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LETTER TO THE EDITOR

Numerical instability in Rayleigh–Schrödinger quantum mechanics

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Abstract
The most physically interesting systems are not exactly solvable in quantum mechanics. For one-dimensional bound systems without exact solutions, we analytically and numerically find that the Rayleigh–Schrödinger perturbed series sensitively depends on an unsolvable integration, which leads to numerical instability in quantum mechanics. By using an exact formal solution of the non-homogeneous Schrödinger equation, we demonstrate the existence of analytically bound states and propose a simple scheme to truncate infinity so that the instability difficulty is avoided.

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It is well known that the fundamental equation of quantum mechanics is the Schrödinger equation, which has no exact solutions for the most physically interesting systems [1, 2]. Therefore, approximation methods are unavoidable in analytical studies of these systems. If a system differs from an exactly solvable system by only a small perturbation, one expects that Rayleigh–Schrödinger expansion [3–5] in powers of a small parameter could give perturbation corrections of the physical quantities. Unfortunately, the Rayleigh series diverges for the most practically perturbed potentials in the previous quantum theory [6–10]. Commonly, only the first-order perturbation result is rational and the higher-order results contain non-physical infinity. Although some improved perturbation techniques have been presented [11–13], convergent wavefunctions have not been included in previous works. Divergence difficulties have caused doubt in the mathematical foundations of the theory in the minds of many physicists. Dirac, among other distinguished physicists, even inferred that the fundamental equation was incorrect and suggested a radical review on the subject [14]. On the other hand, Heisenberg pointed out that the numerical orbits of many nonlinear systems that display numerical instability are ultimately unbounded [15].

Recently, we suggested a different theory for treating quantum perturbation [16–19]. Applying this theoretical method to perturbed Schrödinger systems we have avoided the divergence difficulties of non-relativistic quantum mechanics. In this Letter we will apply this method to the Rayleigh–Schrödinger series for a one-dimensional quantum system without an exact solution. We find that some corrected wavefunctions are analytically bounded but numerically unbounded, i.e. numerically unstable. The instability comes from the sensitive dependence of the numerical solutions on some unsolvable integrations. We will propose a simple scheme to truncate infinity and obtain the correct numerical results.

For simplicity we only consider the one-dimensional stationary and perturbed Schrödinger equation [1–3]

$$\tfrac{1}{2}\psi_{xx} - [V(x) - E]\psi = H'(x)\psi \qquad |H'(x)| \ll |V(x)| \tag{1}$$

where $\psi(x)$ and E are the wavefunction and energy of the system, $V(x)$ is the potential of an exactly solvable system and $H'(x)$ the additional perturbed potential which leads to insolubility. Here and throughout the Letter we adopt atomic units such that $\hbar = \mu = e = 1$. Setting two fundamental solutions of the solvable system as $\psi_k^{(0)}$ and using Refs [16, 17] gives

$$\tilde{\psi}_k^{(0)} = \psi_k^{(0)} \int (\psi_k^{(0)})^{-2}\,\mathrm{d}x \tag{2}$$

where $\psi_k^{(0)}(x)$ is a bound state solution of the unperturbed Schrödinger equation with the boundary conditions $\psi_k^{(0)}(\pm\infty) = \psi_{k,x}^{(0)}(\pm\infty) = 0$. Then applying the l'Hospital rule to equation (2) we derive the limit

$$\lim_{t\to\pm\infty} |\tilde{\psi}_k^{(0)}| = \lim_{t\to\pm\infty} |\psi_{k,x}^{(0)}|^{-1} = \infty \qquad \text{for} \quad \lim_{t\to\pm\infty} \psi_k^{(0)} = \lim_{t\to\pm\infty} \psi_{k,x}^{(0)} = 0. \tag{3}$$

The unbounded $\tilde{\psi}_k^{(0)}$ does not represent any physical state, but it is useful for constructing the exact formal solutions of the non-homogeneous Schrödinger equations.

