EXTENDING THE RANGE OF VALIDITY FOR ASYMPTOTIC ENERGY EXPANSION METHOD BY PADÉ APPROXIMATION

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In general, the Asymptotic Energy Expansion method (AEE) produces accurate eigenvalues for higher eigenstates when parameters of the nonleading power terms of the potential are small. However, the ground state and low eigenstates energies calculated from the AEE method are usually inaccurate. Further, when the parameters of the potential are large, accuracy of the AEE method becomes significantly deteriorated. In this paper we show that by applying the Padé approximation, the accuracy of AEE for the ground state and low eigenstates can be significantly improved and eigenenergies for large parameters can be accurately determined.

Keywords: semiclassical expansion, asymptotic energy expansion, eigenspectra, Padé approximant.

1. Introduction

The Asymptotic Energy Expansion method has useful features which are not available in semiclassical nonperturbative methods such as WKB approximation or perturbative methods like Rayleigh–Schrödinger perturbation expansions [1–3]. Semiclassical methods such as higher order WKB methods are useful not only for solving the time independent Schrödinger equation and obtain accurate eigenvalues numerically but also for some cases, obtaining both lower order as well as higher order terms in the WKB series as algebraic expressions [4–7], enabling these systems to be investigated analytically. As a nonperturbative method, the higher order WKB has been applied successfully for certain types of potentials to obtain analytic expressions for the terms in the WKB series. One of the major difficulties in applying higher order WKB to solve systems such as polynomial potentials is that most of the integrals involved in the higher order terms cannot be evaluated analytically. On the other hand for polynomial potentials having any number of terms, the AEE expansion up to any order can be obtain analytically in term of Gamma functions [3]. As in the case of WKB, eigenenergies obtained by AEE are mainly valid for higher eigenstates. Especially, it fails to predict the ground state

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energies accurately for most of the potentials [4]

$$V(x) = x^{2N} + a_1 x^{2N-1} + a_2 x^{2N-2} + \cdots + a_{2N-2} x^2 + a_{2N-1} x. \tag{1}$$

Perturbative methods such as the Rayleigh–Schrödinger perturbation theory are very valuable in determining eigenenergies numerically for a Hamiltonian system which can be expressed as a sum of an unperturbed Hamiltonian with known eigenstates and a perturbation potential. In other words, the terms in the Rayleigh–Schrödinger perturbation expansion cannot be obtained unless the Hamiltonian can be expressed as a sum of unperturbed Hamiltonian with known eigenstates and a perturbation potential. One example is the general polynomial potential given in (1) when $a_{2N-2} = 0$. Moreover, when parameters of the perturbation potential are not small, usually, the perturbation theory fails to predict accurate eigenvalues.

Similarly to the Rayleigh–Schrödinger perturbation theory, the AEE expansion for the polynomial type systems is also valid when parameters in the not leading terms of the potential are small. When these parameters are large, the accuracy of the AEE significantly deteriorates. Nevertheless, the AEE method is especially suitable for solving polynomial type potentials [3, 8]. Since, in AEE, the quantum momentum function is expanded as a power series in reciprocal of energy, it is found to be very accurate for higher eigenstates. The AEE expansion is identical to higher order WKB expansion for power potentials such as $V(x) = x^{2N}$ [2] while they are completely different for polynomial type potentials. The AEE has also been applied successfully to many systems other than polynomial systems [9, 10]. Recently, the AEE has been successfully utilized to obtain a simple formula for the semiclassical energy of the general odd-degree polynomial potential [11]. Furthermore, the AEE method has been used to show that the complex non-Hermitian PT-symmetric Hamiltonian $H = p^2 - gx^4 + 4i\hbar\sqrt{g}x$ and the conventional Hermitian Hamiltonian $h = p^2 + 4gx^4 + 6\hbar\sqrt{g}x$ have the same eigenspectra [12]. Similarly, using AEE, it was recently shown that the Hamiltonians $H = p^2 - gx^4 + a/x^2$ and $h = p^2 + 4gx^4 + bx$ are isospectral if $a = \left(b^2 - 4g\hbar^2\right)/16g$ [13].

The AEE is a diverging series which is Borel summable. Generally, finite partial sums of the AEE do not show convergence with increasing order, but tend to diverge exponentially for small value of E. Nevertheless, through a simple resummation using the Padé approximants it is possible to extract rapidly converging and highly accurate results for the eigenvalues. Several years ago, Bender et al. [14] have studied the large-order behaviour of the Rayleigh–Schrödinger perturbation theory for the ground-state energy of the complex PT-symmetric Hamiltonian $H = p^2 + \frac{1}{4}x^2 + i\lambda x^3$. The Rayleigh–Schrödinger perturbation series is also Borel summable, and the Padé summation provides excellent agreement with the real energy spectrum. Therefore in this study we test the applicability of Padé to asymptotic series of AEE.

