(II). Referring to Eqs. (3.5a) and (3.5b) as P and Q, respectively, we have

$$\psi(\mathrm{II})=A(b_1Q+b_2P)\ , \qquad (3.7a)$$

where

$$b_1=\tfrac{1}{2}ia_1{}^{-1}\exp(-W_2)\ ,$$
$$b_2=\exp(W_2)-\tfrac{1}{2}ia_1{}^{-1}\sin W_1\exp(-W_2)\ . \qquad (3.7b)$$

Inserting the large-negative-x behavior of P and Q in Eq. (3.7a), we have

$$\psi(\mathrm{II}')=A\,|p\,|^{-1/2}\{b_2a_1\exp[v(a')]+(b_2\sin W_1+b_1)\exp[-v(a')]\}\ . \tag{3.8}$$

Finally from (2.18) and (2.19), $\psi(\mathrm{II}')$ connects to

$$\psi(\mathrm{III}')=Ap^{-1/2}\{2b_2a_1\exp(W_2)\sin[u(b')+\pi/4]+(b_2\sin W_1+b_1)\exp(-W_2)\cos[u(b')+\pi/4]\}. \tag{3.9}$$

Requiring that the coefficient of the incident wave vanish at resonance, we find

$$2ib_2a_1\exp(W_2)+(b_2\sin W_1+b_1)\exp(-W_2)=0\ .$$

Using Eqs. (3.7b), (3.5b), and (2.27), this implies

$$W_1(E_n)=(n+\tfrac{1}{2})\pi \tag{3.10a}$$

and

$$\Gamma(E_n)\simeq 2\hbar v(E_n)\ln[1+\alpha_B{}^{-1}\exp(-2W_2)]\ , \tag{3.10b}$$

where we have ignored the small imaginary part of α_B [which contributes a correction term to $W_1(E_n)$] and have dropped terms of order $\exp(-4W_2)$ since Eq. (3.10b) is not to be used near the top of the well when W_2 is small.

Near the bottom of the well, $W_2 \gg 1$, and

$$\Gamma(E_n)\simeq 2\hbar v(E_n)\alpha_B{}^{-1}\exp(-2W_2)\ . \tag{3.11}$$

In Appendix B, we note that $\alpha_B{}^{-1}$ equals 1.08, 1.03, 1.02 for the first three levels and approaches 1 as n increases,

$$\alpha_B{}^{-1}\sim\exp[+(24n)^{-1}]\ .$$

Thus (3.10b) reduces to (2.17) in the appropriate limit.

C. Decay width near the top of the well

Near the top of a potential barrier, the appropriate comparison equation[10] is

$$\frac{d^2\phi(\sigma)}{d\sigma^2}+(t+\sigma^2)\phi(\sigma)=0\ . \tag{3.12}$$

With t (real <0 for energies below the top of barrier) chosen so that

$$W_2=\hbar^{-1}\int_a^b |p\,|\,dx=\int_{-|t|^{1/2}}^{|t|^{1/2}}(t+\sigma^2)^{1/2}d\sigma$$
$$=-\tfrac{1}{2}\pi t\ , \tag{3.13}$$

the independent solutions of (3.12) are the parabolic cylinder functions

$$\phi(\sigma)=D_{(\pm it-1)/2}(\sqrt{2}\sigma e^{\mp i\pi/4})\ .$$

These yield a uniform approximation for $\psi(x)$ in a region including the top of a barrier. From the asymptotic expansions, Miller and Good[10] derive the two-turning-point connection formula (written in our notation and applying it to one of the barriers in Fig. 1):

$$\{\alpha_T(W_2)\exp(-\tfrac{1}{2}W_2)p^{-1/2}\exp[-iu(a)]+e^{-i\pi/2}p^{-1/2}\exp[iu(a)]\}\underset{x\to-\infty}{\longleftarrow}\gamma_T(W_2)(\sigma')^{-1/2}D_{(it-1)/2}(\sqrt{2}\sigma e^{-i\pi/4})$$
$$\underset{x\to+\infty}{\longrightarrow}p^{-1/2}\exp(-W_2)\exp[iu(b)]\ , \tag{3.14}$$

where

$$\alpha_T(W_2)=(2/\pi)^{1/2}(W_2/\pi e)^{iW_2/\pi}\Gamma(\tfrac{1}{2}-iW_2/\pi)\cosh(-W_2) \tag{3.15a}$$

and

$$\gamma_T(W_2)=(2e^{-i\pi/2})^{1/4}(W_2e^{3i\pi/2}/\pi e)^{iW_2/2\pi}\ . \tag{3.15b}$$

(See Appendix C for further details on α_T.) The complex conjugate of Eq. (3.14) yields another independent connection formula. By joining two of these two-turning-point relations, we are able to cover the whole range of x. (No one-turning-point formulas are used.)

