WKB Approach to Calculating the Lifetime of Quasistationary States

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(Received 25 October 1999)

A novel WKB approach to calculating the lifetime of quasistationary states in the potential wells of the form \( V(x) = P(x) - \mu Q(x) \), where \( P(x) \) is the radial part of the potential for the spherically symmetric harmonic oscillator or the hydrogen atom and \( Q(x) \) is a polynomial, is suggested. In this approach, the usual explicit procedure of the asymptotic matching of the perturbative and WKB wave functions is avoided and a simple formula for the imaginary part of the energy is found. The leading and the first correction terms for the imaginary part of the energy and the related lifetime are analytically calculated.

PACS numbers: 03.65.Sq

The WKB method is one of the oldest approximate methods of quantum mechanics. Despite this fact the standard formulation of the WKB method is difficult to use. The usual explicit procedure of the asymptotic matching of the perturbative and WKB wave functions in the intermediate region leads to very tedious and difficult calculations [1–5]. This procedure must be repeated for different potentials from the very beginning and no general WKB formulas for measurable physical quantities are known. In this approach, the higher order calculations are very difficult.

In this Letter, we suggest a modified approach illustrated in the calculation of the lifetime of the quasistationary states of the Schrödinger equation,

\[
[-d^2/dx^2 + V(x)]\psi(x) = E\psi(x),
\]

for the potential wells of the form

\[
V(x) = P(x) - \mu Q(x).
\]

Here, \( P(x) = \alpha x^{-2} + x^2 \) is the radial part of the potential for the spherically symmetric harmonic oscillator; \( Q(x) = \sum_{l=0}^{m-1} a_l x^{2(m-l)} \) is the perturbation potential. We assume that \( 0 < \mu \ll 1 \) is a small constant so that the potential \( V(x) \) is a smooth function without large oscillations. A similar problem also appears in the case of the hydrogen atom, where \( P(x) = \alpha x^{-2} - x^{-1} \) and \( Q(x) = \sum_{l=0}^{m-2} a_l x^{m-l-1} \). Here, we assume \( m \geq 2 \), \( a_0 = 1 \), and \( \alpha = l(l + D - 2) + (D - 1)(D - 3)/4 \), where \( l \) is the orbital quantum number and \( D \) denotes the number of space dimensions [6]. Some problems of this type have been studied from the point of view of quantum field theory (see, e.g., Refs. [4,7,8]) as well as nonrelativistic hydrogen atom in constant electric field (see, e.g., Refs. [1–3,8]) or models of quark confinement [5,9].

Because of the form of the potential, there is a small probability that the particle escapes through the potential barrier to infinity. Therefore, the energy \( E = \text{Re}E + i\text{Im}E \) has a small imaginary part \( \text{Im}E < 0 \). In this Letter, we first suggest a simple and straightforward way of calculating the WKB wave function for the potentials (2). We then derive a general formula for \( \text{Im}E \) and related lifetime \( \tau = -1/(2\text{Im}E) \). By using this approach, the usual difficulties of the WKB method are avoided and calculations are greatly simplified. For the problems mentioned above, we then find general analytic formulas for \( \text{Im}E \) and \( \text{Re}E \).

The imaginary part of the energy is calculated from the equation (see, e.g., Ref. [4])

\[
\text{Im}E = \frac{1}{2i} \lim_{x \to \infty} \frac{\int_0^x \left[ \psi(x) \left( \frac{d\psi^*(x)}{dx} \right) - \psi^*(x) \left( \frac{d\psi(x)}{dx} \right) \right]}{\int_0^x |\psi(x')|^2 dx'},
\]

where \( \psi(x) \) is the Schrödinger wave function of the perturbing potential.
The wave function \( \psi(x) \) for small \( x \) inside the potential barrier is calculated in the \( n \)th order of the Rayleigh-Schrödinger perturbation theory (RSPT)

\[
\psi_{RSPT}^{(n)}(x) = \sum_{i=0}^{n} \psi_i(x) \mu^i.
\]

Since the dominant contribution to the norm of the quasi-stationary wave function is given by small \( x \), we replace \( \psi(x) \) in the integral \( \int_0^\infty \left| \psi(x') \right|^2 dx' \) by \( \psi_{RSPT}^{(n)}(x) [1,4] \).

The numerator in Eq. (3) is calculated by means of the WKB wave function,

\[
\psi_{WKB}^{(n)}(x) = K \exp \left[ \frac{1}{\mu^{1/(m-1)}} \sum_{i=0}^{1+n(m-1)} S_i(x) \mu^{i/(m-1)} \right],
\]

where \( K \) is a normalization constant discussed below.

