Alternating Wentzel-Krammers-Brillouin Approximation for the Schrödinger Equation: A Rediscovering of the Bremmers Series

Yu-An Tsai∗ and Sheng D. Chao†

Institute of Applied Mechanics,
National Taiwan University, Taipei 106, Taiwan

(Dated: July 6, 2022)

We propose an extension of the Wentzel-Kramers-Brillouin (WKB) approximation for solving the Schrödinger equation. A set of coupled differential equations has been obtained by considering an ansatz of wave function with two auxiliary conditions on gauging the first and the second derivatives of the wave function, respectively. It is shown that an alternating perturbation method can be used to decouple this set of equations, yielding the well known Bremmers series. We derive an analytical scheme to approximate the wave function which consists of the usual WKB approximation as the zeroth order solution with extra correction terms up to the first order perturbation. Therefore, we call this alternative methodology the alternating WKB (a-WKB) approximation. We apply the a-WKB method to solve the eigenvalue problem of a harmonic oscillator and the scattering problem of a repulsive inverse-square (centrifugal) potential and demonstrate its supremacy over the usual WKB approximation.

I. INTRODUCTION

The Wentzel-Krammers-Brillouin theory has been one of the powerful techniques with which one can obtain analytical solutions of moderate accuracy to the Schrödinger equation [1–5]. However, like other approximation methods, the WKB theory has its limited applicability only in specific space regions, normally far away from the classical turning points. It is well known that the WKB theory works well under the conditions of a rapidly-oscillating phase associated with a slowly-varying amplitude in wave mechanics. The problems that can be solved under such conditions are usually referred to be in the semi-classical limits of quantum physics [6].

Let us first review the WKB theory. Consider the time independent Schrödinger equation in one dimension (the x coordinate) with the classical momentum \( p(x) = \sqrt{2m[E - V(x)]} \), where \( m \) is the particle mass, \( E \) is the total energy, and \( V(x) \) is the potential energy function,

\[
\psi''(x) + \frac{p^2}{\hbar^2} \psi(x) = 0
\]  

The first order WKB approximation gives the fundamental solutions,

\[
\psi(x) = \frac{1}{\sqrt{p}} e^{\pm \frac{\pi}{\hbar} \int p \, dt}
\]  

Because the Schrödinger equation is a second order linear differential equation, the complete approximated solution with a relative error of order \( \hbar \) to the exact solution should be a linear combination of the two fundamental solutions,

\[
\psi(x) = \frac{A}{\sqrt{p}} e^{\frac{\pi}{\hbar} \int p \, dt} + \frac{B}{\sqrt{p}} e^{-\frac{\pi}{\hbar} \int p \, dt}
\]  

where \( A \) and \( B \) are two undetermined constants. One can see that the WKB approximation has a simple structure regardless of how complex the potential \( V(x) \) is, as long as the phase integral can be carried out. However, the difficulty in extending the WKB theory emerges as soon as one proceeds to higher order approximations [7–9]. For example, it is a tedious task to derive the connection formulas as the order increases, because the inherent singularity in the neighborhoods of the turning points (where the classical momentum is vanishing) can lead to stronger divergence for the higher order WKB series. In fact, going beyond the leading order of WKB theory without mathematical complications is very difficult, although there exists techniques such as Borel summation of exact WKB analysis [10, 11]. Therefore, it is desirable to keep the simple solution form while improving the applicability range of the usual WKB theory.

In this paper we propose an extended WKB approximation dubbed the alternating WKB (a-WKB) method by considering a heuristic ansatz of the wave function. The theoretical approach of the a-WKB method is presented in Sec. II. In Sec. III, the a-WKB method is applied to the eigenvalue problem of a harmonic oscillator and compared with the usual WKB method. In the a-WKB method, the extra correction terms due to the concept of reflection wave are shown that the contribution appear in only amplitude, instead of in the phase in Sec. IV. The scattering problem of a particle from a repulsive inverse-square potential is investigated in Sec. V. We summarize our main findings and review previous works containing similar coupled differential equations to ours in Sec. VI.

∗ Institute of Applied Mechanics, National Taiwan University, Taipei 106, Taiwan
†sdchao@spring.iam.ntu.edu.tw
II. THEORY OF THE ALTERNATING WKB (A-WKB) APPROXIMATION

We first consider a more general ansatz of the wave function than that of Eq. (3)

\[ \psi(x) = a(x)e^{iS} + b(x)e^{-iS} \]  

(4)

where \( a(x) \) and \( b(x) \) are the two complex amplitude variables which are in general not constants. Then the indefinite phase integral is defined as follows,

\[ S(x) = \frac{1}{\hbar} \int_{x_0}^{x} \rho dt \]  

(5)

We then substitute Eq. (4) into Eq. (1) and require the following two conditions,

\[ \psi'(x) = i\frac{p}{\hbar}[a(x)e^{iS} - b(x)e^{-iS}] \]  