The well known Rayleigh–Schrödinger perturbation expansions read

$$\psi = \sum_{i=0}^{\infty} \lambda^i \psi_k^{(i)} \qquad E = \sum_{i=0}^{\infty} \lambda^i E_k^{(i)} \qquad \text{for} \quad H'(x) = \lambda W(x) \qquad |\lambda| \ll 1 \tag{4}$$

with λ being a small dimensionless parameter. Substituting equations (4) into (1) and equating the coefficients of each power of λ for both sides yields the set of equations

$$\begin{aligned} &\tfrac{1}{2}\psi_{k,xx}^{(i)} - [V(x) - E_k^{(0)}]\psi_k^{(i)} = \varepsilon_k^{(i)} \qquad i = 0, 1, 2, \ldots, \infty \\ &\varepsilon_k^{(0)} = 0 \qquad \varepsilon_k^{(i)} = W(x)\psi_k^{(i-1)} - \sum_{j=1}^{i} E_k^{(j)}\psi_k^{(i-j)} \qquad i = 1, 2, \ldots, \infty. \end{aligned} \tag{5}$$

For sufficiently small λ the Rayleigh series in equation (4) should be convergent, if the solutions $\psi_k^{(i)}$ of equation (5) are bounded. Obviously, equation (5) is a set of non-homogeneous Schrödinger equations with the non-homogeneous terms $\varepsilon_k^{(i)}(x)$. Knowing the solutions $\psi_k^{(0)}$ and $\tilde{\psi}_k^{(0)}$ of the corresponding homogeneous equations, the constant variation method gives the formal general solution [16–19]

$$\psi_k^{(i)} = 2\tilde{\psi}_k^{(0)}\left(A_k^{(i)} + \int_{-\infty}^{x} \psi_k^{(0)}\varepsilon_k^{(i)}\,\mathrm{d}x\right) - 2\psi_k^{(0)}\left(B_k^{(i)} + \int_{0}^{x} \tilde{\psi}_k^{(0)}\varepsilon_k^{(i)}\,\mathrm{d}x\right) \tag{6}$$

of equation (5) for $i = 1, 2, \ldots,$ where $A_k^{(i)}$ and $B_k^{(i)}$ are arbitrary constants adjusted by the boundary conditions and normalization. These exact general solutions contain all of the special solutions, the bounded and unbounded, which are determined by the constants $A_k^{(i)}$ and $B_k^{(i)}$.

The unbounded function $\tilde{\psi}_k^{(0)}$ indicates the existence of infinity in equation (6) at the infinite boundaries and makes no sense of the corrected wavefunctions in equation (6). However, application of the l'Hospital rule can readily prove that these corrections vanish as $x \to \pm\infty$ if and only if the boundary conditions

$$I_{\pm}^{(i)} = \lim_{x\to\pm\infty}\left[A_k^{(i)} + \int_{-\infty}^{x} \psi_k^{(0)}\varepsilon_k^{(i)}\,\mathrm{d}x\right] = 0 \qquad i = 1, 2, \ldots, \infty \tag{7}$$

are satisfied. Under the conditions using l'Hospital rule and equations (3)–(6) yields the limit

