Divergence-free WKB method

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A new semiclassical approach to linear (L) and nonlinear (NL) one-dimensional Schrödinger equation (SE) is presented. Unlike the usual WKB solution, our solution does not diverge at the classical turning point. For LSE, our zeroth-order solution, when expanded in powers of \( \hbar \), agrees with the usual WKB solution \( e^{iS/\hbar}/\sqrt{\det} \) up to \( O(\hbar^0) \), where \( S \) and \( \nu \) are the classical action and the velocity, respectively. For NLSE, our zeroth-order solution includes quantum corrections to the Thomas-Fermi solution, thereby giving a smoothly decaying wave function into the forbidden region.

The WKB method allows us to derive expressions for various quantum-mechanical quantities when the action is much larger than \( \hbar \), and has been widely used in many subfields of physics and chemistry. Nevertheless, the WKB method has a serious flaw of divergence at the classical turning point, which originates from the fact that the classical trajectory is taken as the zeroth-order solution. Considerable efforts have been devoted to overcome this problem, among other things, the complex method and the uniform approximation. However, the former method cannot describe the wave function at the turning point, while the latter one requires us to resort to a comparison function that mimics the original potential and to which an analytic solution is available. This Letter presents a new semiclassical method whose zeroth-order solution is constructed upon a trajectory with quantum corrections such that the aforementioned divergence is absent. Moreover, our method gives a solution to the nonlinear Schrödinger equation (NLSE) on an equal footing.

We begin by reviewing the WKB method for the one-dimensional linear Schrödinger equation (LSE) \( -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \). Rescaling the length and the energy in units of \( l = \sqrt{2mE/\hbar^2} \) and \( h = \sqrt{2mE/\hbar^2} \), respectively, where \( l \) is a characteristic length scale of the potential \( V(x) \), LSE takes the form

\[
-\psi'' + V\psi = E\psi, \tag{1}
\]

where the prime denotes the differentiation with respect to \( x \). In Eq. (1), the length \( x \) and the energies \( E, V \) are proportional to \( \hbar^0 \) and \( \hbar^{-2} \), respectively. We introduce the action function \( \varphi(x) \) through \( \psi(x) = e^{i\varphi(x)} \), where the action is measured in units of \( \hbar \). In terms of \( \varphi(x) \), Eq. (1) takes the form

\[
(\varphi')^2 + (E - V) = -\varphi''. \tag{2}
\]

The zeroth-order WKB solution \( \varphi'_{WKB,0} \), which is obtained by neglecting \( \varphi'' \) in Eq. (2), satisfies the following equation:

\[
(\varphi'_{WKB,0})^2 + (E - V) = 0. \tag{3}
\]

The classical turning point \( x^{(c)} \) is determined by \( V(x^{(c)}) = E \). Incorporating the effect of \( \varphi'' \) perturbatively, the WKB solution \( \varphi'_{WKB} \) takes familiar forms as

\[
\varphi'_{WKB} = \begin{cases} \pm i \sqrt{E - V} - \frac{1}{2} \frac{V'}{\sqrt{E - V}} + \cdots & (V < E), \\ \pm \sqrt{V - E} - \frac{1}{2} \frac{V'}{\sqrt{V - E}} + \cdots & (V > E). \end{cases} \tag{4}
\]

We note that the WKB solution diverges at \( x^{(c)} \). This divergence originates from the fact that the classical trajectory is taken as the zeroth-order solution. Our strategy is to incorporate quantum corrections in the zeroth-order solution so as to remove the divergence.

To carry out this program, we differentiate both sides of Eq. (2) with respect to \( x \), having

\[
2\varphi'\varphi'' - V' = -\varphi''', \tag{5}
\]

and substitute \( \varphi'' \) in Eq. (2) into Eq. (3), obtaining

\[
(\varphi')^3 + (E - V)\varphi' + \frac{1}{2} V'' = \frac{1}{2} \varphi'''. \tag{6}
\]
The Schrödinger equation (11) is sufficient for Eq. (1) to hold, but it is not necessary. To show this, we add \( \varphi' \varphi'' \) to both sides of Eq. (11) and integrate the resulting equation with respect to \( x \). We then get

\[
 g \psi'^2 = (\varphi')^2 + (E - V) + \varphi'' ,
\]

where \( g \) is a constant of integration. Equation (11) can be rewritten as

\[
 - \psi'' + V \psi + g \psi^3 = E \psi .
\]

