WKB and “cubic-WKB” methods as an adiabatic approximation

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Abstract

This paper shows that WKB wave function can be expressed in the form of an adiabatic expansion. To build a bridge between two widely invoked approximation schemes seems pedagogically instructive. Further, “cubic-WKB” method that has been devised in order to overcome the divergence problem of WKB can be also presented in the form of an adiabatic approximation: The adiabatic expansion of a wave function contains a certain parameter. When this parameter is adjusted so as to make the next order correction vanish approximately, the adiabatic wave function becomes equivalent to that of the “cubic-WKB”.
I. INTRODUCTION

WKB method has been widely used in various fields of physics and chemistry. It has also been a reservoir of new ideas, e.g. the supersymmetric WKB, the exact WKB analysis and so on. In this paper we show that WKB method can be formulated as a special case of the adiabatic approximation, another widely invoked approximation scheme. To build a bridge between two seemingly different methods is pedagogically instructive. It may also be useful to improve both methods because findings in the one side could be brought to the other side. Further, the “cubic-WKB” method that has been devised in order to overcome the divergence problem of WKB is also able to be presented in the form of an adiabatic approximation: The adiabatic expansion of a wave function contains a certain parameter. When this parameter is adjusted so as to make the next order correction vanish approximately, the adiabatic wave function becomes equivalent to that of the “cubic-WKB” method.

II. ADIABATIC APPROXIMATION

Let us start with a brief summary of the adiabatic approximation for later use. Consider the following linear differential equation:

\[ \frac{dy(x)}{dx} = M(x)y(x), \]

where \( y \) is an \( N \)-dimensional vector and \( M \) is an \( N \times N \) matrix that depends on \( x \) but not on \( y \). Adiabatic eigenvalues and eigenvectors are given as follows:

\[ M(x)|n(x)\rangle = \lambda_n(x)|n(x)\rangle. \]

The expansion of \( y \) in terms of \( \{|n\rangle\} \),

\[ y(x) = \sum_{n=1}^{N} c_n(x)|n(x)\rangle, \]

is inserted into Eq. (1), and we get the equations for \( \{c_n(x)\} \):

\[ \frac{dc_n(x)}{dx} = \lambda_n(x)c_n(x) - \sum_{\ell=1}^{N} \langle n(x)|\frac{d}{dx}|f(x)\rangle c_\ell(x), \]

(4)
where \( \{ |n(x)\rangle \} \) are dual eigenvectors:

\[
|m(x)\rangle M(x) = \lambda_m(x) |m(x)\rangle ,
\]

\[
|m(x)\rangle |n(x)\rangle = \delta_{m,n} .
\]

Expecting slow variations of \( M(x) \), we introduce a small parameter \( \epsilon \) by changing \( x \) to \( \tau \) as

\[
\tau = \epsilon x .
\]

Then, Eq.(4) becomes

\[
\epsilon \frac{dc_n}{d\tau} = \lambda_n c_n - \epsilon \sum_{\ell=1}^{N} \langle n | \frac{d}{d\tau} | \ell \rangle c_\ell .
\]

We imagine \( c_1 \) is dominant and all the other coefficients \( \{c_\ell; \ell = 2, \cdots, N\} \) are small:

\[
c_1 \sim \mathcal{O}(1) , \quad c_\ell \sim \mathcal{O}(\epsilon) , \quad \ell = 2, \cdots, N ,
\]

and assume following expansions:

\[
c_1 = \exp \left( \frac{1}{\epsilon} S_0 + S_1 + \epsilon S_2 + \cdots \right) ,
\]

\[
c_\ell = \epsilon \left( f_1(\ell) + \epsilon f_2(\ell) + \cdots \right) c_1 , \quad \ell = 2, \cdots, N .
\]

Inserting Eqs. (10) and (11) into Eq.(8), and equating both sides of Eq.(8) in each order of \( \epsilon \), we can sequentially get following expressions:

\[
S_0 = \int^{\tau} \lambda_1 d\sigma = \epsilon \int^{x} \lambda_1 ds ,
\]

\[
S_1 = - \int^{\tau} \langle 1 | \frac{d}{d\sigma} | 1 \rangle d\sigma = - \int^{x} \langle 1 | \frac{d}{ds} | 1 \rangle ds ,
\]

\[
S_2 = - \sum_{m=2}^{N} \int^{\tau} \frac{\langle 1 | \frac{d}{d\sigma} | m \rangle \langle m | \frac{d}{d\sigma} | 1 \rangle}{\lambda_m - \lambda_1} d\sigma
\]

\[
= - \frac{1}{\epsilon} \sum_{m=2}^{N} \int^{x} \frac{\langle 1 | \frac{d}{ds} | m \rangle \langle m | \frac{d}{ds} | 1 \rangle}{\lambda_m - \lambda_1} ds ,
\]

where \( \sigma = \epsilon s \), and

\[
f_1(\ell) = \frac{\langle \ell | \frac{d}{d\tau} | 1 \rangle}{\lambda_\ell - \lambda_1} = \frac{1}{\epsilon} \frac{\langle \ell | \frac{d}{ds} | 1 \rangle}{\lambda_\ell - \lambda_1} , \quad \ell = 2, \cdots, N .
\]