$$\begin{aligned}
\lim_{x\to\pm\infty} \psi_k^{(i)} &= 2 \lim_{x\to\pm\infty}\left[\frac{\psi_k^{(0)}\varepsilon_k^{(i)}}{[(\tilde{\psi}_k^{(0)})^{-1}]_x} - \frac{\tilde{\psi}_k^{(0)}\varepsilon_k^{(i)}}{[(\psi_k^{(0)})^{-1}]_x}\right] \\
&= 2 \lim_{x\to\pm\infty}\left[\frac{(\psi_k^{(0)})^2\tilde{\psi}_k^{(0)}\varepsilon_k^{(i)}}{\psi_{k,x}^{(0)}} - \frac{(\tilde{\psi}_k^{(0)})^2\psi_k^{(0)}\varepsilon_k^{(i)}}{\tilde{\psi}_{k,x}^{(0)}}\right] \\
&= 2 \lim_{x\to\pm\infty}\left[\frac{\psi_k^{(0)}\tilde{\psi}_k^{(0)}\varepsilon_k^{(i)}}{\tilde{\psi}_{k,x}^{(0)}\psi_{k,x}^{(0)}}[\psi_k^{(0)}\tilde{\psi}_{k,x}^{(0)} - \tilde{\psi}_k^{(0)}\psi_{k,x}^{(0)}]\right] \\
&= 2 \lim_{x\to\pm\infty}\left[\frac{\psi_k^{(0)}\tilde{\psi}_k^{(0)}\varepsilon_k^{(i)}}{\tilde{\psi}_{k,x}^{(0)}\psi_{k,x}^{(0)}}\right] \\
&= 2 \lim_{x\to\pm\infty}\left[\frac{\psi_k^{(0)}\tilde{\psi}_{k,x}^{(0)}\varepsilon_k^{(i)} + \tilde{\psi}_k^{(0)}\psi_{k,x}^{(0)}\varepsilon_k^{(i)}}{\tilde{\psi}_{k,x}^{(0)}\psi_{k,xx}^{(0)} + \tilde{\psi}_{k,xx}^{(0)}\psi_{k,x}^{(0)}}\right] \\
&= \lim_{x\to\pm\infty}\left[\frac{\varepsilon_k^{(i)}}{V(x) - E_k^{(0)}}\right] \\
&= \lim_{x\to\pm\infty}\sum_{j=1}^{i} a_k^{(j)}(x)\psi_k^{(i-j)}
\end{aligned} \tag{8}$$

where

$$a_k^{(1)} = \frac{H'(x) - E_k^{(1)}}{V(x) - E_k^{(0)}} \qquad a_k^{(j)} = \frac{-E_k^{(j)}}{V(x) - E_k^{(0)}}$$

for $j = 2, 3, \ldots, \infty$. Given equations (8) and (3), we can check the boundedness of $\psi_k^{(i)}$. For example, equation (8) gives $\lim_{x\to\pm\infty}\psi_k^{(1)}$ being proportional to $\lim_{x\to\pm\infty}\psi_k^{(0)}$, $\lim_{x\to\pm\infty}\psi_k^{(2)}$ proportional to $\lim_{x\to\pm\infty}\psi_k^{(1)}$ and so on. It is apparent that for the most physically interesting potentials and perturbations the ith-order corrected wavefunctions vanish as $x \to \pm\infty$, since $\lim_{x\to\pm\infty}\psi_k^{(0)} = 0$. Thus we have proved the sufficiency of equation (7). In the calculation for the limit only the first term on the right-hand side of equation (6) depends on condition (7). Without equation (7), this term will tend to infinity as $x \to \pm\infty$. This is the proof for the necessity of the conditions. From the condition at $x \to -\infty$ we have the constants $A_k^{(i)} = 0$ for $i = 1, 2, \ldots$. Given $A_k^{(i)}$, the normalization condition can be expanded as the first-order condition

$$\begin{aligned}
0 &= \int_{-\infty}^{\infty} \psi_k^{(0)}\psi_k^{(1)}\,\mathrm{d}x \\
&= 2\int_{-\infty}^{\infty}\psi_k^{(0)}\left[\tilde{\psi}_k^{(0)}\int_{-\infty}^{x}\psi_k^{(0)}\varepsilon_k^{(1)}\,\mathrm{d}x - \psi_k^{(0)}\left(B_k^{(1)} + \int_0^x \tilde{\psi}_k^{(0)}\varepsilon_k^{(1)}\,\mathrm{d}x\right)\right]\mathrm{d}x
\end{aligned} \tag{9}$$

and the second-order condition

$$0 = \int_{-\infty}^{\infty}[2\psi_k^{(0)}\psi_k^{(2)} + (\psi_k^{(1)})^2]\,\mathrm{d}x = 4\int_{-\infty}^{\infty}\psi_k^{(0)}\left[\tilde{\psi}_k^{(0)}\int_{-\infty}^{x}\psi_k^{(0)}\varepsilon_k^{(2)}\,\mathrm{d}x\right.$$

