Divergence-Free WKB Method

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A new semiclassical approach to the linear and nonlinear one-dimensional Schrödinger equation is presented. For both equations our zeroth-order solutions include nonperturbative quantum corrections to the WKB solution and the Thomas-Fermi solution, thereby allowing us to make uniformly converging perturbative expansions of the wave functions. Our method leads to a new quantization condition that yields exact eigenenergies for the harmonic-oscillator and Morse potentials.

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The WKB method allows one to derive expressions for various quantum-mechanical quantities when the action is much larger than $\hbar$, and has been widely used in many fields of physics and chemistry [1–4]. However, the WKB method has a serious flaw in the divergence at the classical turning point because it is based on singular perturbation theory [5,6]. According to theory, only the zeroth-order solution is nonsingular but higher-order solutions are increasingly more singular. Since the WKB method takes the classical action as the zeroth-order solution, the singularity already appears in terms of the order of $\hbar^0$ (prefactor). This Letter presents a new semiclassical method in which nonperturbative quantum corrections are incorporated into the zeroth-order solution. Although our method is also based on singular perturbation theory, it allows us to obtain a uniformly valid wave function by solving the connection problem. Moreover, our method provides a uniformly valid 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 and $\hbar^2/2ml^2$, 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 primes denote 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. Introducing $\varphi(x)$ through $\Psi(x) = e^{\varphi(x)}$, where $\varphi(x)$ is measured in units of $\hbar$, Eq. (1) reduces to

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

We note that $(\varphi')^2$, $E - V$, and φ'' are proportional to $\hbar^{-2}$, $\hbar^{-2}$, and $\hbar^{-1}$, respectively. The zeroth-order WKB solution $\varphi'_{\mathrm{WKB},0}$, which is obtained by neglecting φ'' in Eq. (2), satisfies

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

Incorporating the effect of φ'' perturbatively, the WKB solution φ'_{WKB} takes the familiar form as

$$\varphi'_{\mathrm{WKB}} = \pm i\sqrt{E - V} - \frac{1}{4}\frac{V'}{V - E} + \cdots, \tag{4}$$

where the first and second terms are proportional to $\hbar^{-1}$ and $\hbar^0$, respectively. Equation (4) clearly shows that the singularities of φ'_{WKB} do not move upon improving the order of perturbation. This is an unavoidable feature of singular perturbation theory [5,6].

Our strategy is to incorporate quantum corrections in the zeroth-order solution. To do this, we differentiate both sides of Eq. (2) with respect to x, obtaining $2\varphi'\varphi'' - V' = -\varphi'''$. Substituting φ'' in Eq. (2) into this yields

$$(\varphi')^3 + (E - V)\varphi' + V'/2 = \varphi'''/2. \tag{5}$$

We note that $(\varphi')^3$, $(E - V)\varphi'$, V', and φ''' are proportional to $\hbar^{-3}$, $\hbar^{-3}$, $\hbar^{-2}$, and $\hbar^{-1}$, respectively. The Schrödinger equation (1) is sufficient for Eq. (5) to hold, but it is not necessary. In fact, Eq. (5) can be written as $2\varphi'[\varphi'' + (\varphi')^2 + E - V] = \frac{d}{dx}[\varphi'' + (\varphi')^2 + E - V]$ and integrated as $ge^{2\varphi} = \varphi'' + (\varphi')^2 + E - V$, where g is a constant of integration. This equation is equivalent to

$$-\Psi'' + V\Psi + g\Psi^3 = E\Psi. \tag{6}$$

This is nothing but NLSE, which includes LSE as a particular case of $g = 0$.

Our zeroth-order solution φ'_0, which is obtained by neglecting φ''' in Eq. (5), satisfies

$$(\varphi'_0)^3 + 3p\varphi'_0 + 2q = 0, \tag{7}$$

where $p \equiv (E - V)/3$ and $q \equiv V'/4$. Comparing Eqs. (5) and (7) with Eqs. (2) and (3), respectively, we see that our method is a natural extension of the WKB method. As we show below, our zeroth-order solution φ'_0 includes nonperturbative effects, and, when expanded in powers of $\hbar$, agrees with the WKB solution (4) up to $\mathcal{O}(\hbar^0)$. For $D \equiv p^3 + q^2 > 0$, Eq. (7) has three solutions: one is real and the rest are complex conjugate. For $D < 0$, all three solutions are real. A root of the discriminant of Eq. (7), $D = 0$, therefore determines our turning point $x = x^{(\mathrm{q})}$ [note that $k(x^{(\mathrm{q})}) = 0$ in Eq. (10)].

