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R. L. Monaco and E. Capelas de Oliveira

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Reflection and transmission of waves by a complex potential—a semiclassical Jeffreys–Wentzel–Kramers–Brillouin treatment
A new approach for the Jeffrey-Wentzel-Kramers-Brillouin theory

R. L. Monaco and E. Capelas de Oliveira
Departamento de Matemática Aplicada, IMECC-UNICAMP, 13081-970 Campinas (SP) Brazil

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A new approximation to obtain solutions for the time-independent Schrödinger equation, similar to the classical Jeffrey-Wentzel-Kramers-Brillouin theory, is obtained by means of the theory of continued fractions. A particular case is discussed in detail. © 1994 American Institute of Physics.

INTRODUCTION

The Jeffrey-Wentzel-Kramers-Brillouin (JWKB) method is the most used to find the asymptotic form for the time-independent Schrödinger differential equation. The JWKB method has been a very versatile technique, namely, from quantum mechanical applications to the Sturm-Liouville differential equation for large values of the eigenvalues.

Over the past years, a considerable amount of work has been devoted to modify and extend the JWKB approximation theory, concerning higher order terms. Nevertheless, such efforts have not yielded a compact analytical form, thus, recent applications hinge on the usual JWKB.

In this paper we present a new formulation for the JWKB theory within the scheme of continued fractions. This new technique of approximation, namely, the CM-technique, for solving the linear and homogeneous second order differential equation coincides with the JWKB method until the second order of approximation. Our new method furnishes a simple recurrence relation for the estimation of all orders of approximations. The principal advantage of this new method is to present the higher order corrections in terms of a simple recurrence relation, yielding in a refined fashion the analytical asymptotic solutions.

This paper is organized as follows: In Sec. I we present the CM-technique, while in Sec. II we discuss in all details a numerical example.

I. OUTLINE OF THE METHOD

To solve the differential Schrödinger energy equation (DSEE) for $\psi: \mathbb{R} \to C$ with the potential $V: \mathbb{R} \to R$ and given certain initial conditions, we proceed as follows.

We consider a set $Q_{n+1} \in I$ and for $x_k \in Q_{n+1}$ we write $x_k = \epsilon k$, where $k = 0, 1, 2, \ldots, r$. Let us introduce the notation $\psi_k = \psi(x_k)$ and $V_k = V(x_k)$ and impose the $\psi_k$ to satisfy the following finite difference equation,

$$\frac{-\hbar^2}{2m} (\psi_{k+1} - 2\psi_k + \psi_{k-1})/\epsilon^2 + V_k \psi_k = E \psi_k,$$

where $m$ and $h$ have the usual meaning. We notice that, when we take the limit $\epsilon \to 0$, Eq. (1.1) reduces to the DSEE.

The above difference equation can be written as

$$\psi_{k+1} - \left(2 + \frac{2m}{\hbar^2} e^2(V_k - E)\right) \psi_k + \psi_{k-1} = 0.$$  (1.2)

Now, introducing the $\nabla_n$ symbol, defined as
we cast Eq. (1.2) in the form

\[ \nabla_{k+1} = 2 + \frac{2m}{\hbar^2} \epsilon^2(V_k - E) + \frac{1}{\nabla_k} - 0 \]  

and, then the \( \psi_n \) can be written as follows

\[ \psi_n = \psi_0 \left[ \prod_{k=1}^{n} \nabla_k \right], \]  

where \( \psi_0 \) is a constant.

The above continued fraction for \( \nabla_k \) can be solved via the terminator approximation, and a quadratic equations is obtained, with solutions

\[ \nabla_{0,k} \equiv 1 \pm \epsilon \sqrt{Q_k} + \frac{\epsilon^2}{2} Q_k, \]  

where we defined \( Q_k = (2m/\hbar^2)(E - V_k) \). Then, the product which appears in Eq. (1.4) can be written as follows

\[ \prod_{k=0}^{n} (1 \pm \epsilon \sqrt{Q_k}) = \exp \left( \sum_{k=0}^{n} \epsilon \ln(1 \pm \epsilon \sqrt{Q_k})^{1/2} \right). \]  

In the limit \( \epsilon \rightarrow 0 \) this expression is cast as a Riemann integral.

\[ \exp \left( \pm \sum_{k=0}^{n} \epsilon \sqrt{Q_k} \right) \approx \exp \left( \pm \int_0^x \sqrt{Q(\xi)} \, d\xi \right). \]  

This expression holds to all orders of approximation, and the terms which follow the \( \epsilon^n \) powers, with \( n > 2 \), can be omitted.