(6a)

\[ \psi''(x) = -\frac{p^2}{\hbar^2}[a(x)e^{iS} + b(x)e^{-iS}] \]  

(6b)

This procedure has a part of flavor in the method of variational parameters, but it is not exactly the same. The first condition implies that the variation of amplitudes \( a(x) \) and \( b(x) \) are sufficiently small compared with their respective phase terms. The second condition suggests a plane-wave like solution with the wave number being the classical momentum. Therefore, we obtain a set of coupled differential equations for the amplitude variables,

\[
\begin{cases}
    a'(x) = -\frac{p'}{2p}a(x) + \frac{p'}{2p}b(x)e^{-2iS} \\
    b'(x) = -\frac{p'}{2p}b(x) + \frac{p'}{2p}a(x)e^{2iS}
\end{cases}
\]  

(7)

We interpret these equations as follows. If a particle is moving forward (to the positive x direction from left to right), then the amplitudes \( a(x) \) refers to the forward-going wave amplitude. However, when it confronts a finite potential, a reflection wave would be generated simultaneously as the wave proceeds into the interaction regions. Thus, the amplitude \( b(x) \) refers to the backward-going wave amplitude. Such physics of incoming and reflected waves is governed by the coupling terms. One way to decouple the equations is to employ the method of averaging. Assuming the conditions of highly oscillating phases, the contributions of the inhomogeneous terms with the factors \( e^{2iS} \) and \( e^{-2iS} \), respectively, would fade away in the background. This way we can obtain the first order WKB solutions, but the interference effects are totally ignored. Instead, we use the perturbation method to explore more about the mathematical structure of these equations. Let us rewrite the coupled differential equations in the matrix form by introducing a sufficiently small bookkeeping parameter \( \epsilon \),

\[
\frac{d}{dx} \begin{bmatrix}
    a \\
    b
\end{bmatrix} = -\frac{p'}{2p} \begin{bmatrix}
    1 & e^{-2iS} \\
    -e^{2iS} & 1
\end{bmatrix} \begin{bmatrix}
    a \\
    b
\end{bmatrix} \]  

(8)

Consider now an expansion of the amplitudes, \( a(x) \) and \( b(x) \), up to the first order perturbation in \( \epsilon \),

\[
\frac{d}{dx} \begin{bmatrix}
    a_0 + \epsilon a_1 \\
    b_0 + \epsilon b_1
\end{bmatrix} = -\frac{p'}{2p} \begin{bmatrix}
    1 & -e^{-2iS} \\
    -e^{2iS} & 1
\end{bmatrix} \begin{bmatrix}
    a_0 + \epsilon a_1 \\
    b_0 + \epsilon b_1
\end{bmatrix} \]  

(9)

where \( a_0 \) and \( b_0 \) denote the unperturbed (zeroth order) terms, and \( a_1 \) and \( b_1 \) represent the perturbed terms, respectively. Accordingly, we have the unperturbed equations,

\[
\frac{d}{dx} \begin{bmatrix}
    a_0 \\
    b_0
\end{bmatrix} = -\frac{p'}{2p} \begin{bmatrix}
    a_0 \\
    b_0
\end{bmatrix} \]  

(10)

The solutions to Eq. (10) are easily obtained,

\[
\begin{bmatrix}
    a_0 \\
    b_0
\end{bmatrix} \sim \begin{bmatrix}
    1 \\
    1
\end{bmatrix} \]  

(11)

We see that these are the usual first order WKB solutions. The first order perturbation equations \( (O(\epsilon)) \) are,

\[
\frac{d}{dx} \begin{bmatrix}
    a_1 \\
    b_1
\end{bmatrix} = -\frac{p'}{2p} \begin{bmatrix}
    a_1 - b_0 e^{-2iS} \\
    b_1 - a_0 e^{2iS}
\end{bmatrix} \]  

(12)

By substituting Eq. (11) into Eq. (12), we have,

\[
\frac{d}{dx} \begin{bmatrix}
    a_1 \\
    b_1
\end{bmatrix} = -\frac{p'}{2p} \begin{bmatrix}
    a_1 - \frac{1}{\sqrt{p^2}} e^{-2iS} \\
    b_1 - \frac{1}{\sqrt{p^2}} e^{2iS}
\end{bmatrix} \]  

(13)

Eq. (13) can be solved by the Green’s function method in the region of \([0, x_0]\), namely,

\[
\frac{d}{dx} \begin{bmatrix}
    G_1(x, \xi) \\
    G_2(x, \xi)
\end{bmatrix} + \frac{p'}{2p} \begin{bmatrix}
    G_1(x, \xi) \\
    G_2(x, \xi)
\end{bmatrix} = \delta(x - \xi) \]  

