Variational Perturbation Approach to Resonance-State Wave Functions

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Abstract

The variational perturbation theory for wave functions, which has been shown to work well for bound states of the anharmonic oscillator, is applied to resonance states of the anharmonic oscillator with negative coupling constant. We obtain uniformly accurate wave functions starting from the bound states.

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Perturbation for wave functions of quantum systems is more complicated problem than that for energy eigenvalues since the former deals with functions while the latter only deals with a number. Even for energy eigenvalues, however, naive perturbations by a coupling constant give rise to divergent series in most cases and numerous optimization techniques have been studied [1]. Variational perturbation method, sometimes called the $\delta$ expansion, is one of the successful approaches. It has been found to reproduce energy eigenvalues of quantum anharmonic oscillator (AHO) and double-well potential (DWP) with high accuracy [2]. Characteristic of this method is that one introduces artificial parameters which are not contained in an original Hamiltonian and determines those parameters after calculating a physical quantity perturbatively. One of the advantages of the method is such flexibility that one can choose different value of the parameter depending on the physical quantity one is interested in. One can also choose different value depending on the order of the perturbation one employs. In our previous work, we showed that this advantage could be suitably taken to apply the method to wave functions and obtained uniformly accurate wave functions of AHO and DWP [3].

Recently, it has been shown that a variational perturbation approach can be also adapted to treat systems which accompany quantum tunneling decay processes [4]. In these systems, energy eigenvalues have imaginary parts and naive perturbations fail in general. In this article, motivated by these studies, we attempt to apply our method in [3] to wave functions of a tunneling system. As a simple model, we take anharmonic oscillator with negative coupling constant (NAHO).

We first recall one dimensional AHO to illustrate the variational perturbation treatment for wave functions. The Hamiltonian is

$$H(\lambda) = \frac{1}{2} \left( -\frac{d^2}{dx^2} + x^2 + \lambda x^4 \right).$$  \hspace{1cm} (1)

One defines a new Hamiltonian $H_\delta(\Omega, \lambda) = H_0(\Omega) + \delta H_I(\Omega, \lambda)$ with

$$H_0(\Omega) = \frac{1}{2} \left( -\frac{d^2}{dx^2} + \Omega^2 x^2 \right), \quad H_I(\Omega, \lambda) = \frac{1}{2} \left( (1 - \Omega^2)x^2 + \lambda x^4 \right)$$ \hspace{1cm} (2)

such that $H_{\delta=0}(\Omega, \lambda) = H_0(\Omega)$ and $H_{\delta=1}(\Omega, \lambda) = H(\lambda)$. At first, one employs Rayleigh-Schrödinger (RS) perturbation with $\delta$ as an expansion parameter. Bases of the expansion are the eigenvectors of $H_0(\Omega)$ which is harmonic oscillator (HO) with a trial frequency $\Omega$. The $n$-th order perturbative wave functions thus obtained have the following form

$$\psi_k^{(n)}(x; \Omega) = \sum_j \psi_j^{0}(x; \Omega) \sum_{l=0}^{n} \delta^l C_{jk}^{(l)}(\Omega).$$ \hspace{1cm} (3)

Next step is to choose the parameter $\Omega$ so as to make approximate functions uniformly valid. This can be achieved [3] by

$$\left. \frac{\partial \psi^{(n)}(x; \Omega)}{\partial \Omega} \right|_{\delta=1} = 0.$$ \hspace{1cm} (4)

This condition can be solved for $\Omega$, in principle, as a function of $x$ (and $\lambda$). By substituting the resultant $\Omega(x)$ to (3), we get optimized wave functions $\psi^{(n)}(x; \Omega(x))$. 

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We can interpret the condition (4) in two different ways. First interpretation is a geometrical one. If we regard the obtained functions \( \psi^{(n)}(x; \Omega) \) as a family of curves parametrized by \( \Omega \), Eq.(4) is nothing but the necessary condition for \( \psi^{(n)}(x; \Omega(x)) \) to be an envelope of the family \([3]\). The other interpretation is the principle of minimum sensitivity (PMS) \([5]\); perturbatively calculated quantity should not depend on the artificial parameter \( \Omega \) at \( \delta = 1 \) since the exact one does not depend on \( \Omega \) at all.