Then, the first order approximation is equivalent to the JWKB theory, i.e.,

\[ \psi \approx \exp \left( \pm \int_0^x \sqrt{Q(\xi)} \, d\xi \right). \]  

The terminator can be improved by adding a term \( \alpha_{0,n} \) such that the next iterations is

\[ (\nabla_{0,n} + \alpha_{0,n})(\nabla_{0,n-1} + \alpha_{0,n-1}) - [Q_{n-1}(E^2 + 2)(\nabla_{0,n-1} + \alpha_{0,n-1}) + 1] = 0. \]  

Imposing \( \alpha_{0,n} = \alpha_{0,n-1} \) and introducing

\[ \nabla_{0,n-1} = \nabla_{0,n} - \epsilon \frac{d}{dx} \nabla_{0,n}, \]  

we obtain another quadratic equation for \( \alpha_{0,n} \), which possesses the solutions given by
Using an expansion for the last term in Eq. (1.10), of the type

\[
\sqrt{1 \pm x} = 1 \pm \frac{x}{2} + \cdots,
\]

we get

\[
\alpha_{0,n} = -\frac{1}{4} \varepsilon \frac{1}{Q_n} \frac{d}{dx} Q_n
\]

which is equivalent to

\[
\alpha_{0,n} = -\frac{\varepsilon}{4} \frac{d}{dx} \ln(Q_{n-1}).
\]

Thus, we obtain the second order approximation, given by

\[
\psi \propto \frac{1}{Q^{1/4}} \exp \left\{ \pm \int_0^x \sqrt{Q(\xi)} \, d\xi \right\}
\]

which is exactly the second order approximation obtained also by the JWKB method.

We generalize the above procedure as follows. By considering

\[
(V_{m,n} + \alpha_{m,n})(V_{m,n-1} + \alpha_{m,n-1}) - [Q_{n-1} \varepsilon^2 + 2](V_{m,n-1} + \alpha_{m,n-1}) + 1 = 0,
\]

and introducing the relations

\[
V_{m,n-1} = V_{m,n} - \varepsilon \frac{d}{dx} V_{m,n}
\]

and

\[
V_{m,n} = V_{m+1,n} + \alpha_{m-1,n},
\]

we obtain a quadratic equation for \( \alpha_{m,n} \). Now, considering

\[
\alpha_{m,n} = \alpha_{m,n-1},
\]

we get the solutions of the quadratic equation, given by

\[
\alpha_{m,n} = -V_{m,n} + 1 \pm \sqrt{Q} \sqrt{1 - \frac{1}{eQ} \frac{d}{dx} V_{m,n}}.
\]

By using an expansion for the last term, we obtain the recurrence relation:

\[
V_{m+1,n} = 1 \pm \sqrt{Q} \frac{1}{2\sqrt{Q}} \frac{d}{dx} V_{m,n}
\]

which is equivalent to
\[ \alpha_{m,n} = \frac{1}{2\sqrt{Q}} \frac{d}{dx} (\alpha_{m-1,n}) . \]  

(1.20)

This important result allows us to compute the several iterations for \( V_{m,n} \) [Eq. (1.17)], with \( V_{0n} \) and \( \alpha_{0,n} \) satisfying (1.5) and (1.12), respectively.

As we shall see at the end of this section, the convergence of this method can be assumed for certain cases, thus in this context \( \lim_{m \to \infty} V_{m,n} = V_{\infty,n} \), then the asymptotic solution can be cast as

\[ \psi_n = \psi_0 \prod_{k=1}^{n} V_{\infty,k} , \]  

(1.21)

where \( \psi_0 \) is a constant.

In the \( \lim \epsilon \to 0 \) it can be expressed, following (1.7), in integral form as

\[ \psi_n = \psi_0 \exp \left\{ \int_0^\xi \left( \sqrt{O(\xi)} + \frac{1}{\epsilon} \sum_{m=0}^{\infty} \alpha_m(\xi) \right) d\xi \right\} . \]

When in the continuous notation, \( \alpha_{m,n} = \alpha_m(\xi) \).