(14)

where \( x_0 \) is the nearest turning point in the neighborhood of the initial point \( x = 0 \), and the impulse delta function is applied right at the point of \( x = \xi \). With the homogeneous boundary conditions, we have

\[
\begin{bmatrix}
    G_1(0, \xi) \\
    G_2(0, \xi)
\end{bmatrix} = \begin{bmatrix}
    0 \\
    0
\end{bmatrix} \]  

(15)
and the homogeneous solutions of Eq. (14) are
\[
\begin{bmatrix}
G_1(x, \xi) \\
G_2(x, \xi)
\end{bmatrix} =
\begin{bmatrix}
\frac{C_3}{\sqrt{p(\xi)}} \\
\frac{C_4}{\sqrt{p(\xi)}}
\end{bmatrix}
\text{ for } 0 < x < \xi \quad (16)
\]
and
\[
\begin{bmatrix}
G_1(x, \xi) \\
G_2(x, \xi)
\end{bmatrix} =
\begin{bmatrix}
\frac{C_3}{\sqrt{p(\xi)}} \\
\frac{C_4}{\sqrt{p(\xi)}}
\end{bmatrix}
\text{ for } \xi < x < x_0 \quad (17)
\]
where \(C_1, C_2, C_3, \) and \(C_4\) are the undetermined coefficients. Plugging the homogeneous conditions of Eq. (15) into Eq. (13), we have the Green’s functions associated with the Eq. (13), a result, we have the Green’s functions associated with the conditions are used such that
\[
\begin{bmatrix}
\frac{C_3}{\sqrt{p(\xi)}} \\
\frac{C_4}{\sqrt{p(\xi)}}
\end{bmatrix} =
\begin{bmatrix}
1 \\
1
\end{bmatrix}
\text{ for } \xi < x < x_0 \quad (18)
\]

Hence we obtain the constants \(C_3 = C_4 = \sqrt{p(\xi)}\). As a result, we have the Green’s function associated with the Eq. (19),
\[
\begin{bmatrix}
G_1(x, \xi) \\
G_2(x, \xi)
\end{bmatrix} =
\begin{bmatrix}
0 \\
0
\end{bmatrix}
\text{ for } 0 < x < \xi \quad (19)
\]
and
\[
\begin{bmatrix}
G_1(x, \xi) \\
G_2(x, \xi)
\end{bmatrix} =
\begin{bmatrix}
\frac{\sqrt{p(\xi)}}{\sqrt{p(x)}} \\
\frac{\sqrt{p(\xi)}}{\sqrt{p(x)}}
\end{bmatrix}
\text{ for } \xi < x < x_0 \quad (20)
\]
With these, we can construct the function \(a_1\) and \(b_1\),
\[
\begin{bmatrix}
a_1(x) \\
b_1(x)
\end{bmatrix} =
\begin{bmatrix}
\int_0^{x_0} G_1(x, \xi) \frac{1}{\sqrt{p(\xi)}} \frac{p'(\xi)}{2p(\xi)} e^{-2iS(\xi)} d\xi \\
\int_0^{x_0} G_2(x, \xi) \frac{1}{\sqrt{p(\xi)}} \frac{p'(\xi)}{2p(\xi)} e^{2iS(\xi)} d\xi
\end{bmatrix}
\]
\[
= \begin{bmatrix}
\frac{1}{\sqrt{p(x)}} \int_0^{x} \frac{p'(\xi)}{2p(\xi)} e^{-2iS(\xi)} d\xi \\
\frac{1}{\sqrt{p(x)}} \int_0^{x} \frac{p'(\xi)}{2p(\xi)} e^{2iS(\xi)} d\xi
\end{bmatrix} \quad (21)
\]
Now we set \(\epsilon = 1\), and obtain the first order perturbation for the amplitudes
\[
\begin{bmatrix}
a_0 + a_1 \\
b_0 + b_1
\end{bmatrix} =
\begin{bmatrix}
D_1 \frac{e^{-i\frac{a_0}{p(x)}}}{\sqrt{p(x)}} + \frac{1}{\sqrt{p(x)}} \int_0^{x} f(\xi) d\xi e^{-i\frac{a_0}{p(x)}} \\
D_2 \frac{e^{i\frac{a_0}{p(x)}}}{\sqrt{p(x)}} + \frac{1}{\sqrt{p(x)}} \int_0^{x} g(\xi) d\xi e^{i\frac{a_0}{p(x)}}
\end{bmatrix}
\]
\[
= \begin{bmatrix}
\frac{D_1}{\sqrt{p(x)}} + \frac{1}{\sqrt{p(x)}} \int_0^{x} \frac{p'(\xi)}{2p(\xi)} e^{-2iS(\xi)} d\xi \\
\frac{D_2}{\sqrt{p(x)}} + \frac{1}{\sqrt{p(x)}} \int_0^{x} \frac{p'(\xi)}{2p(\xi)} e^{2iS(\xi)} d\xi
\end{bmatrix}
\]
\[
= \begin{bmatrix}
D_1 p + \int_0^{x} \frac{p'(\xi)}{2p(\xi)} e^{-2iS(\xi)} d\xi \\
D_2 p + \int_0^{x} \frac{p'(\xi)}{2p(\xi)} e^{2iS(\xi)} d\xi
\end{bmatrix}
\]
\[
\quad (22)
\]
According to perturbation theory, it is quite resonable to put the constants \(D_1\) and \(D_2\) at the unperturbed terms instead of putting infront of whole amplitude functions \(a(x)\) and \(b(x)\). Here we properly choose the constants \(D_1\) and \(D_2\) to be the factor \(e^{\pm i\frac{a_0}{p(x)}}\). Therefore, we obtain the first order perturbation solutions of the a-WKB theory with remained constant \(D\), which can be determined by normalization,
\[
\psi_{\text{a-WKB}}(x) = D \left( \frac{e^{-i\frac{a_0}{p(x)}}}{\sqrt{p(x)}} + \frac{1}{\sqrt{p(x)}} \int_0^{x} f(\xi) d\xi \right) e^{i\frac{a_0}{p(x)}} \\
+ D \left( \frac{e^{i\frac{a_0}{p(x)}}}{\sqrt{p(x)}} + \frac{1}{\sqrt{p(x)}} \int_0^{x} g(\xi) d\xi \right) e^{-i\frac{a_0}{p(x)}}
\]
\[
\quad (23)
\]
The function \(f(x)\) and \(g(x)\) are defined as \(\frac{p'(x)}{2p(x)} e^{-2iS(x)}\) and \(\frac{p'(x)}{2p(x)} e^{2iS(x)}\). Notice that in the a-WKB theory, the correction terms appear only in the amplitude. We shall verify this statement in Sec. IV by considering the potential well problem.