The difference between $x^{(q)}$ and the classical turning point $x^{(c)}$ is expanded as

$$x^{(q)} - x^{(c)} = \frac{3}{2}[2V'(x^{(c)})]^{-1/3}\left(1 + \frac{\epsilon}{2} + \mathcal{O}(\epsilon^2, \delta)\right), \tag{8}$$

where $\epsilon \equiv V''(x^{(c)})[2V'(x^{(c)})]^{-4/3}$ and $\delta \equiv V'''(x^{(c)}) \times [2V'(x^{(c)})]^{-5/3}$. We note that the right-hand side of Eq. (8) gives a characteristic decaying length of the wave function in the classically forbidden region [see Eq. (18)]. Our turning point $x^{(q)}$ therefore includes quantum corrections.

In the allowed region ($D > 0$), Eq. (7) has the following three solutions:

$$\varphi_0' = \begin{cases} -\kappa, \\ \kappa/2 + ik \equiv \varphi_+', \\ \kappa/2 - ik \equiv \varphi_-', \end{cases} \tag{9}$$

where $\kappa(x) \equiv (q + \sqrt{D})^{1/3} + (q - \sqrt{D})^{1/3}$ and

$$k(x) \equiv \frac{\sqrt{3}}{2}[(q + \sqrt{D})^{1/3} - (q - \sqrt{D})^{1/3}]. \tag{10}$$

When expanded in powers of $\hbar$, Eq. (9) reduces to

$$\varphi_0' = \begin{cases} -\kappa = \frac{1}{2}\frac{V'}{V-E} + \mathcal{O}(\hbar^2), \\ \varphi_+' = i\sqrt{E - V} - \frac{1}{4}\frac{V'}{V-E} + \mathcal{O}(\hbar^1), \\ \varphi_-' = -i\sqrt{E - V} - \frac{1}{4}\frac{V'}{V-E} + \mathcal{O}(\hbar^1). \end{cases} \tag{11}$$

where $-\kappa$ and $\varphi_\pm'$, respectively, agree with the Thomas-Fermi solution [7–9] and the WKB solutions (4) up to $\mathcal{O}(\hbar^1)$ and $\mathcal{O}(\hbar^0)$. Substituting Eq. (11) into Eq. (6) yields

$$g\Psi^2 = \begin{cases} E - V + \mathcal{O}(\hbar^0) & \text{for } \varphi_0' = -\kappa, \\ \mathcal{O}(\hbar^0) & \text{for } \varphi_0' = \varphi_+', \\ \mathcal{O}(\hbar^0) & \text{for } \varphi_0' = \varphi_-'. \end{cases} \tag{12}$$

In the forbidden region ($D < 0$), Eq. (7) has the following three real solutions:

$$\varphi_0' = \begin{cases} \mp 2\sqrt{-p}\cos(\frac{1}{3}\arctan\frac{\sqrt{-D}}{|q|}) = -\kappa, \\ \mp 2\sqrt{-p}\cos(\frac{1}{3}\arctan\frac{\sqrt{-D}}{|q|} + \frac{2\pi}{3}) \equiv \chi_+', \\ \mp 2\sqrt{-p}\cos(\frac{1}{3}\arctan\frac{\sqrt{-D}}{|q|} - \frac{2\pi}{3}) \equiv \chi_-', \end{cases} \tag{13}$$

where the $-$ and $+$ signs correspond to $V' > 0$ and $V' < 0$, respectively. When expanded in powers of $\hbar$, Eq. (13) reduces to

$$\varphi_0' = \begin{cases} -\kappa = \mp\sqrt{V - E} - \frac{1}{4}\frac{V'}{V-E} + \mathcal{O}(\hbar^1), \\ \chi_+' = \pm\sqrt{V - E} - \frac{1}{4}\frac{V'}{V-E} + \mathcal{O}(\hbar^1), \\ \chi_-' = \frac{1}{2}\frac{V'}{V-E} + \mathcal{O}(\hbar^2). \end{cases} \tag{14}$$