$$-\psi_k^{(0)}\left(B_k^{(2)}+\int_0^x \tilde{\psi}_k^{(0)}\varepsilon_k^{(2)}\,\mathrm{d}x\right)\Bigg]\,\mathrm{d}x+\int_{-\infty}^{\infty}(\psi_k^{(1)})^2\,\mathrm{d}x \qquad (10)$$

and so on. The constants $B_k^{(1)}$ and $B_k^{(2)}$ are given by equations (9) and (10). According to the theory of differential equations, the general solution $\psi_k^{(i)}$ contains all the special solutions of the ith-order equation. Any special solution must satisfy boundary condition (7) of the general solution. For an unsolvable system solution (6) includes some integrations, which cannot be expressed in finite terms of elementary functions. Therefore the integral solution is the final analytical form of the corrected wavefunction. Inserting the third part of equation (5) into (7), from $I_+^{(i)} - I_-^{(i)} = 0$ we obtain the formula of any ith-order energy correction

$$E_k^{(i)} = \int_{-\infty}^{\infty}\psi_k^{(0)}\left[W(x)\psi_k^{(i-1)} - \sum_{j=1}^{i-1}E_k^{(j)}\psi_k^{(i-j)}\right]\mathrm{d}x \qquad i = 1, 2, \ldots, \infty. \qquad (11)$$

This gives the first-order energy correction to be the expectation value of $W(x)$ in the unperturbed state that completely agrees with the common first-order result [1]. Moreover, the above method does not produce any divergence in the analytical results, since conditions (7) and (11) have successfully suppressed infinity in solution (6).

However, the exact and formal general solution (6) of the non-homogeneous Schrödinger equation (5) contains a product between the unbounded function $\tilde{\psi}_k^{(0)}$ and an integration, which cannot always be expressed as a finite form of elementary functions. In numerical computation from equation (6), some small deviations from the unsolvable integration are unavoidable. The different deviations may come from the use of different numerical integration methods and different integration steps, as well as different precisions for the representation of real numbers in the computer. Any infinitesimal deviation will break the boundedness condition (7) and will be amplified by the unbounded function until infinity as $x \to \pm\infty$. Thus we theoretically demonstrate that the corrected wavefunction (6) is analytically bounded but numerically unbounded. This could lead to numerical instability.

Numerical unboundedness is irrational because of its violation of the strict analytical solution (6) under boundedness conditions (7) and (11). In order to use the numerical method in investigating perturbed quantum systems, we must provide a scheme to get rid of this numerical infinity. From equation (8) we find that the ith-order corrected wavefunction $\psi_k^{(i)}$ is proportional to the unperturbed one $\psi_k^{(0)}$ as $x \to \pm\infty$. Ordinarily, the latter exponentially decreases as the spatial coordinate increases and vanishes at $x = \pm\infty$. Therefore, if a corrected solution $\psi_k^{(i)}$ exponentially tends to zero at the point x_0, we certainly have $\psi_k^{(i)}(x) < \psi_k^{(i)}(x_0)$ for all of $|x| > |x_0|$. The infinity appearing in the numerical results for $|x| > |x_0|$ comes from the numerical instability, which should thus be truncated.

Let us take the perturbed reflectionless potential [20,21] and the anharmonic oscillator [22] as two simple examples that exhibit these details. The former contains numerical infinity in the first-order perturbed correction. The first perturbed equation is solvable and the second-order correction leads to numerical infinity for the latter.