When Eq.(11) is a time-dependent Schrödinger equation, \( S_0 \) gives the adiabatic dynamical phase and \( S_1 \) is the origin of so-called Berry’s phase.\(^{10,11}\)
III. WKB AND “CUBIC-WKB” METHODS

We will first show that a usual WKB wave function is obtained in the form of Eq. (10). Consider one-dimensional time-independent Schrödinger equaion for a particle with a mass $m$ and an energy $E$ under a potential $V(x)$:

$$
\psi(x)'' = -k^2(x)\psi(x), \quad k(x) = \sqrt{\frac{2m}{\hbar^2}(E - V(x))},
$$

where and hereafter the prime means differentiation with respect to $x$. Let us introduce following functions:

$$
y_0(x) = \psi(x), \quad y_1(x) = \frac{d\psi(x)}{dx}.
$$

Then, Eq. (16) becomes

$$
\frac{d}{dx} \begin{pmatrix} y_0(x) \\ y_1(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -k^2(x) & 0 \end{pmatrix} \begin{pmatrix} y_0(x) \\ y_1(x) \end{pmatrix}
$$

which is in the form of Eq. (1). Eigenvalues are determined by

$$
0 = \begin{vmatrix} \lambda & -1 \\ k^2(x) & \lambda \end{vmatrix} = \lambda^2 + k^2(x),
$$

from which we get

$$
\lambda_1 = ik, \quad \lambda_2 = -ik.
$$

Eigenvectors and dual eigenvectors are

$$
|\lambda_1\rangle = \begin{pmatrix} 1 \\ ik \end{pmatrix}, \quad |\lambda_2\rangle = \begin{pmatrix} 1 \\ -ik \end{pmatrix},
$$

$$
\langle \lambda_1| = \frac{1}{2} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}, \quad \langle \lambda_2| = \frac{1}{2} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}.
$$

Then we get

$$
\frac{dS_1}{dx} = -\langle \lambda_1| \frac{d}{dx} |\lambda_1\rangle = -\frac{1}{2} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} \begin{pmatrix} 0 \\ i\frac{dk}{dx} \end{pmatrix} = -\frac{1}{2} \frac{d}{dx} \log k.
$$

The approximate wave function up to the 1st order is

$$
\psi(x) = y_0(x) \approx \exp \left( \frac{1}{\epsilon} S_0 + S_1 \right) = \frac{1}{\sqrt{k(x)}} \exp \left( i \int_0^x k(s)ds \right)
$$
which is nothing but a usual WKB wave function. The adiabatic approximation breaks down at the level crossing point that is equal to the classical turning point \(k(x) = 0\). The breakdown manifests itself in the divergence of the approximate wave function, Eq. (24) at the classical turning point.

Various approaches have been devised in order to overcome this divergence problem. Especially, the authors of Ref.s 7 and 8 have successfully obtained wave functions without divergence in the whole coordinate range. Hence they named this method “divergence-free WKB”. The simplest version of this method is called “cubic-WKB” because the 0th-order wave functions are built with the use of roots of a certain cubic algebraic equation (see Eq. (29)). The outline of this method is presented below:

Introducing \(\varphi(x)\) through
\[
\psi(x) = e^{\varphi(x)},
\]
Eq. (16) reduces to
\[
(\varphi')^2 + k^2 = -\varphi''.
\]
When the term \(\varphi''\) is neglected, Eq. (26) gives the 0th-order WKB solutions, Eq. (20).

One more differentiation of Eq. (26),
\[
2\varphi'\varphi'' + 2kk' = -\varphi''',
\]
is again inserted into Eq. (26), and we get
\[
(\varphi')^3 + k^2\varphi' - kk' = \varphi'''/2.
\]
Regarding \(\varphi'''/2\) as a higher order term, the following cubic equation
\[
(\varphi')^3 + k^2\varphi' - kk' = 0
\]
gives the 0th-order “cubic-WKB” solutions. Combining three roots of Eq. (29), the authors of Ref.s 7 and 8 have succeeded in obtaining an approximate wave function without divergence in the whole range of \(x\).