This is nothing but NLSE which includes LSE as a particular case of NLSE. The Schrödinger equation (1) is sufficient for Eq. (6) to hold, but it is not necessary. To show this, we add \( \varphi' \varphi'' \) to both sides of Eq. (6) and integrate the resulting equation with respect to \( x \). We then get

\[
 g \psi'^2 = (\varphi')^2 + (E - V) + \varphi'' ,
\]

where \( g \) is a constant of integration. Equation (7) can be rewritten as

\[
 - \psi'' + V \psi + g \psi^3 = E \psi .
\]

Our zeroth-order solution \( \varphi'_0 \), which is obtained by neglecting \( \varphi'' \) in Eq. (11), satisfies the following cubic equation

\[
 (\varphi'_0)^3 + 3p \varphi'_0 + 2q = 0 ,
\]

where \( p \equiv (E - V)/3 \) and \( q \equiv V'/4 \). Comparing Eqs. (11) and (14) with Eqs. (2) and (3), respectively, we see our zeroth-order solution \( \varphi'_0 \) gives a solution to NLSE and those to LSE, respectively.

Comparing Eqs. (6) and (9) with Eqs. (2) and (3), respectively, we see our zeroth-order solution \( \varphi'_0 \) gives a solution to NLSE and those to LSE, respectively.

From Eq. (14), it is clear that \( -\kappa \) and \( \varphi'_\pm \) give a solution to NLSE and those to LSE, respectively.

In the forbidden region, the cubic equation (14) has the following three real solutions:

\[
 \varphi'_0 = \begin{cases} 
 -\kappa, \\
 \frac{1}{2} \kappa + i k \equiv \varphi'_+, \\
 \frac{1}{2} \kappa - i k \equiv \varphi'_-, 
\end{cases}
\]

where

\[
 \kappa(x) = \frac{1}{2} \left( q + \sqrt{D} \right)^{1/3} + \frac{1}{2} \left( q - \sqrt{D} \right)^{1/3}, \\
 k(x) = \frac{\sqrt{2}}{3} \left[ \left( q + \sqrt{D} \right)^{1/3} - \left( q - \sqrt{D} \right)^{1/3} \right] .
\]

When expanded in powers of \( \hbar \), Eq. (11) reduces to

\[
 \varphi'_0 = \begin{cases} 
 -\kappa = - \frac{2}{3p} + O(\hbar^1) = \frac{1}{2} \sqrt{V'} + O(\hbar^1), \\
 \varphi'_+ = i \sqrt{3p} + \frac{2}{3p} + O(\hbar^1) = i \sqrt{E - V} - \frac{1}{2} \sqrt{V'} + O(\hbar^1), \\
 \varphi'_- = -i \sqrt{3p} + \frac{2}{3p} + O(\hbar^1) = -i \sqrt{E - V} - \frac{1}{2} \sqrt{V'} + O(\hbar^1) ,
\end{cases}
\]

where \( -\kappa \) and \( \varphi'_\pm \), respectively, correspond to the Thomas-Fermi solution (10) and the WKB solutions (4) up to \( O(\hbar^0) \). Substituting Eq. (13) into Eq. (7), we obtain

\[
 g \psi'^2 = \begin{cases} 
 E - V + O(\hbar^0) \text{ for } \varphi'_0 = -\kappa , \\
 O(\hbar^0) \text{ for } \varphi'_0 = \varphi'_+, \\
 O(\hbar^0) \text{ for } \varphi'_0 = \varphi'_-. 
\end{cases}
\]

From Eq. (13), it is clear that \( -\kappa \) and \( \varphi'_\pm \) give a solution to NLSE and those to LSE, respectively.

In the forbidden region, the cubic equation (14) has the following three real solutions:
\[ \varphi_0' = \begin{cases} -\kappa = \mp 2\sqrt{-p} \cos \left( \frac{1}{2} \arctan \frac{\sqrt{p}}{q} \right), \\ \chi_+ = \mp 2\sqrt{-p} \cos \left( \frac{1}{2} \arctan \frac{\sqrt{p}}{q} + 2\pi \right), \\ \chi_- = \mp 2\sqrt{-p} \cos \left( \frac{1}{2} \arctan \frac{\sqrt{p}}{q} - 2\pi \right), \end{cases} \tag{15} \]

where the \(-\) and \(\mp\) signs correspond to \(V' > 0\) and \(V' < 0\), respectively. When expanded in powers of \(\hbar\), Eq. (14) reduces to