Thus $-\kappa$ and χ_+' agree with the WKB solutions (4) up to $O(\hbar^0)$. Substituting Eq. (14) into Eq. (6) yields

$$g\Psi^2 = \begin{cases} \mathcal{O}(\hbar^0) & \text{for } \varphi_0' = -\kappa, \\ \mathcal{O}(\hbar^0) & \text{for } \varphi_0' = \chi_+', \\ E - V + \mathcal{O}(\hbar^0) & \text{for } \varphi_0' = \chi_-'. \end{cases} \tag{15}$$

Because our method is based on singular perturbation theory, $\varphi_\pm'$ in Eq. (9) and $\chi_\pm'$ in Eq. (13) are discontinuous at $x^{(q)}$. However, Eq. (7) has a third solution, $-\kappa$, which is real and has no discontinuities. As we shall see later, this solution $-\kappa$ allows us to construct uniformly valid wave functions for both LSE and NLSE.

To proceed further with our analysis, we assume that $E \gtreqless V(x)$ for $x \lesseqgtr x^{(c)}$ with $E = V(x^{(c)})$. The wave function must then decay to zero as $x \to \infty$, i.e., $\lim_{x\to\infty}\Psi(x) = 0$. Consequently, in the forbidden region ($D < 0$), $-\kappa$ must be chosen as the zeroth-order solution φ_0' for both LSE and NLSE. For NLSE, $g\Psi^2 = \mathcal{O}(\hbar^0)$ in Eq. (15) does not mean $g = 0$ but that the wave function is sufficiently attenuated in the forbidden region.

We are now in a position to construct our zeroth-order solutions to LSE and NLSE. For NLSE, by using Eq. (12) to select the appropriate solution, the zeroth-order solution becomes

$$\Psi_0^{\mathrm{NL}}(x) = N\exp\left(-\int_{x^{(q)}}^{x} dx'\,\kappa(x')\right), \tag{16}$$

where N is a normalization constant. Note that this single solution covers both allowed and forbidden regions. Therefore, Ψ_0^{NL} is uniformly valid.

For LSE, from Eq. (12), we find that the zeroth-order solution $\Psi_0(x)$ is described, in general, as

$$\Psi_0(x) = \begin{cases} \Psi_{\mathrm{I}}(x) \equiv A_+\exp(\int_{x^{(q)}}^{x} dx'\,\varphi_+'(x')) + A_-\exp(\int_{x^{(q)}}^{x} dx'\,\varphi_-'(x')) & (x < x_0), \\ \Psi_{\mathrm{II}}(x) \equiv \exp(-\int_{x^{(q)}}^{x} dx'\,\kappa(x')) & (x > x_0), \end{cases} \tag{17}$$

where $x_0 (< x^{(q)})$ is a connection point to be determined later. The type-I solution $\Psi_{\mathrm{I}}(x)$ is defined for $x < x^{(q)}$, while the type-II solution $\Psi_{\mathrm{II}}(x)$ is smooth for $x \in \boldsymbol{R}$. We now solve the connection problem. To determine the relation between constants A_+ and A_-, we note that, near $x^{(c)}$, LSE (1) reduces to $-d^2\Psi/d\xi^2 + \xi\Psi = 0$, where $\xi \equiv [V'(x^{(c)})]^{1/3}(x - x^{(c)})$. The exact solution to this equation that satisfies the boundary condition $\lim_{\xi\to\infty}\Psi(\xi) = 0$ is the Airy function $\mathrm{Ai}(\xi)$ [10]. In the region $|\xi| \gg 1$, the asymptotic forms of $\mathrm{Ai}(\xi)$ are

$$\mathrm{Ai}(\xi) \sim \begin{cases} \frac{(-\xi)^{-1/4}}{\sqrt{\pi}}\sin(\frac{2}{3}(-\xi)^{3/2} + \frac{\pi}{4}) & (\xi < 0), \\ \frac{\xi^{-1/4}}{2\sqrt{\pi}}\exp(-\frac{2}{3}\xi^{3/2}) & (\xi > 0). \end{cases} \tag{18}$$