For the ground state wave function, first order variational perturbation results in

\[
\psi^{(1)}_0(x; \Omega) = \pi^{-1/4} \Omega^{1/4} \exp \left( -\frac{\Omega}{2} x^2 \right) \times \left[ 1 + \delta \left\{ \frac{1}{8} (1 - \Omega^{-2}) (2\Omega x^2 - 1) - \frac{\lambda}{32} \Omega^{-3} (4\Omega^2 x^4 + 12\Omega x^2 - 9) \right\} \right].
\]

The condition (4) applied to (3) reads

\[
16 x^4 \Omega^5 + 16 x^2 \Omega^4 - 4(2\lambda x^6 + 4x^4 + 7)\Omega^3 - 4(9\lambda x^4 + 4x^2)\Omega^2 - 2(33\lambda x^2 - 14)\Omega + 99\lambda = 0. \tag{6}
\]

Since this is a higher degree algebraic equation for \( \Omega \), one cannot solve it analytically in general. However asymptotic behavior of the physical solution at long distance can be estimated by Eq.(6) and found to be

\[
\Omega(x)^2 \to \frac{\lambda}{2} x^2 \quad (x \to \infty). \tag{7}
\]

Therefore, the perturbative wave function improved by the condition (4) has its asymptotic form

\[
\psi^{(1)}_0(x; \Omega(x)) \to \exp \left( -\sqrt[3]{\frac{\lambda}{8}} |x|^3 \right) \quad (x \to \infty). \tag{8}
\]

The result obtained above has correct \( x \) dependence and only the numerical factor 8 deviates a bit from the exact value 9. A noticeable success of the method in this case can be appreciated by this correct asymptotic behavior. One can never obtain such a behavior by naive RS perturbation since perturbative wave functions obtained by RS at any finite order result in finite superposition of the wave functions of HO. For example, the ground state wave function obtained by naive RS perturbation is of the following expression\(^1\)

\[
\psi_{RS_0}^{(1)}(x) = \pi^{-1/4} \exp \left( -\frac{1}{2} x^2 \right) \left[ 1 - \frac{\lambda}{32} \left( 4x^4 + 12x^2 - 9 \right) \right]. \tag{9}
\]

In the case of \( \lambda > 0 \) the physical solutions of Eq.(8) are to be restricted to real number but this is not the case for \( \lambda < 0 \). The situation is observed by the asymptotic solutions (7); by Eq.(8) with \( \lambda < 0 \) we have

\[
\Omega(x) \to \pm i \sqrt[3]{\frac{\lambda}{8}} |x|, \tag{10}
\]

\(^1\)Note that this form is independent of whether \( \lambda > 0 \) or \( \lambda < 0 \).
that is, pure imaginary at infinity. Substituted them into Eq.(5) reads

\[ \psi_0^{(1)}(x; \Omega(x)) \rightarrow \exp \left( \mp i \sqrt{\frac{|\lambda|}{8} |x|^3} \right), \]  

This oscillatory behavior is of course correct one for NAHO except for the numerical coefficient.

From the consideration above, we may expect to get resonance states of NAHO perturbatively from the bound-state wave functions of HO if we make a novel generalization of our method to allow the trial frequency \( \Omega \) to take complex values. In fact, for the ground state energy of NAHO, it was shown by Karrlein and Kleinert \[4\] that the imaginary part of the energy can be extracted precisely by this complex-valued optimization procedure for energy eigenvalues.

In Fig.1 we show as an example the ground state wave functions obtained in this way for \( \lambda = -0.2 \). There are two wave functions which are complex conjugate each other. Thus, there appear two thick dashed lines in Fig.1 which correspond to the imaginary parts of these two wave functions. The real part contributes high probability density in the vicinity of the potential valley and decreases as the potential barrier becomes high. Outside the barrier, both the real part and imaginary part oscillate as Eq.(11) indicates. Therefore, we successfully get qualitative behavior of the resonant wave functions of NAHO even at the first order perturbation.