\[ \varphi_0' = \begin{cases} -\kappa = \pm \sqrt{-3p} \pm \frac{3q}{3p} + \mathcal{O}(\hbar^1) = \pm \sqrt{V - E} - \frac{1}{3} \sqrt{\frac{V'}{E}} + \mathcal{O}(\hbar^1), \\ \chi_+ = \pm \sqrt{-3p} \pm \frac{3q}{3p} + \mathcal{O}(\hbar^1) = \pm \sqrt{V - E} - \frac{1}{3} \sqrt{\frac{V'}{E}} + \mathcal{O}(\hbar^1), \\ \chi_- = - \sqrt{-3p} + \mathcal{O}(\hbar^1) = \frac{1}{3} \sqrt{\frac{V'}{E}} + \mathcal{O}(\hbar^1), \end{cases} \tag{16} \]

where \(-\kappa\) and \(\chi_+\) correspond to the WKB solutions (4) up to \(O(\hbar^0)\). Substituting Eq. (16) into Eq. (7), we obtain

\[ g\psi^2 = \begin{cases} \mathcal{O}(\hbar^0) \text{ for } \varphi_0' = -\kappa, \\ \mathcal{O}(\hbar^0) \text{ for } \varphi_0' = \chi_+, \\ E - V + \mathcal{O}(\hbar^0) \text{ for } \varphi_0' = \chi_. \end{cases} \tag{17} \]

To proceed further with our analysis, we shall assume that \(V'(x) \geq 0\) \((\forall x)\). Then the wave function must decay to zero as \(x \to \infty\), \textit{i.e.}, \(\lim_{x \to \infty} \psi(x) = 0\). Consequently, in the forbidden region, \(-\kappa\) must be chosen as the zeroth-order solution \(\varphi_0'\) for both cases of LSE and NLSE. Note that, for NLSE, \(g\psi^2 = \mathcal{O}(\hbar^0)\) in Eq. (17) does not mean that \(g = 0\) but that the wave function is well damped in the forbidden region.

We are now in a position to construct our zeroth-order wave functions to LSE and NLSE. For NLSE, the zeroth-order wave function is

\[ \psi_0(x) = N \exp \left( - \int_{x^{(i)}}^x dx' \kappa(x') \right) , \tag{18} \]

where \(N\) is a normalization constant. Note that this single solution covers both allowed and forbidden regions.

For LSE, the zeroth-order wave function can be described, in general, as follows

\[ \psi_0(x) = \begin{cases} A_+ \exp \left( \int_{x^{(i)}}^x dx' \varphi_+'(x') \right) + A_- \exp \left( - \int_{x^{(i)}}^x dx' \varphi_-'(x') \right) \equiv \psi_0^+ (x < x^{(i)}), \\ \exp \left( - \int_{x^{(i)}}^x dx' \kappa(x') \right) \equiv \psi_0^- (x > x^{(i)}). \end{cases} \tag{19} \]

To determine the relation between constants \(A_+\) and \(A_-\), we note that, near \(x^{(c)}\), LSE (1) reduces to

\[ - \frac{d^2\psi}{d\xi^2} + \xi \psi = 0 , \tag{20} \]

where \(\xi \equiv [V'(x^{(c)})]^{1/3} (x - x^{(c)})\). The exact solution of Eq. (20) that satisfies the boundary condition \(\lim_{\xi \to \infty} \psi(\xi) = 0\) is the Airy function \(\text{Ai}(\xi)\) (10). In the region \(|\xi| \gg 1\), the asymptotic forms of \(\text{Ai}(\xi)\) are

\[ \text{Ai}(\xi) \sim \begin{cases} \frac{1}{2 \sqrt{\pi}} (\xi^{-1/4} \sin \left( \frac{2}{3} (\xi^{3/2} + \frac{2}{3}) \right) (\xi < 0), \\ \frac{2}{2 \sqrt{\pi} \xi^{-1/4}} \exp \left( - \frac{2}{3} \xi^{3/2} \right) (\xi > 0). \end{cases} \tag{21} \]