Let us notice that, to justify the expansion \( \sqrt{1 \pm x} \approx 1 \pm x/2 \), we imposed the asymptotic condition, i.e.,

\[ \frac{d}{dx} V_{m,n} \ll 2Q . \]  

(1.22)

The structure of the expressions obtained by us is similar to the JWKB theory, but the numeric coefficients are, in general, different; for example, to third, fourth, and fifth order we have, respectively,

\[ \text{(CM)}_3 = \pm \int \left[ \frac{Q''}{8Q^{3/2}} - \frac{1}{8} \frac{(Q')^2}{Q^{5/2}} \right] d\xi , \]  

(1.23)

\[ \text{(JWKB)}_3 = \pm \int \left[ \frac{Q''}{8Q^{3/2}} - \frac{5}{32} \frac{(Q')^2}{Q^{5/2}} \right] d\xi , \]  

(1.24)

\[ \text{(CM)}_4 = \pm \int \left[ -\frac{Q'''}{16Q^2} + \frac{9}{32} \frac{Q''Q'}{Q^3} - \frac{5}{32} \frac{(Q')^3}{Q^4} \right] d\xi , \]  

(1.25)

\[ \text{(JWKB)}_4 = \pm \int \left[ -\frac{Q'''}{16Q^2} + \frac{9}{32} \frac{Q''Q'}{Q^3} - \frac{15}{64} \frac{(Q')^3}{Q^4} \right] d\xi , \]  

(1.26)

\[ \text{(CM)}_5 = \pm \int \left[ -\frac{Q'''}{32Q^{3/2}} - \frac{11}{64} \frac{Q''Q'}{Q^{5/2}} + \frac{9}{16} \frac{Q'''Q'}{Q^{7/2}} + \frac{7}{64} \frac{(Q')^2}{Q^{9/2}} - \frac{5}{16} \frac{(Q')^4}{Q^{11/2}} \right] d\xi , \]  

(1.27)

\[ \text{(JWKB)}_5 = \pm \int \left[ -\frac{Q'''}{32Q^{3/2}} - \frac{7}{32} \frac{Q''Q'}{Q^{7/2}} + \frac{221}{256} \frac{Q'''Q'}{Q^{9/2}} - \frac{19}{128} \frac{(Q')^2}{Q^{11/2}} + \frac{1105}{2048} \frac{(Q')^4}{Q^{13/2}} \right] d\xi , \]  

(1.28)

where the "prime" denotes differentiation.
By using the recursion relation (1.2), it is straightforward to show that \( h^{m-1} \) is the expansion parameter for the iteration corresponding to \( \alpha_m \), and it is reasonable to expect our method to converge10 in the semiclassical limit (\( \lim h \to 0 \)).

If we consider \( \nabla_n - \nabla_{n-1} = \epsilon \delta_n \) the terminator approximation will introduce errors proportional to the unknown variable \( \nabla_n - \nabla_{n-1} = \epsilon \delta_n \) (obtained by computing the difference of both roots of the quadratic equation). Then, we expect more accurate solutions as we iterate, since from the first iteration we abstract from the error the quantity \( \epsilon (dV_{\alpha,n}/dx) \) [see Eq. (1.10)].

We notice too, that the error may not diminish in the next iteration (a common feature with the JWKB method), meaning our method furnishes the exact (or quasi exact) solution on the first iterations. This feature in our method when the corresponding of the error is less than \( \epsilon (dV_{\alpha,n}/dx) \).

It is instructive to highlight the following: the eigenvalue problem and the turning points \( (Q=0) \) must be treated with the quantum mechanical13,12 continuity conditions.

On the other hand, we can obtain an analytical expression for \( \nabla_{\alpha,n} \), if we assume the series (1.19) to converge. Then, we obtain a first order differential equation, namely,

\[
\nabla_{\alpha}(x) = 1 \pm \epsilon \sqrt{Q + \frac{1}{2Q}} \frac{d
abla_{\alpha}(x)}{dx}.
\]

If we define

\[
\mathcal{F}[x] = \exp[2m(x)] \left( g_0 + 2 \int_0^x Q(\xi) \exp[-2m(\xi)] d\xi \right)
\]

with

\[
m(x) = - \int_0^x Q(\xi) d\xi
\]

thus the asymptotic expression for the wave function is cast as

\[
\psi(x) = \beta \exp \left[ \text{Re} \int_0^x \mathcal{F}(\xi) d\xi \right] \sin \left[ \text{Im} \left[ \int_0^x \mathcal{F}(\xi) d\xi \right] + \alpha \right],
\]

where the constants \( \alpha \) and \( \beta \) are determined by the initial and normalization conditions, for each system under consideration. The constant \( g_0 \) is computed via the initial conditions adjustment of \( \nabla_{\alpha} \) with the general solution of Eq. (1.29). In many cases the former is determined at \( x=0 \), yielding the expression

\[
g_0 = \frac{(\nabla_{\alpha}(0) - 1)^2}{\epsilon} \exp[-2m(0)].
\]

II. A NUMERICAL EXAMPLE

In this section we present a numerical example, by considering the potential given by

\[
Q = x^2 - 2E.
\]

Now we analyze the particular case \( E=0 \).