The reflectionless potential is an exactly solvable quantum system for which some strict solutions have been found [20, 21]. However, this solvability could be easily broken by a periodic perturbation. For the periodically perturbed reflectionless potential, the solvable and perturbed potentials are, respectively

$$V(x) = -\mathrm{sech}^2 x \qquad H'(x) = \lambda W(x) \qquad W(x) = \Omega\sin(kx+\theta) \qquad |\lambda| \ll 1 \qquad (12)$$

where the periodic term describes a standing laser field with Ω being the Rabi frequency and k and θ the wavevector and initial phase, respectively. We consider the simplest ground state to have energy $E^{(0)} = -1/2$. Substituting it and equation (12) into (5) and (2) yields the unperturbed solutions and first-order perturbed function

$$\psi^{(0)} = \frac{1}{\sqrt{2}}\operatorname{sech} x \qquad \tilde{\psi}^{(0)} = \frac{1}{\sqrt{2}}(\sinh x + x\operatorname{sech} x) \tag{13}$$

$$\begin{aligned} \psi^{(1)} &= 2\tilde{\psi}^{(0)} \int_{-\infty}^{x} \psi^{(0)}\varepsilon^{(1)}(x)\,\mathrm{d}x - 2\psi^{(0)}\left[B^{(1)} + \int_{-\infty}^{x} \tilde{\psi}^{(0)}\varepsilon^{(1)}(x)\,\mathrm{d}x\right] \\ \varepsilon^{(1)} &= \frac{1}{\sqrt{2}}[\Omega\sin(kx+\theta) - E^{(1)}]\operatorname{sech} x. \end{aligned} \tag{14}$$

Applying equations (12) and (13) to (11) gives the energy correction

$$E^{(1)} = \frac{1}{2}\pi k\Omega \sin\theta \operatorname{csch}\left(\frac{\pi}{2}k\right). \tag{15}$$

We select the parameter set $k = 4$, $\Omega = 1$ and $\theta = \pi/2$ and insert them into equations (9) and (15), producing the constant $B^{(1)}$ and energy correction $E^{(1)}$ as

$$B^{(1)} = 0.087\,2548 \qquad E^{(1)} = 2\pi\operatorname{csch}(2\pi). \tag{16}$$

Combining these with equation (6) gives the explicit form of the first-order wavefunction

$$\begin{aligned} \psi^{(1)} = \frac{1}{\sqrt{2}}&(\sinh x + x\operatorname{sech} x)\int_{-\infty}^{x} \operatorname{sech}^2 x[\cos(4x) - 2\pi\operatorname{csch}(2\pi)]\,\mathrm{d}x \\ &- \frac{1}{\sqrt{2}}\operatorname{sech} x\left[B^{(1)} + \int_{0}^{x}(\tanh x + x\operatorname{sech}^2 x)[\cos(4x) - 2\pi\operatorname{csch}(2\pi)]\,\mathrm{d}x\right]. \end{aligned} \tag{17}$$

Clearly, the first term in equation (17) has the form $0 \times \infty$ at $|x|$ equating to infinity. Applying the l'Hospital rule to this term we can easily prove its boundedness. But the insolvability of the first integration could produce a deviation to the exact value. Particularly, the irrational number π with its infinite sequence of digits is contained in the integrand and thus cannot precisely take a value in the numerical computation. Any infinitesimal deviation from the precise value can be exponentially amplified by the unbounded function $\tilde{\psi}^{(0)}$ to infinity as $|x|$ tends to infinity. This turns the analytically bounded wavefunction into a numerically unbounded one.

We used 'mathematica' to numerically show the spatial evolution of the first-order solution (17) in figure 1, which includes infinity in the interval $x < -30$ and $x > 10$. Adding the correction to the unperturbed wavefunction $\psi^{(0)}$, we plot the total solution $\psi^{(0)} + \lambda\psi^{(1)}$ for $\lambda = 0.1$ in figure 2(*a*). In figure 1 we see that the periodical perturbation makes the numerical solution periodically increase and decrease for small $|x|$. When $|x|$ approaches 10, it non-periodically tends to zero. The latter decrease is caused by the exponentially decreasing function $\psi^{(0)}$. Therefore, infinity for $|x| > 10$ results from computational instability. Truncating infinity and letting the wavefunction vanish for $|x| > 10$, we obtain the correct numerical solution as shown in figure 2(*b*). In further computations for the second-order correction, we must use the correct solution without infinity. Figure 1 shows $\psi^{(1)}$ being in the order of 10^{-1} so that $\lambda\psi^{(1)}$ is in the order of 10^{-2}. This infers there is no distinct difference between the solution in figure 2(*b*) and the unperturbed solution. In all figures all values are given in atomic units.