Starting with an outgoing wave in region III,

$$\psi(\mathrm{III})=Ap^{-1/2}\exp[iu(b)]\ , \tag{3.16}$$

Eq. (3.14) implies

$$\psi(\mathrm{I})=Ap^{-1/2}\{\alpha_T\exp(\tfrac{1}{2}W_2)\exp[-iu(a)]+e^{-i\pi/2}\exp(W_2)\exp[iu(a)]\} \tag{3.17a}$$

$$=Ap^{-1/2}\{\alpha_T\exp(\tfrac{1}{2}W_2)\exp(-iW_1)\exp[iu(a')]+e^{-i\pi/2}\exp(W_2)\exp(iW_1)\exp[-iu(a')]\}\ . \tag{3.17b}$$

From Eq. (3.14) and its complex conjugate (applied now to the other barrier) we form the linear combination which has the behavior of (3.17b) in region I. Then, assuming $\hbar^{-1}\int_{b'}^{a'}|p|\,dx=W_2$, we have

$$\psi(\mathrm{III'})=Ap^{-1/2}(\alpha_T\exp(\tfrac{3}{2}W_2)\exp(-iW_1)\{\alpha_T\exp[-iu(b')]\exp(-\tfrac{1}{2}W_2)+e^{-i\pi/2}\exp[iu(b')]\}$$
$$+e^{-i\pi/2}\exp(2W_2)\exp(iW_1)\{e^{i\pi/2}\exp[-iu(b')]+\alpha_T^*\exp(-\tfrac{1}{2}W_2)\exp[iu(b')]\})\ . \tag{3.18}$$

For resonance, the coefficient of the incident wave vanishes,

$$\exp(iW_1)\exp(2W_2)+\alpha_T{}^2\exp(-iW_1)\exp(W_2)=0\ ,$$

and thus

$$\exp(2iW_1)=-\alpha_T{}^2\exp(-W_2)\ . \tag{3.19}$$

Using Eqs. (C5) and (2.27), (3.19) implies

$$W_1(E_n)=(n+\tfrac{1}{2})\pi+\phi(E_n) \tag{3.20a}$$

and

$$\Gamma(E_n)=2\hbar\left[T(E_n)-2\hbar\left[\frac{\partial\phi}{\partial E}\right]_{E_n}\right]^{-1}$$
$$\times\ln[1+\exp(-2W_2)]\ . \tag{3.20b}$$

These results are similar to those of Drukarev, Fröman, and Fröman.[19] In Appendix D, we show that although the classical period $T(E_n)$ logarithmically diverges at the top of the well, the denominator in (3.20b) remains finite. Away from the top, the $\partial\phi/\partial E$ term can be neglected.

IV. CONCLUSIONS

Equations (3.10b) and (3.20b) give an improved WKB approximation for the decay width of *any* energy level in a potential well of the general shape of Fig. 1. Thus, except near the very top or bottom, an excellent approximation is simply

$$\Gamma(E_n)=2\hbar\nu(E_n)\ln[1+\exp(-2W_2)]\ .$$

Obviously, the techniques we have used can be applied to other potentials.

In Appendix A we have calculated $\nu(E_n)$ and W_2 (in terms of complete elliptic integrals) for the case of a quartic potential of the form

$$V(x)=\alpha_2x^2-\alpha_4x^4\ .$$

For the low-lying energy levels, a closed-form expression is given for $\Gamma(E_n)$ in Eq. (A14).[20]

It will be very interesting to determine which functional integral methods can reproduce the improved WKB approximation, including the corrections near the top and bottom of the well.

ACKNOWLEDGMENTS

This work was begun in collaboration with Barry Harrington, who contributed much to the formulation and general approach. The research was supported by the National Science Foundation under Grant No. PHY 81-06768.