III. HARMONIC OSCILLATOR

We apply the a-WKB method to the harmonic oscillator problem. We focus on the ground state because the WKB method usually gives worse approximation to the physical system at lower energy states, especially for the ground state energy. Consider a harmonic oscillator with \(m = \omega = 1\), \(E_0 = 1/2\), and the turning points \(x_0 = 1\) (the atomic units) as shown in Fig. 1. Here \(m\) is the mass, \(\omega\) is the angular frequency, \(E_0\) is the ground state energy, and \(x_0\) represents the classical turning point.

There are two distinguishing regions. The classically allowed (forbidden) region is associated with the \(x\) domain where \(E - V(x) > 0\) (\(E - V(x) < 0\)). In this case,
FIG. 2. Comparison of WKB (dotted line) and a-WKB (dashed line) approximation of ground state harmonic oscillator in the atomic unit, \( m = \hbar = 1, E_0 = 0.5 \), and exact solution (solid green line). The classically allowed region is referred to that of \([-1, 1]\). The a-WKB wave function in classical allowed region is,

\[
\psi_{aWKB}(x) = \frac{D}{\sqrt{p(x)}} \left[ e^{-i \frac{x^2}{4}} + \int_0^x f(\xi)d\xi \right] e^{\frac{i}{\hbar} \int_0^x pdt} + c.c.
\]  

(24)

Here we use the abbreviation \( c.c. \) which stands for complex conjugate. In the classically forbidden region (\( |x| > 1 \)), as \( |x| \) increases, the coupled differential equations, Eq. (6a) and Eq. (6b), reduce to a single equation since the potential of harmonic oscillator grows monotonically. Therefore, the a-WKB solution reduces to the same wave function as the first order WKB approximation. One can see that the merit of choosing the constants \( D_1 \) and \( D_2 \) to be the factor \( \mp e^{i \pi \frac{1}{4}} \) can naturally satisfy the matched asymptotic expansion in the leading order at both side of classical allowed and classical forbidden region. The overall constant \( D \) is then determined by the normalization condition. In Fig. 2 we compare the a-WKB solution with the usual WKB approximation, as well as the exact wave function. We see a significant improvement on the wave function, thus demonstrating the utility of the a-WKB approximation.

Because the a-WKB approximation contains the extra integration terms in the amplitude, it is interesting to study the well-known deficiency of the second order WKB approximation (see Fig. 3). We see that the second order WKB approximation does not even have the correct behavior around the turning point. This should be contrasted to the a-WKB approximation. The a-WKB approximation gives a better solution than the first order WKB approximation in the classical allowed region. As can be seen from Eq. (24), the a-WKB wave function is identical to the first order WKB wave function at the initial point \( x = 0 \). The perturbation due to the reflection wave starts to develop as the wave approaches to the turning point. The amplitudes in correction terms perform negative contribution, thus gradually reducing the divergent wave function and improving the solution. In contrast, the 2\(^{nd}\) order WKB wave function is a correction in the phase term so the (wrong) diverging behavior cannot be rectified.