When we try to compare the perturbatively obtained results with the exact ones, we encounter two difficulties. Firstly, it is difficult to compute numerically an eigenstate which oscillates rapidly at boundaries. Secondly, the wave functions under consideration are not normalizable and therefore it becomes meaningless to compare numerical values of the wave functions at each point. To avoid these problems, we invoke the complex-coordinate method (CCM) \[7\]. This tool is often used for computing complex eigenvalues for resonance states numerically. The essence of CCM is as follows. The ordinary Schrödinger equations in configuration space

\[ \hat{H}\psi(x) = E\psi(x) \]  

are defined on the real \( x \) axis. Then, one rotates this support of \( \psi(x) \) in complex \( x \) plane as \( x \rightarrow xe^{i\theta} \). One determines the argument of the rotation \( \theta \) such that the rotated wave functions \( \psi(xe^{i\theta}) = \hat{U}(\theta)\psi(x) \) tend to 0 at infinity, that is,

\[ \hat{U}(\theta)\hat{H}\hat{U}^{-1}(\theta)\psi(xe^{i\theta}) = E\psi(xe^{i\theta}) \]  

\[ \psi(xe^{i\theta}) \rightarrow 0 \quad (|x| \rightarrow \infty) \]  

where \( \hat{U}(\theta) \) denotes the rotation operator in complex \( x \) plane. Thanks to \[4\], numerical calculation turns out to be easier and the rotated wave functions become normalizable.

In order that the wave functions of quartic AHO satisfy the boundary condition \[\text{(14)}\], the following inequality must holds \[4\]

\[ \left| (\arg \pm x) + \frac{1}{6} (\arg \lambda) \right| < \frac{\pi}{6}, \]  

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For NAHO, \( \arg \lambda = \pi \), and the inequality (15) reads

\[-\frac{\pi}{3} < \theta < 0. \tag{16}\]

We fix the argument at \( \theta = -\pi/6 \) for our calculations. The normalized ground-state wave function in CCM for \( \lambda = -0.2 \) calculated numerically is shown in Fig.2.

Finally, we combine perturbation theory with CCM. The procedure is that we rotates Eq.(5) in the complex \( x \) plane by the same argument as that for the exact one Eq.(13) (\( \theta = -\pi/6 \) in our case).

\[\psi^{(n)}(x; \Omega) \rightarrow \psi^{(n)}(xe^{i\theta}; \Omega) \tag{17}\]

The optimization condition Eq.(4) thus changes in the same manner. If the physical solutions of Eq.(4) are written formally as \( \Omega = \Omega(x) \), the solutions in the rotated coordinate are \( \Omega = \Omega(xe^{i\theta}) \). Therefore we eventually get the optimized wave functions combined with CCM

\[\phi^{(n)}_{VP}(x) = \psi^{(n)}(xe^{i\theta}; \Omega(xe^{i\theta})). \tag{18}\]

In Fig.3, we show the 1st-order ground-state wave function for NAHO with \( \lambda = -0.2 \) and \( \theta = -\pi/6 \), obtained by Eq.(18). The comparison of it to the exact one in Fig.2 exhibits excellent agreement in the whole of a domain calculated. To make more quantitative comparison, (squared) norm defined by

\[\|\phi^{\text{exact}} - \phi^{(1)}\|^2 = \int dx |\phi^{\text{exact}}(x) - \phi^{(1)}(x)|^2 \tag{19}\]

are represented in Table I and the expectation value of the (rotated) Hamiltonian are represented in Table II. The agreement is excellent as a first-order perturbation.

For the purpose of comparing our variational results with naive RS ones, we also show the results obtained from RS perturbation. We calculate RS wave functions Eq.(9) on complex coordinate

\[\phi^{(0)}_{RS}(x) = \psi^{(0)}_{RS}(xe^{i\theta}) \tag{20}\]

with \( \theta = -\pi/6 \). In Fig.4, \( \phi^{(0)}_{RS} \) thus obtained with \( \lambda = -0.2 \) is shown. Squared norm Eq.(19) and the expectation value of the (rotated) Hamiltonian for \( \phi^{(0)}_{RS} \) are also shown in Table I and II respectively.

Some remarks are in order here.