To calculate \( \psi_{WKB}^{(n)}(x) \) we suggest a new simple approach. For the sake of simplicity, we discuss here only the case of the perturbed harmonic oscillator. The dominant contribution to the numerator in Eq. (3) comes from the region \( V(x) \gg \text{Re} E \), where \( x^2 = \mu a^2 [1-5] \). To make these terms of the same order in \( \mu \), we perform the scaling \( x = \mu^{-1/2(m-1)} u \) in Eq. (1), which then becomes

\[
\mu^{2/(m-1)} \frac{d^2}{du^2} \psi = \left[ u^2 - u^{2m} - (E_0 + a_1 u^{2(m-1)}) \right] \times \mu^{1/(m-1)} + \ldots \psi.
\]

Here, the RSPT expansion of the real part of the energy \( \text{Re} E = E_0 + E_1 \mu + E_2 \mu^2 + \ldots \) was used. By searching for the solution of this equation in the form (5) and comparing the terms of the same power of \( \mu^{1/(m-1)} \), we obtain equations from which the \( S_i \) terms can easily be calculated. Here, we give the resulting expressions for the first two terms only:

\[
S_0(u) = - \int u \left[ u^2 - u^{2m} \right]^{1/2} du + s_0
\]

and

\[
S_1(u) = \frac{1}{4} \ln(u^2 - u^{2m}) - \frac{E_0}{4(m-1)} \ln \left[ 1 + (1 - u^{2(m-1)})^{1/2} \right] - \frac{a_1}{2} \frac{1 - u^{2(m-1)})^{1/2}}{m-1} + s_1,
\]

where \( s_i \) are integration constants. These solutions correspond to the wave going through the barrier to infinity. The form of our WKB wave function \( \psi_{WKB}^{(n)} \) is the same as that obtained by taking the first \( 2 + n(m-1) \) terms of the usual WKB expansion and expanding them up to the \( n \)th order of \( \mu \). However, our approach is much simpler.

We now suggest a simple new method of the asymptotic matching of the functions \( \psi_{RSPT}^{(n)}(x) \) and \( \psi_{WKB}^{(n)}(x) \). These functions must equal in an overlap region of their mutual validity defined by the inequalities \( \text{Re} E \ll x^2 \ll \mu^{-1/(m-1)} \). Therefore, the logarithm of these functions expanded up to the \( n \)th order of \( \mu \) must be asymptotically (for large \( x \)) equal:

\[
\sum_{i=0}^{1+n(m-1)} S_i(x) \mu^{(i-1)/(m-1)} = \ln \psi_{RSPT}^{(n)}(x) + \sum_{i=0}^{1+n(m-1)} A_i \mu^{(i-1)/(m-1)} + O(1/x^2),
\]

where we have introduced

\[
\sum_{i=0}^{1+n(m-1)} A_i \mu^{(i-1)/(m-1)} = - \ln K.
\]

The right-hand side of Eq. (9) can be considered as the asymptotic expansion of the left-hand side. Generally, this expansion contains \( x \)-dependent terms, constant terms, and terms negligible in the overlap region. Henceforth, we normalize \( \psi_{RSPT}^{(n)}(x) \) in such a way that the asymptotic expansion of \( \ln \psi_{RSPT}^{(n)}(x) \) does not contain a constant additive term in any order of \( \mu \). Furthermore, we put \( s_i = -A_i^{(0)} \), where \( A_i^{(0)} \) is a constant term of the asymptotic expansion of \( S_i(x) \) for the bound state potential \( V(x) = P(x) \). This choice of the normalization of \( \psi_{RSPT}^{(n)}(x) \) and constants \( s_i \) leads to \( K = 1 \) for \( \mu = 0 \) so that the asymptotic matching is also obeyed in this case. Then, it follows from Eq. (9) that \( A_i \) is a constant term of the asymptotic expansion of \( S_i(x) \) in the overlap region. Since the \( S_i(x) \) depend on \( \mu \) and \( x \) via the variable \( u = \mu^{1/(2(m-1))} x \) and all of the terms \( A_i, i \neq 1 \) do not depend on \( x \) and \( \mu \) it is seen that all \( A_i, i \neq 1 \), can be calculated as the constant terms of the expansion of \( S_i(u) \) near \( u = 0 \) and \( s_i = 0 \) for \( i \neq 1 \). To calculate \( A_1 \) we return to the variable \( x \),

\[
S_1(x) = - \frac{1}{4} \ln(x^2 - \mu x^{2m}) - \frac{E_0}{4(m-1)} \ln \left[ \frac{4}{u^{2(m-1)}} \right]^{1/2} + \frac{a_1}{2(m-1)} + O(a^2),
\]

and get

\[
A_1 = - \frac{E_0}{4(m-1)} \ln \frac{4}{\mu} - \frac{a_1}{2(m-1)}.
\]