To see more closely the details, the WKB series up to the second order is written as

\[
\psi(x) = e^{\frac{i}{\hbar} S_0(x) + S_1(x) + hS_2(x)}
\]  

(25)

where \( S_0, S_1, S_2 \) refer to the phase integral of \( \int^x pdx' \), first and second order of WKB series, repectively. By definition, the series behaves asymptotically if the following relations are satisfied,

\[
\frac{1}{\hbar} S_0(x) \gg S_1(x) \\
S_1(x) \gg hS_2(x) \\
hS_2(x) < O(1)
\]  

(26)

In Fig. 4, we compare the functions \( S_0, S_1 \) and \( S_2 \) in the classical region. We see clearly that the 2\(^{nd}\) order WKB series does not behave asymptotically in the whole region. The function \( S_2 \) is actually larger than \( S_1(x) \), and exhibits stronger divergence than the first order WKB approximation near the turning point. It is thus
clear why the a-WKB theory has its supremacy over the usual WKB approximation.

IV. QUANTIZATION CONDITION OF THE A-WKB APPROXIMATION

We found that the main contribution of correction terms in a-WKB wave function is on the amplitudes. Does it also improve the phase parts of the wave function? Infact, the quantization condition of the WKB approximation comes from the phase parts of exponent of wave function. Therefore we should derive the quantization condition associated to the a-WKB approximation to see if there has any extra correction. Consider a potential well with two simple turning points. The n-th order a-WKB wave function(n times reflections) has the form in classical allowed region

\[
\psi_{a\text{-WKB}}(z) \sim A(z) e^{i\phi(z)} \equiv e^{i\frac{S_0 + \hbar S_a}{\hbar}}
\]  

(27)

where \(S_a(z)\) is defined as

\[
e^{iS_a(z)} = \frac{1}{\sqrt{p}} e^{-i\frac{z^2}{2p}} + \int_0^z dt_1 \frac{p'}{2p} e^{-2iS_0} \int_0^{t_1} dt_2 \frac{p'}{2p} e^{2iS_0} \int_0^{t_2} dt_3 \cdots \int_0^{t_{n-1}} dt_n \frac{p'}{2p} e^{(-1)^n2iS_0}
\]  

(28)

the amplitude \(A(z) = e^{iS_a(z)}\) corresponds to reflection waves. \(S_0(z) = \frac{1}{2} \int dz \sqrt{E - V(z)}\) is now denoted as the phase integral. We raise the independent variable \(x\) to be complex variable \(z\). To represent a physical state, the a-WKB wave function should be single valued as the state evaluating along the contour \(\gamma\) which encircles the two turning points. Therefore, we have to require(Keller has suggested the same condition satisfied by the 1st order of WKB wave function)\[12\]

\[
\Delta [(S_0 + \hbar S_a)] = \oint_\gamma \frac{dz}{z} (S_0 + \hbar S_a) dz = 2n\pi\hbar
\]  

(29)

It is shown that the Eq. (29) gives the Bohr-Sommerfield quantization condition with 1/2 phase shift. Therefore, the a-WKB wave function with all order of reflections contains no extra contribution to the quantization condition(see Appendix for the derivation). This verifies the statement that the correction of the a-WKB wave function is presented purely on amplitude.

V. SCATTERING BY CENTRIFUGAL POTENTIAL

Consider a particle scattering from a three dimensional centrifugal potential of the form of \(l(l+1)/r^2\)[13][14]. The particle beam is incident from infinity, with a total energy \(E\) and the angular momentum \(l\). The classical turning point is denoted as \(r_0 = \sqrt{(l(l+1)/E)}\). We shall focus on the classically allowed region which contains the essential information we need for the scattering problem. Following the same steps of the a-WKB theory in deriving Eqs. (5) to (13), we have the Green’s function problem, now in a different spatial domain, \(r \in [r_0, \infty]\)

\[
G(r; \xi) = \begin{bmatrix} G_1(r; \xi) \\ G_2(r; \xi) \end{bmatrix} = \begin{bmatrix} C_1 \sqrt{p(\xi)} \\ C_2 \sqrt{p(\xi)} \end{bmatrix} \quad \text{for} \quad r_0 < r < \xi
\]  

(30)

\[
\tilde{G}(r; \xi) = \begin{bmatrix} G_1(r; \xi) \\ G_2(r; \xi) \end{bmatrix} = \begin{bmatrix} C_3 \sqrt{p(r)} \\ C_4 \sqrt{p(r)} \end{bmatrix} \quad \text{for} \quad \xi < r < \infty
\]  

(31)

By applying the homogeneous boundary condition at \(r \to \infty\), we have

\[
C_3 = C_4 = 0
\]  

(32)

The constants \(C_1\) and \(C_2\) can then be determined by the jump condition

\[
C_1 = C_2 = -\sqrt{p(\xi)}
\]  

(33)