For the linear potential, where $p = -[V'(x^{(c)})]^{2/3}\xi/3$ and $q = V'(x^{(c)})/4$, one can perform integrations in Eq. (17)

to obtain asymptotic behavior for $|\xi| \gg 1$ as [11]

$$\Psi_0 = \begin{cases} \Psi_{\rm I} \sim (2e^2)^{-1/3}(-\xi)^{-1/4}[A_+ \exp(-i\{\frac{2}{3}(-\xi)^{3/2} + \frac{\pi}{4}\}) + A_- \exp(i\{\frac{2}{3}(-\xi)^{3/2} + \frac{\pi}{4}\})] & (\xi < 0), \\ \Psi_{\rm II} \sim (2e^5)^{1/6}\xi^{-1/4}\exp(-\frac{2}{3}\xi^{3/2}) & (\xi > 0). \end{cases} \tag{19}$$

For Eq. (19) to match Eq. (18), we must choose $A_+/A_- = -1$. The zeroth-order solution (17) can thus be described as

$$\Psi_0(x) = \begin{cases} \Psi_{\rm I}(x) = A\exp(\frac{1}{2}\int_{x^{(q)}}^{x} dx'\,\kappa(x'))\sin(\int_x^{x^{(q)}} dx'\,k(x')), \\ \Psi_{\rm II}(x) = \exp(-\int_{x^{(q)}}^{x} dx'\,\kappa(x')), \end{cases} \tag{20}$$

where $A \equiv \mp 2iA_\pm$. In Eq. (20), for Ψ_0 and Ψ_0' to be continuous at a certain point x_0, i.e., $\Psi_{\rm I}(x_0) = \Psi_{\rm II}(x_0)$ and $\Psi_{\rm I}'(x_0) = \Psi_{\rm II}'(x_0)$, A and x_0 must satisfy [12]

$$\tan\left(\int_{x_0}^{x^{(q)}} dx\,k(x)\right) = \frac{2k(x_0)}{3\kappa(x_0)} \quad \text{and} \quad A = \exp\left(\frac{3}{2}\int_{x_0}^{x^{(q)}} dx\,\kappa(x)\right)\csc\left(\int_{x_0}^{x^{(q)}} dx\,k(x)\right). \tag{21}$$

Equations (21) have a unique solution x_0 near $x^{(q)}$ such that $x_0 < x^{(q)}$, because $\Psi_{\rm I}$ is upwardly convex and $\Psi_{\rm II}$ is downwardly convex there. While $\Psi_{\rm I}$ ceases to be valid at $x^{(q)}$, we have avoided using it at $x^{(q)}$ by matching the wave functions at $x_0(<x^{(q)})$. Our solution Ψ_0 constructed above is therefore uniformly valid. Our method is based on the cubic algebraic equation that yields a third, nonsingular solution $-\kappa$ and shifts the connection point from $x^{(q)}$ to x_0. It is due to this shift of the connection point that our connected wave function Ψ_0 is free from divergence in any order of perturbation.

We now derive a quantization condition by assuming that $\lim_{|x|\to\infty} V(x) > E$. Since Eq. (20) vanishes at $x^{(q)}$ for any potential, we have

$$\frac{1}{2\pi}\oint dx\,k(x) = \frac{1}{\pi}\int_{x_{\rm L}^{(q)}}^{x_{\rm R}^{(q)}} dx\,k(x) = n + 1, \tag{22}$$

where $k(x)$ is defined in Eq. (10), $n = 0, 1, 2, \ldots$ is the number of nodes of the wave function, and the suffixes L and R refer to the left and right turning points, respectively. Equation (22) is to be contrasted with the WKB quantization condition $\frac{1}{2\pi}\oint dx\sqrt{E - V(x)} = \frac{1}{\pi}\int_{x_{\rm L}^{(c)}}^{x_{\rm R}^{(c)}} dx\sqrt{E - V(x)} = n + \frac{1}{2}$. For the harmonic-oscillator and Morse potentials, we can evaluate the integral in Eq. (22) by transforming it to a contour integral on the complex torus that is defined by the algebraic equation derived from Eq. (7). For the harmonic-oscillator and Morse potentials, the eigenvalues thus calculated are found to be exact [11].