Here, we put \( s_1 = \ln \mu/[4(m-1)] \).
By calculating $K$ from Eq. (10), we obtain from Eq. (5) the WKB approximation of the wave function $\psi(x)$ needed in the numerator of Eq. (3):

$$
\psi_{\text{WKB}}^{(n)}(x) = \exp \left[ \sum_{i=0}^{1+n(m-1)} [S_i(x) - A_i] \mu^{(i-1)/(m-1)} \right].
$$

(13)

Taking into account the asymptotics of the WKB wave function for $x \to \infty$,

$$
\psi_{\text{WKB}}^{(n)}(x) = \exp \left[ \sum_{i=0}^{1+n(m-1)} (C_i - A_i) \mu^{(i-1)/(m-1)} \right] \times \exp \left[ i \mu^{1/2} x^{m+1}/(m+1) \right] \left[ 1 + O(1/x^2) \right],
$$

(14)

where $C_i$ denotes a constant term of the asymptotic expansion of $S_i(u)$ for $u \to \infty$; we obtain from Eqs. (3) and (14) the final formula for the imaginary part of the energy $\text{Im}E$:

$$
\text{Im}E = \frac{\exp \left[ 2 \text{Re} \sum_{i=0}^{1+n(m-1)} (C_i - A_i) \mu^{(i-1)/(m-1)} \right]}{\int_0^1 |\psi_{\text{RSPT}}^{(n)}(x)|^2 dx}.
$$

(15)

The real part of the $C_1$ term equals zero.

For $m = 2, 3$ all of the $S_i(u)$ terms can be calculated analytically. For $m > 3$ the numerator in Eq. (15) can be calculated for $i \neq 1$ as follows: We split the $S_i(u)$ term into two parts $S_i(u) = \int b_i(u) du + D_i(u)$, where the first term obeys the condition $\int_0^1 b_i(u) du \to \infty$. Since the $b_i$ terms are real for $u < 1$ and purely imaginary for $u > 1$, we can write

$$
\text{Re}(C_i - A_i) = \int_0^1 b_i(u) du + \text{Re}(V_i - P_i), \quad i \neq 1,
$$

(16)

where $P_i$ and $V_i$ denote the constant terms of the expansion of $D_i(u)$ near zero and infinity, respectively. If the integrals in the $S_i(u)$ terms cannot be calculated analytically we integrate them by parts until Eq. (16) can be used.

Our formula (15) has the following advantages. First, a general result similar to Eq. (15) has not been known till now and any problem had to be solved from the very beginning. Second, the explicit asymptotic matching of the functions $\psi_{\text{RSPT}}^{(n)}(x)$ and $\psi_{\text{WKB}}^{(n)}(x)$ is avoided. Further, this formula offers a systematic way of performing calculations to an arbitrary order of $\mu^{1/(m-1)}$. Finally, the advantage of Eq. (15) is that it uses only the minimal information necessary for the calculation of $\text{Im}E$.

To illustrate the use of Eq. (15) we first consider the perturbed harmonic oscillator. For this problem, we obtained, from Eq. (15),

$$
\text{Im}E = \frac{-2e^{a_1/(m-1)}(\frac{4}{\mu})^{2N/(m-1)}}{K! \Gamma(2N - K)} \times e^{-d \mu^{1/(m-1)}} \left[ 1 + R_1 \mu^{1/(m-1)} + R_2 \mu^{2/(m-1)} + \ldots \right],
$$

(17)

where

$$
d = \frac{\Gamma(\frac{1}{m-1}) \Gamma(\frac{3}{2})}{(m-1) \Gamma(\frac{3m-5}{2(m-1)})},
$$

(18)

$N = K + 1/2 + D/4$ is the principal quantum number, and $K = 0, 1, \ldots$ denotes the radial quantum number. For $m = 2$, the first correction coefficient equals

$$
R_1 = \frac{-17N^2}{2} - 3N + \frac{3\xi}{2} - \frac{5}{12} - 3Na_1 - \frac{a_1^2 - a_1}{2}. \quad (19)
$$