The associated Green’s functions are

\[
\tilde{G}(r; \xi) = \begin{bmatrix} \sqrt{p(\xi)} \\ \sqrt{p(\xi)} \end{bmatrix} \quad \text{for} \quad r_0 < r < \xi
\]  

(34)

The particular solution of Eq. (13) corresponding to the repulsive potential is

\[
\tilde{A}_{1,p}(r) = \begin{bmatrix} a_{1,p} \\ b_{1,p} \end{bmatrix} = \int_{r_0}^{\infty} \hat{g}(r; \xi) \hat{F}(\xi) d\xi
\]  

(35)

where \(\hat{g}\) stands for a 2 by 2 matrix, and \(\hat{F}\) refers to the source term.
\[
\begin{bmatrix}
g(r; \xi) = \begin{bmatrix} G_1(r; \xi) & 0 \\ G_2(r; \xi) & 0 \end{bmatrix}
\end{bmatrix}
\]

Therefore, the particular solution is,

\[
\begin{bmatrix}
A_1^\dagger(r) = \begin{bmatrix} a_{1,p}(r) \\ b_{1,p}(r) \end{bmatrix} = \begin{bmatrix} D_1 + \frac{1}{\sqrt{\hbar}} \int_r^\infty \frac{p'}{2p} e^{-2i\xi} d\xi \\
D_2 + \frac{1}{\sqrt{\hbar}} f^\infty_r \frac{p'}{2p} e^{2i\xi} d\xi \end{bmatrix}
\end{bmatrix}
\]

where \( D_1, D_2 \) are then chosen as the factor of \( e^{\mp i\frac{\pi}{4}} \).

Finally, the a-WKB wave function is

\[
\psi_{\text{aWKB}}(r) = \frac{D}{\sqrt{p(r)}} \left( e^{-i\frac{\pi}{4}} - \int_r^\infty \frac{p'}{2p} e^{-2i\xi} d\xi \right) e^{i\frac{\pi}{4}} f^\infty_r \rho d\tau + \text{c.c.} \tag{40}
\]

where \( f^\infty_r = \sqrt{2mE - \frac{(l+1/2)^2}{r^2}} \) into the effective momentum \( p^{\text{eff}} = \sqrt{2mE - \frac{(l+1/2)^2}{r^2}} \), and the a-WKB wave function is written as,

\[
\psi_{\text{aWKB}}(r) = \frac{D}{\sqrt{p^{\text{eff}}(r)}} \left( e^{-i\frac{\pi}{4}} - \int_r^\infty \frac{p'}{2p^{\text{eff}}} e^{-2i\xi} d\xi \right) e^{i\frac{\pi}{4}} f^\infty_r \rho^{\text{eff}} d\tau + \text{c.c.} \tag{41}
\]

Setting \( m = \hbar = l = 1, \) and \( E = 0.5 \). In this case, the turning point is \( x_0 = 1.5 \), and the effective potential is

\[
p^{\text{eff}}(r) = \sqrt{(1 - \frac{4/9}{r^2})} \tag{42}
\]

In Fig. 5 we compare the a-WKB and the WKB wave functions, as well as the exact solution. We see that the a-WKB wave function performs better approximation than the usual WKB near the turning point.

VI. CONCLUDING REMARKS AND THE HISTORICAL REVIEW OF DIFFERENT APPROACHES OF THE WKB THEORY

Historically, the coupled differential equation of Eq. (7) or a similar one has been derived in several earlier works with different approaches. Each of them is very instructive to us for developing the a-WKB approximation. Therefore we intend to review these methods, briefly, in this section. Zwaan was the first one who introduced complex variables to explore the WKB theory. Following the Zwaan’s treatment, Kemble, Fröman and Fröman provided a fine analysis [7, 8, 16]. First, they give the approximate solution to the Schrödinger equation in the similar form of Eq. (4).

\[
\psi(z) = a_i(z) f_i(z) + a_v(z) f_v(z) \tag{43}
\]

where \( z \) is the complex variables, \( f_i \) and \( f_v \) are defined as

\[
\begin{cases}
f_i(z) = \frac{1}{\sqrt{\rho}} e^{i\xi} \\
f_v(z) = \frac{1}{\sqrt{\rho}} e^{-i\xi} \tag{44}
\end{cases}
\]

Impose the condition

\[
\psi'(z) = a_i f'_i + a_v f'_v \tag{45}
\]

This is physically equivalent to the short wave limit of our condition Eq. (6a), albeit using complex coordinate.
On the second condition, Kemble, Fröman and Fröman found the governing equation of \( f(z) \), which is different from our condition of Eq. (6b).

\[
f'' + \left[ \frac{p'}{p} \right]^2 - Q f = 0 \tag{46}
\]

where

\[
Q = \frac{3}{4} \left( \frac{p'}{p} \right)^2 - \frac{p''}{2p} \tag{47}
\]