For the first and second orders our results are the same as in the ordinary JWKB approximation. The iterations higher than the second order of Eq. (1.18) are given by the following series
FIG. 1. The difference $d(x)$ between the exact solution and the JWKB approximation up to second order is represented by the pointed line $d(x) = \psi_+(x) - \text{JWKB}_2$; the difference between the same exact solution and the one furnished by the CM-approximation up to the tenth order is represented by the full line $d(x) = \psi_+(x) - \text{CM}_{10}$. Finally, the difference between the same exact solution and the JWKB$_{10}$ is represented by the dotted line $d(x) = \psi_+(x) - \text{JWKB}_{10}$.

\begin{equation}
- \frac{1}{2x} \sum_{n=1}^{\infty} \frac{1.3.5 \ldots (2n-1)}{(2x^2)^n}, \tag{2.2}
\end{equation}

\begin{equation}
- \frac{1}{2x} \sum_{n=1}^{\infty} \frac{(-1)^n1.3.5 \ldots (2n-1)}{(2x^2)^n}. \tag{2.3}
\end{equation}

The above expressions can be compacted using the asymptotic expansions for the integrals of the error function since for $x \gg 1$, condition (1.22) is satisfied

\begin{equation}
\int_0^x e^{-t^2} \, dt \sim \frac{1}{2x} e^{x^2} \left[ 1 + \sum_{n=1}^{\infty} \frac{1.3.5 \ldots (2n-1)}{(2x^2)^n} \right]. \tag{2.4}
\end{equation}

\begin{equation}
\int_0^x t^{-1/2} e^{-t} \, dt \sim \sqrt{\pi} \frac{e^{-x^2}}{x} \left[ 1 + \sum_{n=1}^{\infty} \frac{(-1)^n1.3.5 \ldots (2n-1)}{(2x^2)^n} \right]. \tag{2.5}
\end{equation}

Then, the asymptotic solutions can be written as

\begin{equation}
\psi_+ = \sqrt{\frac{1}{\pi x}} \exp \left[ \frac{x^2}{2} - \frac{\sqrt{\pi}}{2} \int_0^x \text{Erf}(t) e^{-t^2} \, dt + \ln \sqrt{x} \right], \tag{2.6}
\end{equation}

\begin{equation}
\psi_- = \sqrt{\frac{\pi}{x}} \exp \left[ -\frac{x^2}{2} + \frac{\sqrt{\pi}}{2} \int_0^x [\text{Erf}(t) - 1] \, dt + \ln \sqrt{x} \right], \tag{2.7}
\end{equation}

where we have used the definition for the error function

\[ \frac{\sqrt{\pi}}{2} \text{Erfi}[x] = \int_0^x e^{t^2} \, dt \]  

(2.8)

and

\[ \sqrt{\pi} \text{Erf}[x] = \int_0^{x^2} t^{-1/2} e^{-t} \, dt. \]  

(2.9)

In Fig. 1 we show the comparison between the solution given by our new method and the exact solution expressed in terms of Bessel functions

\[ \psi_+(x) = \sqrt{2} i e^{x^2/2} / \sqrt{\pi x}, \quad x \to \infty. \]  

(2.10)

Both, the asymptotic solutions (2.6) (2.7) and our CM-approximation up to the tenth order, yield essentially identical numerical values, in the interval [2, \infty).

In this example, applying our method, we did obtain an asymptotic analytical expression, avoiding the cumbersome higher order analytical scheme of the usual JWKB method.\textsuperscript{12}

It is straightforward to show that the solution obtained with the terminator approximation (1.29) yields equivalent results.

To conclude, we numerically analyze the fourth excited state of the harmonic oscillator (\( E = 9/2 \)). In Fig. 2, near the turn points, we notice a minute difference when compared to the exact solution. We remark that exactly at those points our method is at its worst [see condition (1.22)]. Nevertheless at the turning points no singularities are present, therefore it is unnecessary to define...
other approximation zones as in the JWKB theory. We believe it is instructive to remark that in the case $E=0$ [see Eqs. (2.6) and (2.7)] the logarithmic terms exactly cancel the singularities at $x=0$.

The normalizability condition for $\psi$ [see (1.32)], turns out to be extremely sensitive to the value of $g_0$, thus the eigenvalue problem requires a very sharp computational algorithm, a matter to be discussed in a future work, where we shall compare our method with other techniques.\(^4\)

Finally, we remark that the wave function amplitude decreases when the argument of the trigonometric function [see (1.32)] takes its asymptotic value $n\pi$, at the turning points.

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