Hybrid Taylor-WKB series

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Abstract. A generalized WKB approach for constructing WKB series endowed with some properties of Taylor ones is presented. Apart from the Riccati equation itself its formalism involves also the Riccati-equation’s derivatives (REDs) obtained by differentiating of the former with respect to a spatial variable. For any smooth potential barrier given in the finite spatial interval to include turning points, the zeroth-order term of presented WKB series is regular everywhere in this interval. Moreover, the more REDs are used, the more exact the zeroth-order solution is.

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1. Introduction

In 1994 year two generalized WKB approaches has been proposed - in the paper [1], for solving the Helmholtz equation, and in the papers [2, 3] (see also [4]), for solving the one-dimensional Schrödinger equation (OSE). Both are based on the same idea - to use the REDs in order to obtain WKB series regular at the turning points (later, in 2002 year, this idea has been reopened in [5]). However, despite the common idea, these approaches differ from each other, because they treat the REDs in a different way. For example, in the approach [1] the searched-for solutions are expanded traditionally in integer powers of Plank’s constant $\hbar$. While in the formalism [2, 3] the role of a small parameter is played by some function $\epsilon(x; \hbar)$ of the spatial variable $x$ and Plank’s constant. In this paper we develop the approach [2, 3, 4].

2. Formalism

Let us consider the OSE

$$\frac{d^2 \Psi}{dx^2} - Q^{(0)}(x; \hbar) \Psi = 0, \quad Q^{(0)}(x; \hbar) = \frac{2m_e}{\hbar^2} (V(x) - E);$$

where the potential $V(x)$ is zero beyond the interval $[a, b]$ and is a bounded infinitely differentiable function; $E$ is the energy of a particle; $m_e$ is its mass. It is also assumed that there are turning points in the interval $[a, b]$ whose order does not exceed $N$. Remind, if $x_0$ is the turning point of the $n$-th order (here $0 \leq n \leq N$), then

$$Q^{(0)}(x_0) = \ldots = Q^{(n-1)}(x_0) = 0; \quad Q^{(n)}(x_0) \neq 0;$$

$Q^{(k)} = d[Q^{(0)}]^k/dx^k$; if $n = 0$, points $x_0$ can be formally considered as zeroth-order turning points.

Letting, as in the standard WKB approach, $\Psi(x) = e^{S(x)}$ and $y(x) = dS(x)/dx$, we reduce solving Eq. (1) to solving the Riccati equation. However, unlike the standard WKB approach, we write down this equation together with the first $N$ REDs:

$$y^{(m+1)} + \sum_{k=0}^{m} C_k^m y^{(m-k)}y^{(k)} - Q^{(m)} = 0; \quad \frac{dy^{(N)}}{dx} + \sum_{k=0}^{N} C_k^N y^{(N-k)}y^{(k)} - Q^{(N)} = 0;$$

$m = 0, \ldots, N-1$; $y^{(k)} = dy^k/dx^k$; $C_k^m$ are the binomial coefficients. The derivatives

$$y^{(m)}(x; \hbar) \quad (m = 1, \ldots, N)$$

are considered here as independent functions to obey the set of Eqs. (3); the equality $y^{(m+1)}(x; \hbar) = dy^{(m)}(x; \hbar)/dx$ holds, provided that Eqs. (3) are solved exactly.

Let now

$$y^{(m)}(x; \hbar) = \epsilon^{-m-1}(x; \hbar)u_m(x; \hbar) \quad (m = 0, \ldots, N),$$

where $\epsilon(x; \hbar)$ is some function whose norm $\|\epsilon(x; \hbar)\|$ diminishes when $\hbar \to 0$; thereinafter the norm $\|f(x)\|$ of any function $f(x)$ is determined as the maximum value of $|f|$ in the interval $[a, b]$. Substitution of Exp. (4) into Eq. (3) yields

$$u_{m+1} + \sum_{k=0}^{m} C_k^m u_{m-k}u_k - Q_m = 0; \quad \epsilon u_N' - (N+1)\epsilon' u_N + \sum_{k=0}^{N} C_k^N u_{N-k}u_k - Q_N = 0$$

(5)
where \( m = 0, \ldots, N - 1 \); \( Q_\ell = \epsilon^{\ell+2}Q^{(\ell)}; \ell = 0, \ldots, N \); the primes denote the differentiation with respect to \( x \).