On the other hand, for the linear potential, where \(p = -[V'(x^{(c)})]^{2/3} / 3\) and \(q = V'(x^{(c)}) / 4\), one can integrate \(\varphi_\pm\) and \(\kappa\) in Eq. (13); then the asymptotic behavior of Eq. (13) for \(|\xi| \gg 1\) becomes

\[ \psi_0 = \begin{cases} \psi_0^+ \sim (2e)^{-2/3} \xi^{-1/4} [A_+ \exp \left( -i \left( \frac{2}{3} (-\xi)^{3/2} + \frac{2}{3} \right) \right) + A_- \exp \left( i \left( \frac{2}{3} (-\xi)^{3/2} + \frac{2}{3} \right) \right)], \\ \psi_0^- \sim \frac{i}{2} (2e)^{5/6} \xi^{-1/4} \exp \left( - \frac{2}{3} \xi^{3/2} \right), \end{cases} \tag{22} \]

For Eq. (22) to match Eq. (21), we must choose \(A_+/A_- = -1\). The zeroth-order solution (19) can thus be described as

\[ \psi_0(x) = N \exp \left( - \int_{x^{(i)}}^x dx' \kappa(x') \right) , \tag{23} \]

where

\[ \kappa = \mp \sqrt{-p} \cos \left( \frac{1}{2} \arctan \frac{\sqrt{p}}{q} \right) , \tag{24} \]

and

\[ \psi_0(x) = \begin{cases} A_+ \exp \left( \int_{x^{(i)}}^x dx' \mp \sqrt{-p} \cos \left( \frac{1}{2} \arctan \frac{\sqrt{p}}{q} + 2\pi \right) \right) \equiv \psi_0^+ (x < x^{(i)}), \\ \exp \left( - \int_{x^{(i)}}^x dx' \mp \sqrt{-p} \cos \left( \frac{1}{2} \arctan \frac{\sqrt{p}}{q} - 2\pi \right) \right) \equiv \psi_0^- (x > x^{(i)}). \end{cases} \tag{25} \]
\[ \psi_0(x) = \begin{cases} 
\psi_1 = A \exp \left( \frac{1}{2} \int_{x_0}^{x'} dx' \kappa(x') \right) \sin \left( \int_{x_0}^{x'} dx' k(x') \right) & (x < x_0), \\
\psi_{II} = \exp \left( - \frac{1}{2} \int_{x_0}^{x} dx' \kappa(x') \right) & (x > x_0), 
\end{cases} \tag{23} \]

where \( A \equiv \mp 2iA_\pm \). For \( \psi_1 \) and \( \psi_{II} \) and their first derivatives to be continuous at a certain point \( x_0 \), \( \psi_1(x_0) = \psi_{II}(x_0) \) and \( \psi_1'(x_0) = \psi_{II}'(x_0) \), \( x_0 \) and \( A \) must satisfy
\[
\tan \left( \int_{x_0}^{x} dx \kappa(x) \right) = \frac{2k(x_0)}{3\kappa(x_0)} \quad \text{and} \quad A = \exp \left( \frac{1}{2} \int_{x_0}^{x} dx \kappa(x) \right) \sec \left( \int_{x_0}^{x} dx \kappa(x) \right). 
\]

These simultaneous equations can be solved approximately, giving \( x_0 = x^{(n)} + O(\epsilon) \) and \( A = (2\epsilon)^{3/2} + O(\epsilon) \). For the linear potential \( (\epsilon = 0) \), the asymptotic behavior of \( \psi_1 (\psi_{II}) \) in Eq. (22) for \( \xi \to -\infty \) \((+\infty)\) with \( A_\pm = \mp (2\epsilon)^{3/2}/2i \) exactly agrees with that of \( \text{Ai}(\xi) \) in Eq. (21) except for an overall factor.

Our zeroth-order wave function (23) vanishes at \( x^{(n)} \) for any potential, which gives us a new quantization condition (compared with the WKB quantization condition)
\[
\frac{1}{2\pi} \oint dx \kappa(x) = \frac{1}{2} \int_{x_L^{(n)}}^{x_R^{(n)}} dx \ k(x) = n + 1 
\quad \text{(Our method)}, 
\tag{24}
\]
\[
\frac{1}{2\pi} \oint dx \kappa_{\text{WKB}}(x) = \frac{1}{2} \int_{x_L^{(n)}}^{x_R^{(n)}} dx \ k_{\text{WKB}}(x) = n + \frac{1}{2} 
\quad \text{(the WKB method)},
\]

where \( k(x) \) is given in Eq. (12), \( k_{\text{WKB}}(x) \equiv \sqrt{E - V(x)} \), \( n = 0, 1, 2, \cdots \) is the number of nodes of the wave function, and the suffixes \( L \) and \( R \) denote the left- and right-side turning points, respectively. We note that \( k(x) \) and \( x^{(n)} \) include quantum corrections, which accounts for an extra 1/2 in our quantization condition.