Another interesting system is the anharmonic oscillator that was often used for illustrating the divergence difficulties in quantum mechanics [12] and the quantum field [22]. In these cases the solvable potential and the perturbed potential are, respectively

$$V(x) = x^2/2 \qquad H'(x) = \lambda W(x) \qquad W(x) = x^4 \qquad |\lambda| \ll 1. \tag{18}$$

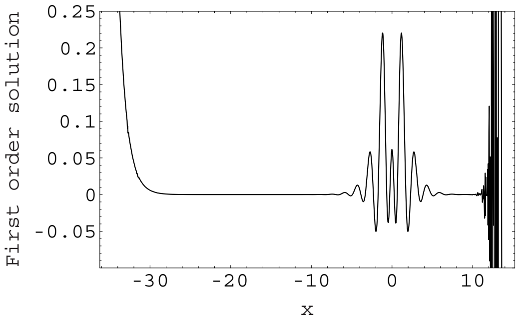

Figure 1. A plot of the space evolution of the first-order corrected wavefunction from equation (17) for the periodically perturbed reflectionless potential. Here and in all other figures all values are given in atomic units.

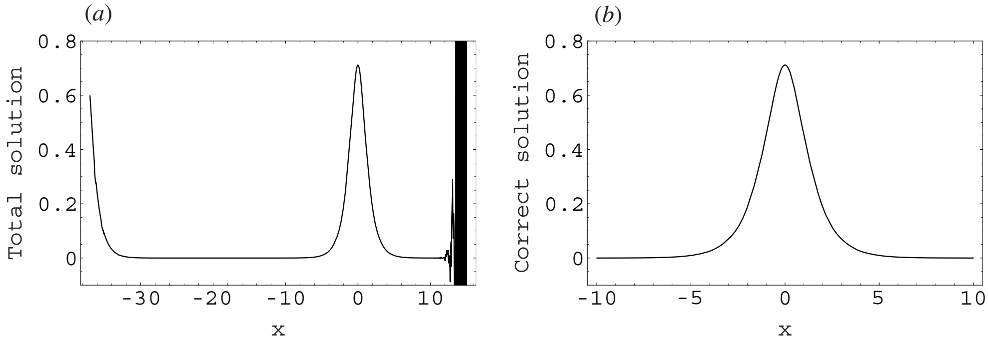

Figure 2. Plots of the space evolution of the periodically perturbed reflectionless potential for (*a*) the total wavefunction up to first-order correction and (*b*) the correct wavefunction after truncating numerical infinity.

Consider the unperturbed ground state with quantum number $n = 0$. The unperturbed wavefunction and the corresponding unbounded solution (2) then read

$$\psi_0^{(0)} = \pi^{-1/4}\mathrm{e}^{-x^2/2} \qquad \tilde{\psi}_0^{(0)} = \tfrac{1}{2}\pi^{3/4}\mathrm{e}^{-x^2/2}\mathrm{Erfi}(x) \tag{19}$$

where $\mathrm{Erfi}(x)$ denotes the imaginary error function. Applying equations (18) and (19) to (11) yields the first-order energy correction $E_0^{(1)} = 3/4$. Furthermore, inserting them into equations (9) and (5) gives the first-order normalization constant $B_0^{(1)} = -0.281\,25$ numerically and the first-order perturbed function $\varepsilon_0^{(1)} = \pi^{-1/4}\mathrm{e}^{-x^2/2}(x^4 - 3/4)$ analytically. Therefore, from equations (6) and (19) the first-order corrected wavefunction becomes