We have so far ignored the term $\varphi'''/2$ on the right-hand side of Eq. (5). The effect of this term can be evaluated perturbatively, giving $\varphi_1' = \varphi_0'''/[6((\varphi_0')^2 + p)]$. The first-order solution $\Psi_1(x)$ can be constructed by using $\varphi_0' + \varphi_1'$ instead of φ_0'. We apply Ψ_0 [see Eqs. (16) and (20)] and Ψ_1 to the linear (Figs. 1 and 2), harmonic-oscillator (Fig. 3), and Morse (Fig. 4) potentials. We also compare them with the exact, WKB, and combined Thomas-Fermi and WKB solutions. The zeroth-order connected wave function Ψ_0 does not diverge at any point, as expected from singular perturbation theory, whereas the error is discernible at about $x^{(c)}$. We remark that the

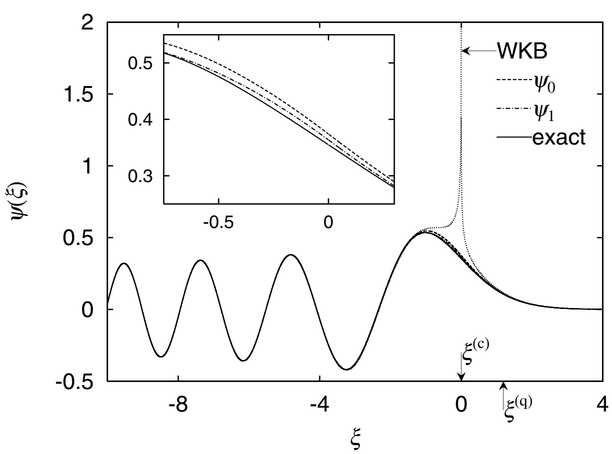

FIG. 1. Zeroth-order Ψ_0 (dashed curve) and first-order Ψ_1 (dot-dashed curve) solutions to LSE for the linear potential $-d^2\Psi/d\xi^2 + \xi\Psi = 0$. The exact solution (solid curve) and the usual WKB solution (dotted curve) are superimposed for comparison. The region around the turning point is enlarged in the inset.

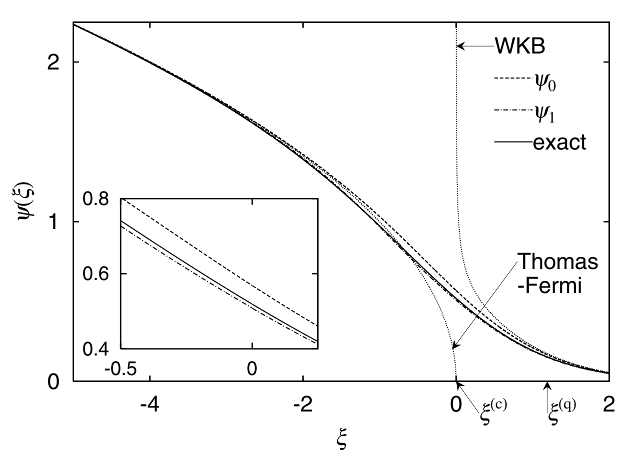

FIG. 2. Zeroth-order Ψ_0 (dashed curve) and first-order Ψ_1 (dot-dashed curve) solutions to NLSE for the linear potential $-d^2\Psi/d\xi^2 + \xi\Psi + \Psi^3 = 0$ [13]. The exact solution (solid curve) and a combined Thomas-Fermi and WKB solution (dotted curve) are superimposed for comparison. The region around the turning point is enlarged in the inset.