Now let us search for the solution of Eqs. (5) in the form of the expansion in integer powers of \( \epsilon(x; \hbar) \),

\[
u_n(x; \hbar) = \sum_{k=0}^m u_{m,k}(x; \hbar)\epsilon^k(x; \hbar),
\]

supposing that for any \( k \) and \( m \) the following relations are valid

\[
\left\| \frac{d^k \epsilon(x; \hbar)}{dx^k} \right\| \sim \| \epsilon(x; \hbar) \|, \quad \| Q_k(x; \hbar) \| = O(1), \quad \| u_{m,k}(x; \hbar) \| = O(1).
\]

Keeping the zeroth-order terms, we obtain

\[
u_{m+1,0} + \sum_{k=0}^m C_m^k u_{m-k,0}u_{k,0} = Q_m \quad (m = 0, \ldots, N - 1);
\]

\[
\sum_{k=0}^N C_N^k u_{N-k,0}u_{k,0} = Q_N
\]

(we have to stress once more that the functions \( Q_0, \ldots, Q_N \) are of the same order, by norm; it should be taken into account that the function \( |Q_N(x; \hbar)| \) takes its maximal value at the turning point (of the \( N \)-th order), however the ones \( |Q_0(x; \hbar)|, \ldots, |Q_{N-1}(x; \hbar)| \) approach their maxima beyond this point). In the \( \alpha \)-th order \( (\alpha = 1, 2, \ldots) \),

\[
u_{m+1,\alpha} + \sum_{k=0}^m \sum_{\gamma=0}^\alpha C_m^k u_{m-k,\gamma}u_{k,\alpha-\gamma} = 0 \quad (m = 0, \ldots, N - 1);
\]

\[
\frac{du_{N,\alpha-1}}{dx} - (N + 2 - \alpha)\frac{\epsilon'}{\epsilon}u_{N,\alpha-1} + \sum_{k=0}^N C_N^k \sum_{\gamma=0}^\alpha u_{N-k,\gamma}u_{k,\alpha-\gamma} = 0.
\]

Now we have to define the unknown function \( \epsilon(x; \hbar) \) to enter Eqs. (8) via the functions \( Q_m(x; \hbar) \) \( (m = 0, \ldots, N) \). For this purpose we will suppose that for all \( m \), \( u_{m,0} = m!a_m \) where \( a_0 = 1 \). Besides, for convenience let further \( \kappa = \epsilon^{-1} \). Then, from Eqs. (8), we obtain

\[
(m + 1)a_{m+1} + \sum_{k=0}^m a_{m-k}a_k = \frac{Q^{(m)}}{m!\kappa^{m+2}} \quad (m = 0, \ldots, N - 1);
\]

\[
\sum_{k=0}^N a_{N-k}a_k = \frac{Q^{(N)}}{N!\kappa^{N+2}}.
\]

These equations can be reduced to the algebraic equation of the \( (N+2) \)-th order for \( \kappa(x; \hbar) \). For example, for \( N = 0, \ N = 1 \) and \( N = 2 \) we have, respectively,

\[
\kappa^2 = Q^{(0)}, \quad \kappa^3 - \kappa Q^{(0)} + \frac{Q^{(1)}}{2} = 0, \quad 3\kappa^4 - 4\kappa^2 Q^{(0)} + \kappa Q^{(1)} + \left( Q^{(0)} \right)^2 - \frac{Q^{(2)}}{2} = 0.
\]

3. The relationship between small parameters \( \epsilon(x; \hbar) \) and \( \hbar \) at the turning point of the \( n \)-th order