1. For \( \lambda \leq -0.12 \) the physical solutions of Eq.(4) with real \( x \) can be obtained as a complex conjugate pair in the whole \( x \) domain calculated. They correspond to out-going and incoming states respectively. For weak negative coupling \( \lambda \geq -0.12 \), that is, high potential

\[\text{After we calculate the optimized wave function Eq. (18), we make a (global) phase transformation so that the phase of the optimized wave function becomes the same as that of the exact wave function at the origin.} \]
barrier case, there appear domains where the physical solutions split into two different real values and one cannot judge which solution should be taken. Therefore naive application of the optimization condition (4) do not work well in high-barrier case. This situation is similar to that for the same optimization scheme for eigenvalues of NAHO [4].

2. In the case of the optimized perturbation combined with CCM, the physical solutions of Eq. (2) with complex \( x \) can be determined uniquely as a complex number since the coefficients of the algebraic equation (3) are now complex. For \( \lambda \leq -0.12 \), imaginary parts of those physical solutions are all positive in the whole domain calculated. For \( \lambda \geq -0.12 \), on the other hand, imaginary parts of the physical solutions turn to be negative in a domain \( |x| \leq x_0 \) with a certain point \( x_0 \). However, no difficulties arise in the method with CCM in contrast to in the case of the method with real \( x \).

3. From Table 1 we can see that the errors for our method take its maximum around \( \lambda = -0.2 \). Even at this point, however, the error defined by Eq. (19) is about 0.0016, which indicates that our method is applicable to both the tunnel regime and the sliding regime of the coupling constant space. On the contrary, in the case of the optimization for eigenvalues of NAHO, it was proved that there exists lower bound \( \lambda_0 \) so that optimized perturbation series converge to the exact ones for \( |\lambda| \geq \lambda_0 \) [8]. Therefore, it may be said that convergence property of the method for eigenfunctions with CCM is different from that for eigenvalues.

4. We have also calculated the 2nd-order variational perturbation. The results only exhibit slight quantitative improvement from the 1st-order ones. This feature indicates rapid convergence property of the method although whether perturbative wave functions really converge into the exact ones or not is of course another problem.

5. In view of both perturbation theory and physical problem, Zeeman and Stark effects are interesting problems. These systems accompany quantum tunneling and thus the method presented in this paper will be applicable.

In summary, we have generalized the variational perturbation method for wave functions of bound states to treat those of resonant states and applied it for NAHO. We can obtain qualitative nature of resonance states such as oscillatory asymptotic behavior and reproduction of complex energy, only by a 1st-order perturbation based on the bound states of HO. The method with CCM can overcome the difficulty in the method with real \( x \) for \( \lambda \geq -0.12 \) and can give uniformly accurate wave functions in both the tunneling and the sliding regime.

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\[ ^3 \text{Some authors characterize the tunneling (sliding) regime of the coupling constant space as the real part of the ground state energy lower (higher) than the potential barrier height and we follow this definition here. For our Hamiltonian Eq. (1), the border of the two regime is at } \lambda \approx -0.3387. \]

\[ ^4 \text{An interesting resummation approach for Stark effect is found in Ref. [9].} \]
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FIGURES

FIG. 1. The perturbative wave functions $\psi^{(1)}(x, \Omega(x))$ for the ground state with $\lambda = -0.2$. The thick solid line is their real part and the thick dashed lines are their imaginary parts. (See text for the meaning of two lines.) The thin dashed line is the potential with $\lambda = -0.2$. Relation between types of lines and their meanings is common to all the figures in this article.

FIG. 2. The exact wave function $\phi^{\text{exact}}(x) = \psi^{\text{exact}}(xe^{i\theta})$ for the ground state with $\lambda = -0.2$ calculated by CCM. The rotation argument $\theta$ equals $-\pi/6$.

FIG. 3. The variational perturbation wave function $\phi^{(1)}_{VP}(x)$ combined with CCM for the ground state with $\lambda = -0.2$.

FIG. 4. The RS perturbation wave function $\phi^{(1)}_{RS}(x)$ combined with CCM for the ground state with $\lambda = -0.2$. 
### TABLE I. Squared norm defined by Eq.(19).