For $m > 2$, we obtained

$$
R_1 = \frac{\left[ N^2(m + 1) - \xi(m - 1) - \frac{m^2}{12} - \frac{m}{4} + \frac{1}{6} + Na_1 \right]}{\left( 3 - m \right) - \frac{a_1^2(m - 2)}{4} + \frac{a_2(m - 1)}{2}} \times \frac{1}{(m - 1)^2} \frac{\Gamma^{m-5/2}(m-1)}{\Gamma^{m-5/2}(m-1)}. \quad (20)
$$

For $m = 2$ and $a_i = 0$ for $i > 0$ we also derived the second correction coefficient,

$$
R_2 = \frac{1}{16} \left[ 578N^4 - 92N^3 - \frac{442}{3} N^2 - 90N + 18\xi^2 + (-204N^2 + 100N + 26)\xi - \frac{155}{18} \right]. \quad (21)
$$

where $\xi = \alpha/4 - 3/18$. The RSPT coefficients of the energy can be for large $n$ calculated via the dispersion relation [4,8,10]

$$
E_n = \frac{1}{\pi} \int_0^\infty \frac{\text{Im}E(\mu)}{\mu^{n+1}} d\mu. \quad (22)
$$

By inserting formula (17) into this equation, we obtain the large-order behavior of the RSPT coefficients:

$$
E_n = -\frac{e^{a_1/(m-1)} 2^{2N/(m-1)} (m-1)}{\pi K! \Gamma(2N - K)} \times \Gamma(m - 1) n + 2N \delta \times \left[ 1 + \frac{R_1 d}{(m - 1)n + 2N - 1} + \ldots \right]. \quad (23)
$$

Special cases of Eqs. (17)–(23) can be found in [1–4,7,9]. Only a slightly different derivation leads to Eq. (15) also in the case of the perturbed hydrogen atom. The imaginary
part of the energy equals, in this case,

$$\text{Im}E = -\frac{e^{a_i/[m-1)N]}N^{-2N-4N/(m-1)}\mu^{-2N/(m-1)}}{4K! \Gamma(2N - K)} \exp[-(2N)^{-1-2/(m-1)}d\mu^{-1/(m-1)} + (E_1/N)\delta_{m,2}]$$

$$\times \left[ 1 + R_1\mu^{1/(m-1)} + R_2\mu^{2/(m-1)} + \ldots \right],$$

(24)

where the principal quantum number equals \( N = K + l + (D - 1)/2 \), \( E_1 = -3N^2 + \alpha \), and \( a_1 = 0 \) for \( m = 2 \). The constant \( d \) is given by Eq. (18). For \( m = 2 \), we found the coefficients

$$R_1 = -14N^5 - 12N^4 - \frac{20}{3}N^3 + 2N\alpha^2$$

(25)

and

$$R_2 = \frac{2}{9}N^2[441N^8 + 261N^7 + 42N^6 - 540N^5 - 80N^4 + 9\alpha^4 + 60N\alpha^3 - (126N^4 + 45N^3 + 6N^2)\alpha^2].$$

(26)

For \( m = 3 \) and \( a_i = 0 \) for \( i > 0 \) we obtained

$$R_1 = -\pi N^2(5N^2 + 1 - 3\alpha).$$

(27)

By using Eq. (22), we also derived the large-order behavior of the RSPT coefficients:

$$E_n = -\frac{e^{a_i/[m-1)N]}N^{-2N-4N/(m-1)}\mu^{-2N/(m-1)}}{4K! \Gamma(2N - K)\pi} \left[ 2\exp[(E_1/N)\delta_{m,2}] \right]$$

$$\times \left[ 1 + \frac{2(2N)^{-1-2/(m-1)}dR_1}{(m-1)n + 2N - 1} + \ldots \right].$$

(28)

The particular cases of Eqs. (24)–(28) can be found in [5,9]. Equations (17)–(28) were also verified numerically.

We note that Eqs. (17) and (24) and Eqs. (23) and (28) are asymptotic series valid for sufficiently small \( \mu \) and large \( n \), respectively.

A more detailed report, including additional results, will be published elsewhere. Finally, we note that our method can also be extended to the problems such as those in [11].

We thank Professor H.J. Silverstone and Professor C.R. Handy for discussions. This work was supported in part by the NSERC, CFCSU, and the GACR (Grant No. 202/00/1026).