Having Eq. (43) to Eq. (47), they obtained the coupled differential equation

\[
\begin{align*}
\{ a'_1(z) &= \frac{i\hbar}{2} \frac{Q}{p} [a_i + a_e e^{-2iS}] \\
\{ a'_2(z) &= -\frac{i\hbar}{2} \frac{Q}{p} [a_i + a_e e^{2iS}] \tag{48}
\end{align*}
\]

The Eq. (48) is similar to our coupled differential equation of Eq. (7), but it is not exactly the same because Eq. (46) and Eq. (6b) are different. On the other hand, it is shown that Bremmer’s method can be used to derive the same coupled differential equation as Eq. (7). We follow the M. V. Berry’s procedure [6] which is more straightforward. Start from the wave function

\[
\psi(x) = \psi_+ + \psi_- = \frac{b_+(x)}{\sqrt{p(x)}} e^{iS(x)} + \frac{b_-(x)}{\sqrt{p(x)}} e^{-iS(x)} \tag{49}
\]

associated with the following two conditions

\[
\psi'_+(x) = -\frac{p'}{2p} \psi_+ + \frac{i\hbar}{p} \psi_+ + \frac{p'}{2p} \psi_- \tag{50}
\]

and

\[
\psi'_-(x) = -\frac{p'}{2p} \psi_- + \frac{i\hbar}{p} \psi_- + \frac{p'}{2p} \psi_+ \tag{51}
\]

Combing from Eq. (49) to Eq. (51), we have the coupled differential equations

\[
b'_\pm(x) = \frac{p'}{2p} b_\pm(x) e^{\mp 2iS} \tag{52}
\]

Eq. (52) is essentially equivalent to the coupled differential equation we derived in Eq. (7). Notice that the function \( b_-(x) \) and \( b_+(x) \) have the same effect to our amplitude functions in Eq. (4) which describe reflections when the wave confronts a nonzero potential. Instead of considering the B.C.s from Berry (\( b_+(\infty) = 1 \) and \( b_-(\infty) = 0 \)), we assume that neither \( b_+(x) \) nor \( b_-(x) \) would dominate the other one, and we give them the same weighting at the reference point, say \( x=0 \).

\[
b_+(0) = b_-(0) = 1 \tag{53}
\]

Use the conditions of Eq. (53) and integrate from \( x = 0 \), we have

\[
b_\pm(x) = 1 + \int_0^x \frac{p'}{2p} e^{\mp 2iS} dt \tag{54}
\]

Substitute into Eq. (49)

\[
\psi(x) \sim \frac{1}{\sqrt{p}} \left( 1 + \int_0^x \frac{p'}{2p} e^{-2iS} dt \right) e^{\mp \int_0^x p dt} + c.c. \tag{55}
\]

Eq. (55) corresponds to the a-WKB wave function in the pure classical allowed region. On the turning point problem, we use the connection formulas to match the wave function at classical allowed and classical forbidden region in the leading order. This essentially gives the a-WKB approximation modified by the constant \( D \) from the classical forbidden side, which can be determined by normalization condition.

\[
\psi(x) = \frac{D}{\sqrt{p}} \left( e^{-i\frac{\pi}{4}} + \int_0^x \frac{p'}{2p} e^{-2iS} dt \right) e^{\mp \int_0^x p dt} + c.c. \tag{56}
\]

The conditions of Eq. (50) and Eq. (51) proposed by Berry come from the idea of dividing the potential function into a series of steps so that we can successfully express the related function with a constant in each step. Such method was also performed by the numerical approach so-called transfer matrix [18]. In the transfer matrix method, the wave function takes the form of

\[
\psi(x) = t(x)e^{\mp p(x)x} + r(x)e^{-\mp p(x)x} \tag{57}
\]

where \( p(x) \) is the classical momentum as usual. For instance, we can write the wave function in \( j \)-th step

\[
\psi(x) = \sum_{j} t_j e^{\mp p_j(x)x} + r_j e^{-\mp p_j(x)x} \tag{58}
\]

By applying the continuous conditions on the \( \psi(x) \) and \( \psi'(x) \) at the joint between \( j \)-th, \( j+1 \)-th step and taking the first order of Taylor expansion, one can obtain

\[
\frac{d}{dx} \begin{bmatrix} t(x) \\ r(x) \end{bmatrix} = \Gamma(x) \begin{bmatrix} t(x) \\ r(x) \end{bmatrix} \tag{59}
\]