We have so far ignored the term \( \varphi''/2 \) on the right-hand side of Eq. (4). The effect of this term may be evaluated perturbatively, giving [1]
\[
\varphi_1' = \frac{1}{27} \left[ -\varphi_0''(V')^2 \left( \varphi_0' - \frac{\varphi_0''}{2V'} \right)^2 \left( \varphi_0' - \frac{\varphi_0''}{2V'} \right) \frac{(V')^2}{((\varphi_0')^2 + p)^3} \left( \varphi_0' - \frac{\varphi_0''}{2V'} \right)^2 \left( \varphi_0' - \frac{\varphi_0''}{2V'} \right)^2 \right] . 
\tag{25}
\]

The first-order wave function \( \psi_1(x) \) can be constructed by using \( \varphi_0' + \varphi_1' \) instead of \( \varphi_0' \).

We finally apply the zeroth-order solution \( \psi_0(x) \) and the first-order solution \( \psi_1(x) \) to a linear potential (Figs. 1 and 2), a parabolic potential \( V = x^2 \) with \( E = 17 \) (Figs. 3 and 4), and the Morse potential \( V = 900[\exp(-2x) - 2\exp(-x)] \) with \( E = -(39/2)^2 \) (Fig. 5). We also compare them with the exact solution and the WKB solution or a solution in which the Thomas-Fermi and WKB ones are combined.

As shown in the figures, the zeroth-order wave function \( \psi_0 \) does not diverge at the turning point but the error is discernible around the classical turning point \( x^{(c)} \). This small discrepancy is drastically improved by using the first-order wave function \( \psi_1 \). The error associated with the zeroth-order solution is estimated to be [1]
\[
\max \left| \frac{\psi_0 - \psi_{\text{exact}}}{\psi_{\text{exact}}} \right| \simeq 0.028 - 0.36\epsilon + O(\epsilon^2, \delta) . 
\tag{26}
\]

Equation (26) implies that our zeroth-order wave functions (18) and (23) are suitable for \( \epsilon > 0 \) rather than \( \epsilon < 0 \); when \( \epsilon < 0 \), the wave function is unstable against a small perturbation.

In conclusion, we proposed a divergence-free semiclassical method that enables us to solve LSE and NLSE on an equal footing. Our zeroth-order solution is constructed upon a trajectory that includes quantum corrections and therefore allows a rapidly converging perturbative expansion of the wave function. Our method may therefore be applied to drastically improving related semiclassical methods such as instantons [12] and periodic orbital theory [13]. The results of these subjects will be reported elsewhere.

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FIG. 1. Zeroth-order solution $\psi_0$ (dashed curve) and first-order solution $\psi_1$ (dot-dashed curve) to LSE for a linear potential, $-d^2\psi/d\xi^2 + \xi\psi = 0$. The exact solution (solid curve) and the usual WKB solution (dotted curve) are superimposed for comparison. The region around the turning point is enlarged in the inset.
FIG. 2. Zeroth-order solution $\psi_0$ (dashed curve) and first-order solution $\psi_1$ (dot-dashed curve) to NLSE for a linear potential, $-\frac{d^2\psi}{d\xi^2} + \xi\psi + \psi^3 = 0$. The exact solution (solid curve) and a solution in which the Thomas-Fermi and WKB ones are combined (dotted curve) are superimposed for comparison. The region around the turning point is enlarged in the inset.

FIG. 3. Solutions to LSE for a parabolic potential, $V = x^2$ with $E = 17$ and $\epsilon = 0.0476$. The notations are the same as FIG. 1. The region around the turning point is enlarged in the inset.
FIG. 4. Solutions to NLSE for a parabolic potential, \( V = x^2 \) with \( E = 17 \) and \( \epsilon = 0.0476 \). The notations are the same as FIG. 2. The region around the turning point is enlarged in the inset.

FIG. 5. Solutions to LSE for the Morse potential, \( V = 900[\exp(-2x) - 2\exp(-x)] \) with \( E = -(39/2)^2 \), \( \epsilon_L = 0.0982 \) and \( \epsilon_R = -0.0394 \). The notations are the same as FIG. 1. The regions around the two turning points are enlarged in the insets.