APPENDIX A

In this appendix, we give explicit expressions for $\nu(E_n)$, $W_1(E_n)$, and $W_2(E_n)$ for a quartic potential of the form shown in Fig. 1. We expand these exact results to obtain $\Gamma(E_n)$ for E_n near the bottom of the well. With

$$V(x)=\alpha_2x^2-\alpha_4x^4\ , \tag{A1}$$

$$p(x)=[2m(E_n-\alpha_2x^2+\alpha_4x^4)]^{1/2}$$
$$=(2m\alpha_4)^{1/2}[(x^2-a^2)(x^2-b^2)]^{1/2}\ , \tag{A2}$$

where $x=a,b$ are the turning points and $a'=-a$ and $b'=-b$ for the symmetric potential of (A1) and (A2) implies

$$a^2+b^2=(\alpha_2/\alpha_4)$$
and (A3)
$$a^2b^2=E_n/\alpha_4\ .$$

Now,

$$[\nu(E_n)]^{-1}=T(E_n)=2\int_{a'}^{a}\frac{dx}{v(E_n)}=2m\int_{-a}^{a}dx/p(x)$$
$$=4(m/2\alpha_4)^{1/2}\int_0^a dx[(b^2-x^2)(a^2-x^2)]^{-1/2}=4(m/2\alpha_4)^{1/2}b^{-1}F(\pi/2,a/b)\ , \tag{A4}$$

where $F(\pi/2,a/b)\equiv K(a/b)$ is a complete elliptic integral, and we are using the notation of Gradshteyn and

Ryzhik[21]:

$$W_1(E_n)=\hbar^{-1}\int_{a'}^{a}p(x)dx=(2/\hbar)(2m\alpha_4)^{1/2}\int_0^a[(x^2-a^2)(x^2-b^2)]^{1/2}dx$$
$$=(2/\hbar)(2m\alpha_4)^{1/2}(b/3)[(a^2+b^2)E(\pi/2,a/b)-(b^2-a^2)F(\pi/2,a/b)]\,, \tag{A5}$$

where $E(\pi/2,a/b)=E(a/b)$ is another of the complete elliptic integrals of Ref. 21. From the definitions, one can relate $W_1(E_n)$ and $T(E_n)$:

$$\frac{\partial W_1(E_n)}{\partial E_n}=\frac{T(E_n)}{2\hbar}\,. \tag{A6}$$

Finally,

$$W_2(E_n)=\hbar^{-1}\int_a^b|p|\,dx=\hbar^{-1}\int_{b'}^{a'}|p|\,dx=\hbar^{-1}(2m\alpha_4)^{1/2}\int_a^b[(x^2-a^2)(b^2-x^2)]^{1/2}dx$$
$$=\hbar^{-1}(2m\alpha_4)^{1/2}(b/3)[(a^2+b^2)E(\pi/2,q)-2a^2F(\pi/2,q)]\,, \tag{A7}$$

where $q=(1-a^2/b^2)^{1/2}$.

Near the bottom of the well, $a/b\ll 1$, and thus (from Ref. 21)

$$K(a/b)\to\tfrac{1}{2}\pi[1+\tfrac{1}{4}(a/b)^2+\cdots]\,,\quad E(a/b)\to\tfrac{1}{2}\pi[1-\tfrac{1}{4}(a/b)^2+\cdots]\,,$$
$$K(q)\to\ln\frac{4b}{a}+\frac{1}{4}\left[\ln\frac{4b}{a}-1\right](a/b)^2+\cdots\,,\quad E(q)\to 1+\frac{1}{2}\left[\ln\frac{4b}{a}-\tfrac{1}{2}\right](a/b)^2+\cdots\,. \tag{A8}$$

These imply

$$T(E_n)\to(4/b)(m/2\alpha_4)^{1/2}\tfrac{1}{2}\pi(1+a^2/4b^2)\,,$$
$$W_1(E_n)\to(2m\alpha_4)^{1/2}(\pi/2\hbar)a^2b,\quad W_2(E_n)\to(2m\alpha_4)^{1/2}(b^3/3\hbar)\left[1-(3a^2/2b^2)\ln\frac{4b}{a}\right]\,, \tag{A9}$$

where, for $a/b\ll 1$,

$$a^2\simeq E_n/\alpha_2,\quad b^2\simeq\alpha_2/\alpha_4\,. \tag{A10}$$

Combining (A9), (A10), and (2.28a), we have

$$E_n\simeq(n+\tfrac{1}{2})\hbar(2\alpha_2/m)^{1/2} \tag{A11}$$

near the bottom of the well, corresponding to the energy levels of a simple harmonic oscillator. Equations (A9)–(A11) imply