Since both $\phi^{\text{exact}}$ and $\phi^{(1)}$ are normalized to unity, the squared norm takes a value in the interval $[0,2]$. 

| $\lambda$     | $\|\phi^{\text{exact}} - \phi^{(1)}_{VP}\|^2$ | $\|\phi^{\text{exact}} - \phi^{(1)}_{RS}\|^2$ |
|---------------|-----------------------------------------------|-----------------------------------------------|
| $-0.05$       | 1.29994 E-5                                  | 1.04105 E-3                                  |
| $-0.06$       | 3.34356 E-5                                  | 1.98414 E-3                                  |
| $-0.07$       | 7.73821 E-5                                  | 3.38198 E-3                                  |
| $-0.08$       | 1.59194 E-4                                  | 5.31350 E-3                                  |
| $-0.09$       | 2.89919 E-4                                  | 7.84056 E-3                                  |
| $-0.1$        | 4.75445 E-4                                  | 1.10032 E-2                                  |
| $-0.2$        | 1.56666 E-3                                  | 7.65252 E-2                                  |
| $-0.3$        | 1.18456 E-3                                  | 1.90267 E-1                                  |
| $-0.4$        | 9.16755 E-4                                  | 3.32428 E-1                                  |
| $-0.5$        | 7.57480 E-4                                  | 4.84690 E-1                                  |
| $-0.6$        | 6.56376 E-4                                  | 6.33762 E-1                                  |
| $-0.7$        | 5.87611 E-4                                  | 7.72179 E-1                                  |
| $-0.8$        | 5.38161 E-4                                  | 8.96876 E-1                                  |
| $-0.9$        | 5.01007 E-4                                  | 1.00742 E0                                   |
| $-1.0$        | 4.72111 E-4                                  | 1.10469 E0                                   |
| $\lambda$ | $\langle H \rangle^{\text{exact}}$ | $\langle H \rangle_{VP}^{(1)}$ | $\langle H \rangle_{RS}^{(1)}$ |
|---------|----------------|----------------|----------------|
| $-0.05$ | $0.47912 + i 0.00001$ | $0.47971 + i 0.00036$ | $0.50328 - i 0.00369$ |
| $-0.06$ | $0.47416 + i 0.00006$ | $0.47519 + i 0.00061$ | $0.51141 - i 0.00176$ |
| $-0.07$ | $0.46879 + i 0.00026$ | $0.47050 + i 0.00098$ | $0.52287 + i 0.00248$ |
| $-0.08$ | $0.46297 + i 0.00077$ | $0.46564 + i 0.00150$ | $0.53799 + i 0.00961$ |
| $-0.09$ | $0.45677 + i 0.00176$ | $0.46062 + i 0.00219$ | $0.55712 + i 0.02025$ |
| $-0.1$  | $0.45034 + i 0.00335$ | $0.45551 + i 0.00308$ | $0.58058 + i 0.03497$ |
| $-0.2$  | $0.39744 + i 0.04471$ | $0.39512 + i 0.03694$ | $1.11140 + i 0.52301$ |
| $-0.3$  | $0.37377 + i 0.09506$ | $0.36928 + i 0.09092$ | $2.28179 + i 1.88598$ |
| $-0.4$  | $0.36441 + i 0.13868$ | $0.35999 + i 0.13638$ | $4.06817 + i 4.22403$ |
| $-0.5$  | $0.36146 + i 0.17576$ | $0.35740 + i 0.17444$ | $6.30746 + i 7.37246$ |
| $-0.6$  | $0.36169 + i 0.20780$ | $0.35798 + i 0.20704$ | $8.81116 + i 11.06949$ |
| $-0.7$  | $0.36363 + i 0.23600$ | $0.36022 + i 0.23560$ | $11.43170 + i 15.07917$ |
| $-0.8$  | $0.36655 + i 0.26122$ | $0.36339 + i 0.26106$ | $14.07565 + i 19.23405$ |
| $-0.9$  | $0.37004 + i 0.28407$ | $0.36710 + i 0.28408$ | $16.69183 + i 23.42979$ |
| $-1.0$  | $0.37387 + i 0.30499$ | $0.37111 + i 0.30512$ | $19.25816 + i 27.61088$ |

TABLE II. Expectation value of (rotated) Hamiltonian with respect to the exact wave function $\langle H \rangle^{\text{exact}}$ and that with respect to the perturbative one $\langle H \rangle^{(1)}$. 
Fig. 1
Fig. 3
Fig. 4