Let us now show that there are at least two roots \( \kappa \) of Eqs. (10), such that

\[
\lim_{\hbar \to 0} |\kappa^{-1}(x; \hbar)| = 0
\]
for any point \( x \in [a, b] \). For example, let \( x \) be the turning point of the \( n \)-th order; 
\[
|Q^{(n+1)}(x)/Q^{(n)}(x)| \ll |\kappa(x; \hbar)|.
\]
The solution of Eqs. (10), at this point, can be found in the form
\[
\kappa(x; \hbar) = \hbar^{-\beta} \sum_{s=0}^\infty \tilde{\kappa}_s(x) \hbar^{s\beta}; \quad a_m(x; \hbar) = \sum_{s=0}^\infty a_{m,s}(x) \hbar^{s\beta} \quad (m = 1, \ldots, N) \tag{13}
\]
where \( \beta \) is an arbitrary positive constant. The substitution of Exps. (13) into Eqs. (10), with taking into account (2) and keeping only the main-order terms, yields that the series (13) are justified only for \( \beta = 2/(n + 2) \). In this case
\[
(m + 1)a_{m+1,0} + \sum_{k=0}^m a_{m-k,0}a_{k,0} = 0 \quad (m = 0, \ldots, n - 1, n + 1, \ldots, N - 1);
\]
and
\[
\sum_{k=0}^N a_{N-k,0}a_{k,0} = 0 \tag{14}
\]
where it is assumed that \( a_0 = a_{0,0} = 1 \). When Eqs. (14) have been solved one can find \( \tilde{\kappa}_0 \) from the equation
\[
\left[(n + 1)a_{n+1,0} + \sum_{k=0}^n a_{n-k,0}a_{k,0}\right] \tilde{\kappa}_0^{n+2} = \frac{2m_e}{n!} V^{(n)}(x_0). \tag{15}
\]
From Eq. (13) it follows that there are \( n + 2 \) complex roots \( \tilde{\kappa}_0 \) with equal absolute values at the turning point of the \( n \)-th order. This means that there are \( n + 2 \) different functions \( \kappa(x; \hbar) \) such that at this point
\[
|\kappa(x; \hbar)| \sim \hbar^{-2/(n+2)}, \tag{16}
\]
thereby the condition (12) is fulfilled for these roots. If \( n = 0 \), i.e., if \( x \) is not a turning point, then there are two roots to satisfy (12).

So, the expansion in the integer powers of \( \epsilon(x; \hbar) \) at the turning point of the \( n \)-th order is equivalent to that in the small parameter \( \hbar^{2/(n+2)} \). This is in a full agreement with the existing approaches. Far from the turning points the expansion (6) is equivalent to that in integer powers of \( \hbar \), as in the WKB-approach.

What is important, one of two relevant roots \( \kappa(x; \hbar) \) of Eqs. (10) obeys the condition (12) for any point \( x \in [a, b] \) (hereinafter this root will be denoted as \( \kappa^{(1)}(x; \hbar) \)). For other roots this condition breaks when \( x \) crosses turning points. Thus, only one root of these equations yields the function \( \epsilon(x; \hbar) \) to have a small norm in the interval \([a, b]\).

The zeroth-order solution, \( y \approx [\epsilon(x; \hbar)]^{-1} = \kappa^{(1)}(x; \hbar) \), associated with this root yields a good approximation of the exact solution of the Riccati equation in the whole interval \([a, b]\). In this case, the more the REDs are taken into account, the more precise this approximation is. We do not give a strong proof of this statement. Instead we pay reader’s attention to the fact that for a smooth potential, in the limit \( N \to \infty \), the set of Eqs. (10) for the zeroth order solution coincides with the exact set of Eqs. (3), considering that in the zeroth order \( y^{(m)} = m!a_m \kappa^{m+1} \).

As is seen, the presented WKB series like the Taylor ones includes the derivatives of the function expanded; and the larger the number considered derivatives, the more
precise the zeroth-order WKB-approximation is. In this sense the presented generalized WKB series can be considered as a hybrid Taylor-WKB series. A distinctive feature of such series is the possibility to improve the exactness of the zeroth-order WKB-approximation. Such possibility is very important, because considering of nonzero terms in asymptotic approaches is usually associated with serious mathematical problems (and our approach is not an exclusion; however, in our approach, Eqs. (9) are extra in fact).

4. Example: a linear potential

To exemplify our approach, let us consider the case when an electron with the energy $E = 0.1 \text{eV}$ impinges the linear potential $V(x) = (1 + x/d)V_0$ to be nonzero in the interval $[-d/2, d/2]$; $V_0 = 0.1 \text{eV}$, $d = 100 \text{nm}$. In such setting the point $x = 0$ is a turning point of the first order.