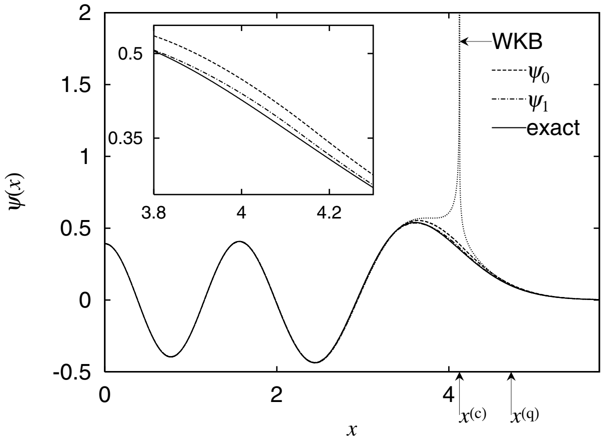

FIG. 3. Solutions to LSE for the harmonic-oscillator potential $V = x^2$ with $E = 17$. The notations are the same as those in Fig. 1. The region around the turning point is enlarged in the inset.

first-order connected wave function Ψ_1 also does not diverge anywhere [14], and the small discrepancy is seen to be drastically improved by Ψ_1.

In conclusion, we have proposed a new "cubic-WKB" method that enables us to solve LSE and NLSE on an equal footing. Our zeroth-order solution is constructed upon a trajectory that includes nonperturbative quantum corrections, thereby allowing a uniformly converging perturbative expansion of the wave function. Our method is based on singular perturbation theory and is thus a natural extension of the WKB method [15]. It may be applied to drastically improving related semiclassical methods such as instantons [16–19] and periodic orbit theory [20].

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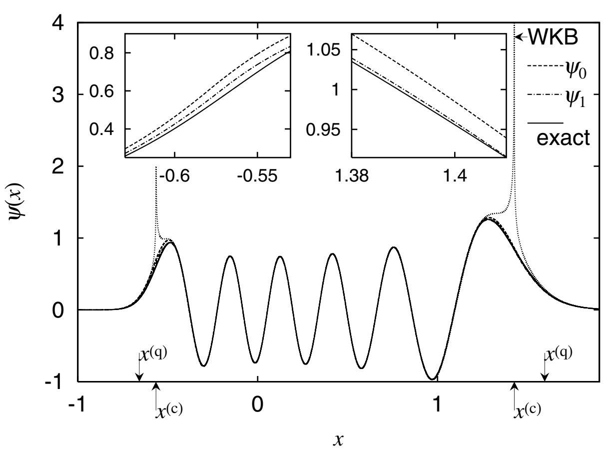

FIG. 4. Solutions to LSE for the Morse potential $V = 900[\exp(-2x) - 2\exp(-x)]$ with $E = -(39/2)^2$. The notations are the same as those in Fig. 1. The regions around the two turning points are enlarged in the insets.

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[12] For the linear potential, the simultaneous equations (21) can be solved, giving $x_0 = x^{(c)}$ and $A = (2e)^{3/2}$. Then the asymptotic behavior of Ψ_0 in Eq. (19) for $|\xi| \gg 1$ with $A_\pm = \mp(2e)^{3/2}/2i$ exactly agrees with that of $\mathrm{Ai}(\xi)$ in Eq. (18), except for an overall numerical factor.

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[14] Before the connection, the type-I first-order solution $\Psi_{1,\mathrm{I}}(x)$ defined for $x < x^{(q)}$ diverges at the turning point $x^{(q)}$, whereas the type-II first-order solution $\Psi_{1,\mathrm{II}}(x)$ does not diverge anywhere. After connecting these solutions $\Psi_{1,\mathrm{I}}(x)$ and $\Psi_{1,\mathrm{II}}(x)$ at the first-order connection point x_1, the divergence of $\Psi_{1,\mathrm{I}}(x)$ at $x^{(q)}$ does not appear in the final connected wave function $\Psi_1(x)$, since $x_1 < x^{(q)}$ (see Figs. 1, 3, and 4). Similarly, the connected wave function $\Psi_n(x)$ ($n = 0, 1, 2, \ldots$) calculated by our nth-order perturbation theory is free from the divergence anywhere. The method proposed in this Letter is therefore named the "divergence-free WKB method."

[15] For further generalization, we obtain ($n = 2, 3, \ldots$) $(\varphi')^n + \sum_{m=0}^{n-2} a_m(x)\,(\varphi')^m = (-1)^{n-1}\varphi^{(n)}/(n-1)!$ instead of Eq. (5). By neglecting $\varphi^{(n)}$, higher-order quantum corrections can be incorporated in the zeroth-order solution.

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