$$T(E_n)\to\pi(2m/\alpha_2)^{1/2}[1+(n+\tfrac{1}{2})\hbar\alpha_4 m^{-1/2}(2\alpha_2)^{-3/2}]\,,$$
$$W_2(E_n)\to(2m)^{1/2}\alpha_2^{3/2}(3\hbar\alpha_4)^{-1}-\tfrac{1}{2}(n+\tfrac{1}{2})\ln\left[\frac{2^{7/2}\alpha_2^{3/2}m^{1/2}}{(n+\frac{1}{2})\hbar\alpha_4}\right]\,. \tag{A12}$$

Then, the barrier penetration factor becomes

$$\exp(-2W_2)\simeq\left[\frac{2^{7/2}\alpha_2^{3/2}m^{1/2}}{\hbar(n+\frac{1}{2})\alpha_4}\right]^{n+1/2}\exp\left[-\frac{m^{1/2}(2\alpha_2)^{3/2}}{3\hbar\alpha_4}\right]\,. \tag{A13}$$

From Eqs. (A12), (A13), and (3.11), we find

$$\Gamma(E_n)\simeq 2\hbar(\pi\alpha_B)^{-1}(\alpha_2/2m)^{1/2}\left[\frac{2^{7/2}\alpha_2^{3/2}m^{1/2}}{\hbar(n+\frac{1}{2})\alpha_4}\right]^{n+1/2}\exp\left[-\frac{m^{1/2}(2\alpha_2)^{3/2}}{3\hbar\alpha_4}\right]\,. \tag{A14}$$

APPENDIX B

We discuss the quantity $\alpha_B(W_1)$ which was introduced in Eq. (3.6). Using the quantization condition on W_1,

$$W_1(E_n)=(n+\tfrac{1}{2})\pi ,$$

we can write

$$\alpha_B(E)\simeq\alpha_B(E_n)$$
$$=(2\pi)^{-1/2}[e/(n+\tfrac{1}{2})]^{n+1/2}\Gamma(n+1) , \qquad \text{(B1)}$$

or

$$\alpha_B{}^{-1}=\frac{1}{n!}(2\pi)^{1/2}[(n+1/2)/e]^{n+1/2} . \qquad \text{(B2)}$$

This can be explicitly evaluated for any n, e.g.,

$$\alpha_B{}^{-1}\ (n=0)=(\pi/e)^{1/2}=1.075 ,$$
$$\alpha_B{}^{-1}\ (n=1)=1.027 ,$$
$$\alpha_B{}^{-1}\ (n=2)=1.017, \text{ etc.}$$

For large n, we can use Stirling's formula for the Γ function to show

$$\alpha_B{}^{-1}\underset{n\to\infty}{\sim}\exp(1/24n) , \qquad \text{(B3)}$$

and thus $\alpha_B{}^{-1}\to 1$ for large n.

APPENDIX C

We discuss $\alpha_T(W_2)$ defined by Eq. (3.15a). (See also Connor[13] who introduces a related quantity.) Using standard identities,

$$\alpha_T(W_2)=(2/\pi)^{1/2}\cosh(-W_2)\,|\,\Gamma(\tfrac{1}{2}-iW_2/\pi)\,|\,\exp[i\phi(W_2)] ,$$

where

$$\phi(W_2)=\arg\Gamma(\tfrac{1}{2}-iW_2/\pi)+\frac{W_2}{\pi}\left[\ln\frac{W_2}{\pi}-1\right] . \qquad \text{(C1)}$$

For large W_2,

$$\phi(W_2)\to-(\pi/24W_2) .$$

Since

$$|\,\Gamma(\tfrac{1}{2}-iW_2/\pi)\,|=[\pi/\cosh(-W_2)]^{1/2} ,$$

we have

$$\alpha_T(W_2)=[2\cosh(-W_2)]^{1/2}\exp[i\phi(W_2)]=[\exp(-W_2)+\exp(W_2)]^{1/2}\exp[i\phi(W_2)] . \qquad \text{(C2)}$$

Hence,

$$\alpha_T{}^2(W_2)=\exp(W_2)[1+\exp(-2W_2)]\exp[2i\phi(W_2)] . \qquad \text{(C3)}$$