We now try to express the above result in the form of Eq. (10). Since the key equation (29) is cubic instead of quadratic, we need a \(3 \times 3\) matrix \(M(x)\) and, in turn, need one more equation in addition to Eq. (18). Differentiating Eq. (16), we get
\[
\psi''' = -2kk'\psi - k^2\psi'.
\]
In addition to $y_0$ and $y_1$, we introduce $y_2 = \psi''$. Then (30) becomes

$$\begin{align*}
y''_2 &= -2kk'y_0 - k^2y_1.
\end{align*}$$

(31)

Since $y'_1$ ( = $\psi''$) is equal to both $-k^2y_0$ and $y_2$, there is room for one parameter which we denote as $\alpha$:

$$\begin{align*}
y'_1 &= \alpha y_2 - (1 - \alpha)k^2y_0.
\end{align*}$$

(32)

The parameter $\alpha$ needs not to be a constant but can depend on $x$. From Eqs. (31) and (32) together with $y'_0 = y_1$, we get

$$\begin{align*}
\frac{d}{dx}\begin{bmatrix}
y_0 \\
y_1 \\
y_2
\end{bmatrix} = \begin{bmatrix}
0 & 1 & 0 \\
(\alpha - 1)k^2 & 0 & \alpha \\
-2kk' & -k^2 & 0
\end{bmatrix}\begin{bmatrix}
y_0 \\
y_1 \\
y_2
\end{bmatrix}.
\end{align*}$$

(33)

It should be noted that the solution of Eq.(16) is also a solution of Eq.(33), but the converse statement does not hold. Hence additional conditions are necessary to select proper solutions of Eq.(33). From Eq.(33), we get

$$\begin{align*}
\frac{d}{dx}\left(\frac{y''_0 + k^2y_0}{\alpha}\right) = 0.
\end{align*}$$

(34)

Therefore, we can see that the solution of Eq.(33) with the initial condition satisfying $y_2(0) + k^2(0)y_0(0) = 0$ becomes the solution of Eq.(16).

The adiabatic eigenvalues of (33) are determined by

$$\lambda^3 + k^2\lambda + 2\alpha kk' = 0$$

(35)

which coincides with Eq.(29) if $\alpha = -1/2$. The reason of this choice will be explained below Eq.(40).

The eigenvector and dual eigenvector with eigenvalue $\lambda$ are

$$\begin{align*}
|\lambda\rangle &= \begin{bmatrix}
1 \\
\lambda \\
\frac{\lambda^2 + (1 - \alpha)k^2}{\alpha}
\end{bmatrix} = \begin{bmatrix}
1 \\
\lambda \\
-\frac{2kk' - \alpha k^2}{\lambda}
\end{bmatrix},
\end{align*}$$

(36)

$$\langle\lambda| = N^{-1}\begin{bmatrix}
\lambda + \frac{\alpha k^2}{\lambda} \\
1 \\
\frac{\alpha}{\lambda}
\end{bmatrix}, \quad N = 3\lambda + \frac{k^2}{\lambda}.$$
Then, from Eq. (13), the 1st-order term becomes
\[
\frac{dS_1}{dx} = -\langle \lambda | \frac{d}{d x} | \lambda \rangle = -\frac{3\lambda \lambda' + 2(1 - \alpha)kk' - \frac{\alpha'}{\alpha}(\lambda^2 + k^2)}{3\lambda^2 + k^2}.
\] (38)

Far away from the classical turning point, the eigenvalues which are necessary to build approximate wave functions are \( \lambda \approx \pm ik \) and
\[
\lambda^2 \approx -k^2, \quad \lambda \lambda' \approx -kk'.
\] (39)

In this case,
\[
\frac{dS_1}{dx} \approx -\frac{(1 + 2\alpha)k'}{2k}.
\] (40)

We can see the choice \( \alpha = -1/2 \) makes the 1st-order correction vanish approximately. Since the smallness of the 1st-order correction usually means small errors of the lowest-order result, this choice seems reasonable.

IV. CONCLUSION

In this work we have shown WKB as well as “cubic-WKB” methods can be expressed in the form of an adiabatic expansion. As for the “cubic-WKB” method, the adiabatic expansion of a wave function contains a certain parameter. When this parameter is chosen so as to make the 1st-order term vanish approximately, the lowest-order adiabatic wave function becomes equal to the lowest-order “cubic-WKB” wave function.

Comments on further study are in order; Since the parameter \( \alpha \) is in general a function of \( x \), we may be able to choose \( \alpha(x) \) so that the 1st-order term vanishes not approximately but exactly if we focus on a specific eigenvector. To examine what happens in this case would be worth pursuing. An \( N \)th-order WKB method, the extension of “cubic-WKB”, has been presented in Ref. 8. To extend the present result toward this direction is interesting. The authors of Refs. 7 and 8 have further extended their idea in the context of the steepest descent method.\(^{14,15}\) To investigate a relation between the present results and theirs seems also interesting.

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An additional note

After this manuscript was published in *Mod. Phys. Lett. A* 34, 1950250 (2019), I have noticed papers 16,17 discussing the relation between WKB and adiabatic approximations. I thank the author of Ref.s 16 and 17 for informing me of this work.

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