$$\begin{aligned}\psi_0^{(1)} &= \pi^{1/4}\mathrm{e}^{-x^2/2}\left[\mathrm{Erfi}(x)\int_{-\infty}^{x}\mathrm{e}^{-x^2}(x^4 - \tfrac{3}{4})\,\mathrm{d}x - \int_0^x \mathrm{e}^{-x^2}\mathrm{Erfi}(x)\left(x^4 - \frac{3}{4}\right)\mathrm{d}x - 2\frac{B_0^{(1)}}{\sqrt{\pi}}\right] \\ &= -\pi^{-1/4}\mathrm{e}^{-x^2/2}[2B_0^{(1)} + \tfrac{1}{4}x^2(3 + x^2)].\end{aligned} \tag{20}$$

Here numerical infinity does not exist since the integration multiplied by the unbounded function $\mathrm{Erfi}(x)$ is solvable. Applying equations (19) and (20) to (11) and noting that equation (9) produces the second-order energy correction gives

$$E_0^{(2)} = \int_{-\infty}^{\infty}\psi_0^{(0)}x^4\psi_0^{(1)}\,\mathrm{d}x = -(2.658\,68B_0^{(1)} + 5.400\,45)/\sqrt{\pi}. \tag{21}$$

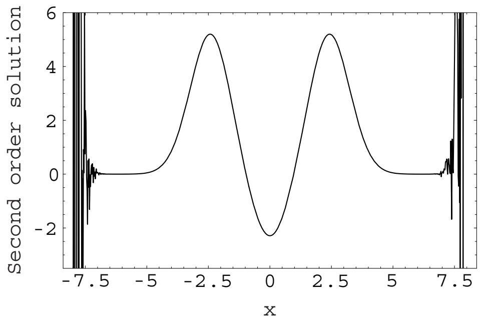

Figure 3. Plot of the space evolution of the anharmonic oscillator for the numerically unbounded second-order correction of the wavefunction in equations (19), (20), (22) and (23).

Setting $\lambda = 0.1$, up to second order the total energy reads $E_0 = E_0^{(0)} + \lambda E_0^{(1)} + \lambda^2 E_0^{(2)} = 1/2 + 0.1 \times 3/4 - 0.01 \times (2.658\,68 B_0^{(1)} + 5.400\,45)/\sqrt{\pi} \approx 0.548\,75$. Given equations (20) and (21), from equations (5) and (10) we have, respectively, the second-order perturbed function and normalization constant

$$\varepsilon_0^{(2)} = (H' - E_0^{(1)})\psi_0^{(1)} - E_0^{(2)}\psi_0^{(0)} = \left(x^4 - \frac{3}{4}\right)\psi_0^{(1)} + \frac{(2.658\,68 B_0^{(1)} + 5.400\,45)}{\sqrt{\pi}}\psi_0^{(0)} \qquad B_0^{(2)} = 1.522\,46 \qquad \text{for} \quad B_0^{(1)} = -0.281\,25. \tag{22}$$

Substitution of equations (19), (20) and (22) into (6) for $i = 2$ readily gives the integral form of the second-order corrected wavefunction

$$\begin{aligned}\psi_0^{(2)} &= 2\tilde{\psi}_0^{(0)} \int_{-\infty}^{x} \psi_0^{(0)} \varepsilon_0^{(2)}\, \mathrm{d}x - 2\psi_0^{(0)}\left[B_0^{(2)} + \int_0^x \tilde{\psi}_0^{(0)} \varepsilon_0^{(2)}\, \mathrm{d}x\right] \\ &= 2\tilde{\psi}_0^{(0)} \int_{-\infty}^{x} \psi_0^{(0)} \left[\left(x^4 - \frac{3}{4}\right)\psi_0^{(1)} + \frac{(2.658\,68 B_0^{(1)} + 5.400\,45)}{\sqrt{\pi}}\psi_0^{(0)}\right] \mathrm{d}x \\ &\quad -2\psi_0^{(0)}\left[B_0^{(2)} + \int_0^x \tilde{\psi}_0^{(0)}\left((x^4 - \tfrac{3}{4})\psi_0^{(1)} + \frac{(2.658\,68 B_0^{(1)} + 5.400\,45)}{\sqrt{\pi}}\psi_0^{(0)}\right)\mathrm{d}x\right]\end{aligned} \tag{23}$$