Expanding $\phi(W_2)$ near the resonance energy,

$$\phi(W_2)\simeq\phi(E_n)+(E-E_n)(\partial\phi/\partial E)_{E_n}$$
$$=\phi(E_n)-(i/2)\Gamma(E_n)(\partial\phi/\partial E)_{E_n} . \qquad \text{(C4)}$$

Inserting this in (C3), we have

$$\alpha_T{}^2(W_2)=\exp(W_2)\exp\left[\Gamma(E_n)\left[\frac{\partial\phi}{\partial E}\right]_{E_n}\right][1+\exp(-2W_2)]\exp[2i\phi(E_n)] . \qquad \text{(C5)}$$

APPENDIX D

We examine equation (3.20b) for $\Gamma(E)$ near the top of the well and show that Γ remains finite and nonzero as we approach the top.

Write

$$\frac{\partial\phi}{\partial E}=\frac{\partial\phi}{\partial W_2}\frac{\partial W_2}{\partial E} . \qquad \text{(D1)}$$

From

$$W_2=\frac{1}{\hbar}\int_a^b[2m(V-E)]^{1/2}dx\ ,$$
$$\frac{\partial W_2}{\partial E}=-\frac{1}{\hbar}\int_a^b m[2m(V-E)]^{-1/2}dx\ . \tag{D2}$$

For E near $V_{\max}$, we find

$$W_2\simeq(\pi/\hbar)(m/|V''|)^{1/2}(V_{\max}-E) \tag{D3}$$

and, hence,

$$\frac{\partial W_2}{\partial E}\simeq-(\pi/\hbar)(m/|V''|)^{1/2}\ , \tag{D4}$$

where $|V''|$ is evaluated at $V_{\max}$. From (C1),

$$\frac{\partial\phi}{\partial W_2}=-\frac{1}{\pi}\mathrm{Re}\psi\left[\frac{1}{2}-i\frac{W_2}{\pi}\right]+\frac{1}{\pi}\ln\left[\frac{W_2}{\pi}\right], \tag{D5}$$

where[22]

$$\psi(z)\equiv\frac{\partial}{\partial z}\ln\Gamma(z)\ .$$

Since W_2 approaches zero at the top of the barrier, we can expand

$$\psi\left[\frac{1}{2}-i\frac{W_2}{\pi}\right]\simeq\psi(\tfrac{1}{2})-(i/\pi)W_2\psi'(\tfrac{1}{2})+\cdots\ ,$$

and thus[22]

$$\mathrm{Re}\psi\left[\tfrac{1}{2}-i\frac{W_2}{\pi}\right]\simeq\psi(\tfrac{1}{2})=-1.9635\ . \tag{D6}$$

Using (D3) and (D6), (D5) implies

$$\frac{\partial\phi}{\partial W_2}\simeq-(1/\pi)\psi(\tfrac{1}{2})+\frac{1}{\pi}\ln(W_2/\pi)$$
$$\simeq\frac{1}{\pi}\ln\left[(V_{\max}-E_n)\frac{1}{\hbar}(m/|V''|)^{1/2}\right] \tag{D7}$$

for E_n near $V_{\max}$. Putting (D4) and (D7) into (D1), we have

$$\left[\frac{\partial\phi}{\partial E}\right]_{E_n}\simeq-(1/\hbar)(m/|V''|)^{1/2}$$
$$\times\ln\left[(V_{\max}-E_n)\frac{1}{\hbar}(m/|V''|)^{1/2}\right] \tag{D8}$$

very close to the top of the well. From Eq. (A4), one can show that near the top of the well

$$T(E_n)\simeq-2(m/|V''|)^{1/2}\ln[(V_{\max}-E_n)/64V_{\max}]\ . \tag{D9}$$

Thus, (D8) and (D9) when inserted in the denominator of Eq. (3.20b), imply that as we approach the top of the well,

$$T-2\hbar\left[\frac{\partial\phi}{\partial E}\right]_{E_n}\to2(m/|V''|)^{1/2}$$
$$\times\ln\left[\frac{1}{\hbar}64V_{\max}(m/|V''|)^{1/2}\right], \tag{D10}$$

and hence $\Gamma(E_n)$ remains finite and nonzero. For the quartic potential

$$V(x)=\alpha_2x^2-\alpha_4x^4\ ,$$

$$V_{\max}=(\alpha_2{}^2/4\alpha_4)\ \text{and}\ |V''|=4\alpha_2\ .$$

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