Figs. 1 and 2 show, respectively, the absolute values of the solutions of the second and first equations (11) as well as those of the exact solution of the Riccati equation
\[ y(x) = \rho \frac{Bi'(\rho x) + i \cdot Ai'(\rho x)}{Bi(\rho x) + i \cdot Ai(\rho x)} \]  
(17)
where $Ai$ and $Bi$ are the Airy functions, $Ai'$ and $Bi'$ are their first derivatives, respectively; $i = \sqrt{-1}$, $\rho \approx 7.055 \cdot 10^{-2} \text{nm}^{-1}$; the solution is obtained with the help of the Maple programme. Solution (17) is evident to correspond to the solution $\Psi(x) = Bi(\rho x) + i \cdot Ai(\rho x)$ of Eq. (1).

Fig. 1 shows that in the limit $x \to \infty$ the condition (12) holds for the roots 1 and 3, while in the limit $x \to \infty$ it does for the roots 1 and 2 which are the complex conjugates to each other in this region. Thus, $\kappa^{(1)}(x; \hbar)$ is the root 1 for $N = 1$. For $N = 2$ (see Fig. 2) the same numeration is used for relevant roots.

The roots $\kappa^{(1)}(x; \hbar)$ of Eqs. (11) which give the best approximation of $y(x)$ for $N = 0$, $N = 1$ and $N = 2$ can be presented in an analytical form as follows. For $N = 0$ (the first equation in the set (11)), $\kappa^{(1)}(x; \hbar) = [(Q^{(0)}(x; \hbar))^1/2]$; hereinafter, $-\pi/n \leq \text{arg}(z^{1/n}) \leq \pi/n$ for any complex $z$ and integer $n$; besides, we take into account here that if $z$ is a complex root of an algebraic equation with real coefficients, then its complex conjugate $z^*$ is its root too.

For $N = 1$ (the second equation in the set of Eqs. (11))
\[ \kappa^{(1)}(x; \hbar) = \frac{1}{2}(A_1 + A_2) - \frac{\sqrt{3}}{2}(A_1 - A_2), \] 
(18)
$A_{1,2} = \text{surd}(r \pm \sqrt{q^3 + r^2}, 3)$; $q = -\frac{Q^{(0)}(x)}{3}$, $r = -\frac{Q^{(1)}(x)}{4}$;

here $\text{surd}(z, 3)$ is the Maple’s function of a complex variable $z$: if $\Re(z) \geq 0$ then $\text{surd}(z, 3) = z^{1/3}$; otherwise, $\text{surd}(z, 3) = -(z)^{1/3}$; note that when the function $z^{1/3}$ is used straightforwardly in the Exps. (18), this analytical expression yields different roots in the different parts of the interval $[a, b]$.

From Exps. (18) it follows that far from the turning point $x = 0$ (when the term with $Q^{(1)}$, in the expression for $A_{1,2}$, is negligible) $|\kappa^{(1)}(x; \hbar)| \sim \hbar^{-1}$; but at the turning
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point itself, where \( Q^{(0)} = 0 \), \( |\kappa^{(1)}| = \sqrt{|Q^{(1)}/2|} \sim \hbar^{-2/3} \) (see also (16)).

Lastly, for \( N = 2 \) (the third equation in the set (11)) we have

\[
\kappa^{(1)}(x; \hbar) = -u(x) + \sqrt{(u(x))^2 - v(x)},
\]

\[
u = \frac{1}{2} \sqrt{z(x) - a_2(x)}, \quad v = \frac{z(x)}{2} + \sqrt{\left(\frac{z(x)}{2}\right)^2 - a_0(x)},
\]

\[
a_2 = -\frac{4}{3}Q^{(0)}(x); \quad a_1 = \frac{1}{3}Q^{(1)}(x), \quad a_0 = \frac{1}{3} \left[ (Q^{(0)}(x))^2 - \frac{1}{2}Q^{(2)}(x) \right];
\]

here \( z \) is the solution of the auxiliary equation

\[
z^3 + b_2(x)z^2 + b_1(x)z + b_0(x) = 0;
\]

where \( b_2 = -a_2(x), \ b_1 = -4a_0(x), \ b_0 = 4a_0(x)a_2(x) - (a_1(x))^2 \). This solution is defined as follows

\[
z = s_1(x) + s_2(x) - \frac{b_2(x)}{3}, \quad s_{1,2} = \left[ \nu(x) \pm \sqrt{\mu(x)^3 + \nu(x)^2} \right]^{1/3},
\]

\[
\mu = \frac{b_1(x)}{3} - \frac{b_2(x)^2}{9}, \quad \nu = \frac{1}{6} [b_1(x)b_2(x) - 3b_0(x)] - \frac{b_2(x)^3}{27}.
\]