which includes some unsolvable integrations. Equation (19) shows $\tilde{\psi}_0^{(0)}$ tending to infinity, and equation (7) gives the first integration in equation (23) as tending to zero as $|x| \to \infty$. Therefore, the first term of equation (23) possesses the form $0 \times \infty$ at $x = \pm\infty$. Although use of the l'Hospital rule can easily prove its boundedness, numerical instability could incorrectly lead to unboundedness.

We can now numerically illustrate the instability of the anharmonic oscillator by figures 3 and 4. In figure 3 we show the space evolution of the second-order correction of the wavefunction. From the two plots we find that as in figure 1 the second-order solution exponentially and non-periodically approaches zero at $x = \pm 6$ but tends to infinity for $|x| > 6$. Therefore we can truncate infinity and let the second-order correction be zero for $|x| > 6$ so that the numerical plots correctly describe the analytically bounded solution. In figure 4(a) we plot the space evolution of the total wavefunction up to second order, $\psi_0 = \psi_0^{(0)} + \lambda\psi_0^{(1)} + \lambda^2\psi_0^{(2)}$ for $\lambda = 0.1$. Similarly, infinity exists for $|x| > 6$ in the plot. Truncating infinity at $|x| = 6$ and letting the wavefunction vanish for $|x| > 6$, figure 4(b) becomes figure 4(b) and agrees with the analytically bounded solution. Clearly, to avoid infinity we must use the wavefunction

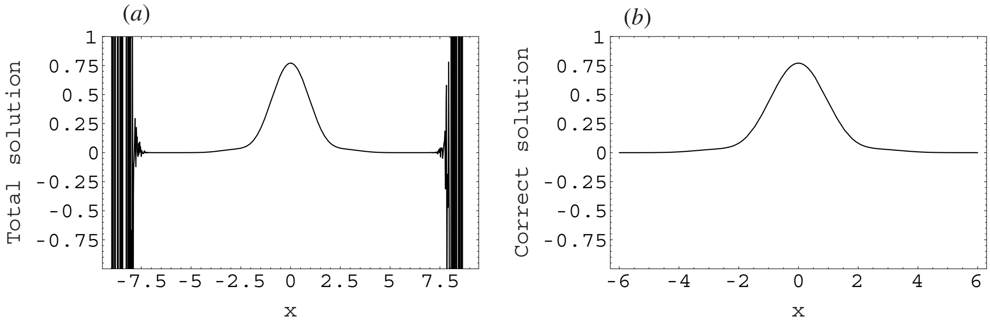

Figure 4. Plots of the space evolution of the anharmonic oscillator for (*a*) the total wavefunction up to second order, $\psi_0 = \psi_0^{(0)} + \lambda\psi_0^{(1)} + \lambda^2\psi_0^{(2)}$ for $\lambda = 0.1$ and (*b*) the corrected solution after truncating numerical infinity.

shown in figure 4(*b*) in further computations for ith-order ($i > 2$) corrections of energy and the wavefunction.

In summary, we have considered analytically unsolvable quantum systems, such as the periodically perturbed reflectionless potential, the anharmonic oscillator and other physically interesting systems. We used a different quantum perturbation method to seek the exact and formal general solution of the corresponding non-homogeneous Schrödinger equation. Applying this exact formal solution we have analytically and numerically revealed that the boundedness of the solution sensitively depends on some unsolvable integrations, which lead to the numerical instability. By proposing a simple scheme to truncate infinity we have avoided the unboundedness of the numerical results. Although we only give the one-dimensional result here, the idea on which the numerical instability and the method for truncating numerical infinity is based can be extended to multi-dimensional and time-dependent cases.

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