with

\[
\Gamma(x) = \begin{bmatrix} -\frac{1}{2} xp'(x) - \frac{p'}{2p} e^{-2i\pi x/\hbar} & \frac{p'}{2p} e^{-2i\pi x/\hbar} \\ \frac{p'}{2p} e^{-2i\pi x/\hbar} & \frac{1}{2} xp'(x) - \frac{p'}{2p} \end{bmatrix} \tag{60}
\]
As can be seen, the coupled differential equation of Eq. (59) is identical to Eq. (7) if we simply replace \( t(x) \) and \( r(x) \) by \( a(x) e^{-\frac{i}{2}xp}e^{iS} \) and \( b(x) e^{\frac{p}{2}xp}e^{-iS} \). However, the transfer matrix \( \Gamma(x) \) is useful to calculate the wave function only with the uncoupled differential equation, namely, ignoring off diagonal terms. As one go further to solve the wave function with the transfer matrix containing off diagonal terms, the integrands of \( \frac{\pi}{2p} e^{-2i\gamma(x)/\hbar} \) and \( \frac{p'}{2p} e^{2i\gamma(x)/\hbar} \) become mathematically cumbersome. Bremmer and Berry’s coupled differential equation of Eq. (52), as well as ours of Eq. (7) seems to be more intuitive because the complicated coupled terms in the transfer matrix \( \Gamma(x) \) are now naturally formulated in the phase integral \( e^{\pm 2iS} \) and amplitude function \( \frac{p'}{2p} \).

We have developed an alternating approximate scheme dubbed the a-WKB method by proposing an ansatz for the wave function together with two auxiliary conditions. This method is based on an extension of the usual WKB approximation with the extra perturbative correction terms in the amplitude. It is shown that a-WKB method is equivalent to the and Berry’s treamnet by using the different conditions. We have demonstrated that the a-WKB method can be applied to the harmonic oscillator problem and a scattering problem. In particular, the a-WKB approximation serves as a proper way to avoid the more involved connection formulas as one proceeds to use higher order WKB approximations. In general, the a-WKB method performs much better than the first order WKB approximation around the turning points and the resulting analytical formulas are still quite manageable mathematically.

\section*{ACKNOWLEDGMENTS}

This work was supported by the Ministry of Science and Technology of Taiwan through MOST 108-2221-E-002-002-MY3. We acknowledge the National Center for High-performance Computing (NCHC) for providing computing resources.

\section*{Appendix: Evaluating the a-WKB quantization condition}

The difference between a-WKB and Bohr-Sommerfield quantization condition has to be the second integrand of Eq. (32), which can be written as

\[
\hbar \oint_\gamma \frac{dS_1}{dz} dz = \hbar i \oint_\gamma \frac{d}{dz} \ln \left[ \frac{1}{\sqrt{p}} e^{-i\frac{\pi}{4}} + \int_0^x dt_1 \frac{p'}{2p} e^{-2iS_0} \int_0^{t_1} dt_2 \frac{p'}{2p} e^{2iS_0} \int_0^{t_2} dt_3 \ldots \int_0^{t_n} dt_{n-1} \frac{p'}{2p} e^{(-1)^n2iS_0} \right] dz \\
= \hbar i \left[ -\ln(p^{\frac{1}{2}}) \right] \text{evaluated once around the contour} + \hbar i \left[ \frac{e^{i\frac{\pi}{4}} p'}{2p} e^{-2iS_0} \int_0^{t_1} dt_1 \frac{p'}{2p} e^{2iS_0} \ldots \int_0^{t_n} dt_{n-1} \frac{p'}{2p} e^{(-1)^n2iS_0} \right] dz \tag{A.1}
\]

Because the contour encloses two turning points, we can use the argument principle such that

\[
-h i \oint_\gamma d\left(\frac{\pi}{4}\right) = -h i \ln(p^{\frac{1}{2}}) \right| \text{evaluated once around the contour} = -h i \oint_\gamma \frac{p'}{2p} dz = \hbar \frac{1}{2} \times 4\pi i = 2\pi h \tag{A.2}
\]

The remained term of the Eq. (A.1)
\[
\frac{\hbar}{i} \oint_{\Gamma} e^{i\pi \frac{p'}{2p}} e^{-2it_0} e^{2iS_0} \int_0^{t_1} dt_2 e^{2it_2} \int_0^{t_3} dt_3 \ldots \int_0^{t_n} dt_{n-1} \frac{p'}{2p} e^{(-1)^n 2it_0} d\gamma
\]

\[
\approx \frac{\hbar}{i} \oint_{\Gamma} \left( e^{i\pi \frac{p'}{2p}} e^{-2it_0} \int_0^x dt_2 e^{2it_2} \int_0^{t_3} dt_3 \ldots \int_0^{t_n} dt_{n-1} \frac{p'}{2p} e^{(-1)^n 2it_0} \right) e^{-i\pi \frac{p'}{2p}} \int_0^{t_1} dt_2 e^{2it_2} \int_0^{t_3} dt_3 \ldots \int_0^{t_n} dt_{n-1} \frac{p'}{2p} e^{(-1)^n 2it_0} d\gamma = 0
\]

(A.3)

The Eq. (A.2) gives the part of 1/2 correction to the Bohr-Sommerfield quantization condition, and the Eq. (A.3), caused by the reflection waves, turns out to be the total derivative, which is zero while evaluating once around the contour.