Figs. 3 and 4 show the \( x \)-dependence of the absolute values and imaginary parts, respectively, of \( \kappa^{(1)}(x; \hbar) \) obtained for \( N = 0, \ N = 1 \) and \( N = 2 \). As is seen, the more the REDs are used in the formalism, the better the zeroth-order approximation is.

We have to stress that for the potential at hand and for any \( N \) there is always such a point \( x_b \) in the region \( x > 0 \) (the below-barrier region) that \( \Im (\kappa^{(1)}(x; \hbar)) = 0 \) for \( x \geq x_b \) (see Fig. 4). At the same time for the exact solution \( y(x) \) considered here there are no regions on the \( OX \)-axis where \( \Im(y(x)) \equiv 0 \). Though \(|\Im(y(x))| \ll |\Re(y(x))|\)
Figure 2. Absolute values of the exact solution $y(x)$ (circles) and the all four roots $\kappa(x; \hbar)$ of Eq. (11) for $N = 2$.

Figure 3. Absolute values of the exact solution $y(x)$ (circles) and the roots $\kappa^{(1)}(x; \hbar)$ for $N = 0$, $N = 1$ and $N = 2$. 
Figure 4. Imaginary parts of the exact solution $y(x)$ (circles) and the roots $\kappa_1(x;\hbar)$ for $N = 0$, $N = 1$ and $N = 2$.

Figure 5. Real parts of the exact wave function $\Psi(x)$ (circles) and its zeroth-order approximations for $N = 0$, $N = 1$ and $N = 2$. 
in the below barrier region, $\Im(y(x))$ cannot be neglected in any case, because it yields the second independent real solution to the OSE, i.e., the function $Ai(\rho x)$. As regards the approximate solution $\kappa^{(1)}(x; \hbar)$, if $x_b \in [a, b]$ then in the region $[x_b, b]$ it loses this solution. However, as is seen from Fig. 4 this point shifts to the right on the OX axis when $N$ increases. Thus, to eliminate the above shortcoming, one has to include the next RED’s into the formalism of the zeroth-order approximation. For a given potential $V(x)$ and given spatial interval $[a, b]$, there exist such a value of $N$ for which $x_b > b$. This property exemplifies the above statement that the zeroth-order approximation $\kappa^{(1)}(x; \hbar)$ becomes precise in the limit $N \to \infty$.

On Figs. 5 and 6 we show, respectively, the real and imaginary parts of the exact solution $Bi(\rho x) + iAi(\rho x)$ of the OSE and its zeroth-order generalized WKB-approximations for $N = 0$, $N = 1$ and $N = 2$. As is seen, even for the exponentially decaying (for $x > 0$) function Airy $Ai(\rho x)$ the zeroth-order approximation for $N = 2$ gives a good exactness. Moreover, the real part of this approximation fits perfectly the Airy function $Bi(\rho x)$. As regards the zeroth-order approximation at $N = 0$, for this case there is no root $\kappa^{(1)}(x; \hbar)$ which would fit both the independent real solutions of the OSE in the below-barrier region ($x > 0$).

5. Conclusion

So, for constructing everywhere regular WKB-series it is suggested to include into the WKB formalism the spatial derivatives of a potential-energy function under study. WKB-series obtained in such a way are named here the Taylor-WKB ones. For a smooth potential given in the finite spatial interval the zeroth-order term of the Taylor-WKB
series yields a good approximation in the whole interval under study, including turning points if they exist. The more the derivatives of the potential are involved into the formalism, the more exact the zeroth-order approximation is. Of importance is the fact that for smooth potentials to have only the first- and/or second-order turning points, in the considered spatial region, the presented approach yields an analytical expression to be the regular approximate complex solution to the one-dimensional Schrödinger equation.

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References

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