In this paper we show that the accuracy of eigenenergies of the ground state and lower eigenstates obtained with AEE can be vastly improved by using the Padé summation of AEE. Further we show that even when parameters of the potential are large, the Padé summation of AEE produces accurate eigenenergies. As two

illustrations, we study the AEE for the quantum action variable J of the quartic Hamiltonian $p^2+x^4+ax^2$ and the complex PT-symmetric Hamiltonian p^2+ix^3+bx and compare the results with exact eigenenergies of the same systems obtained with the matrix diagonalization method. However, for these Hamiltonians, we find that the AEE is divergent (zero radius of convergence).

The outline of the paper is as follows. In Section 2, the AEE for the quantum action variable J of the even and odd degree polynomial potential are discussed. In Section 3, we apply an alternative approach based on a rational approximation to sum the AEE expansion. The ccuracies of lowest eigenvalues are illustrated by using two example in Section 4. Concluding remarks are given in Section 5.

2. Description of the AEE method

In order for this paper to be self-contained, first we describe the AEE method and derive the necessary equations. Since the method is slightly different for odd degree and even degree potentials, derivations of recurrence relations are divided into two steps. First consider the one-dimensional Schrödinger equation ($2m = 1$)

$$-\hbar^2 \frac{\partial^2 U(x,E)}{\partial x^2} + V(x)\,U(x,E) = EU(x,E)\,, \tag{2}$$

where $V(x)$ is a potential and assume $V(x) = \sum_{k=0}^{N} V_k\ (x)$, where $V_k(x)$ has the scaling property that $V_k(\lambda x) = \lambda^{n_k} V_k(x)$ and n_k are distinct integers.

Substituting

$$P(x,E) = \frac{\hbar}{i}\frac{\partial U(x,E)/\partial x}{U(x,E)}$$

in the above equation, we get

$$\frac{\hbar}{i}\frac{\partial P(x,E)}{\partial x} + P^2(x,E) = E - V(x) = P_c(x,E)\,. \tag{3}$$

Note that $P(x,E)$ above corresponds to the derivative of the action in the usual WKB ansatz. The quantity $J(E)$ is now defined as

$$J(E) = \frac{1}{2\pi}\int_{\gamma} P(x,E)\,dx, \tag{4}$$

with the quantization condition $J(E) = n\hbar$. The contour γ encloses two physical turning points of $P_c = \sqrt{E - V(x)}$. However, depending on the system this contour becomes branch points of appropriate square root function [3, 11]. Boundary condition imposed upon $P(x,E)$ is $P(x,E) \to P_c(x,E)$ as $\hbar \to 0$ [15, 16].

Also assume that $V_k\ (x)$ are ordered in such a way that $n_0 > n_1 > n_2 > \cdots > n_N$. Now Eq. (3) becomes

$$\frac{\hbar}{i}\frac{\partial P(x,E)}{\partial x} + P^2(x,E) = E - V_0(x) - \sum_{k=1}^{N} V_k\ (x). \tag{5}$$

2.1. Even degree potentials

Assume that the potential is of even degree (i.e. n_0 is even). Let $n_0 = 2m_0$ for some $m_0 \in N$. Let $\epsilon = E^{-1/2m_0}$ and $y = \epsilon x$. Then (5) becomes, after simplification,

$$\frac{\hbar}{i}\epsilon^{2m_0}\frac{\partial P(y,\epsilon)}{\partial y} + \epsilon^{2m_0}P^2(y,\epsilon) = 1 - V_0(y) - \sum_{k=1}^{N}\epsilon^{2m_0-n_k}V_k(y). \tag{6}$$

Now we expand $P(y,\epsilon)$ as a power series in ϵ,

$$P(y,\epsilon) = \epsilon^s\sum_{n=0}^{\infty}a_n(y)\epsilon^n. \tag{7}$$

Substituting (7) in (6) and equating coefficients of ϵ^n, we obtain $s = -m_0$, $a_0 = \sqrt{1 - V_0(y)}$ and

$$a_n = \frac{-1}{2a_0}\left[\sum_{i=1}^{n-1}a_i a_{n-i} + \hbar\frac{da_{n-m_0-1}}{dy} + \sum_{k=1}^{N}V_k\ (y)\delta_{2m_0-n_k,n}\right]. \tag{8}$$

In the above formula $a_n = 0\ \forall n < 0$.

Now $J(E)$ becomes, after simplification,

$$J(E) = \frac{\epsilon^{-m_0-1}}{2\pi}\sum_{m=0}^{\infty}\epsilon^m\int_{\gamma_y}P(y,\in)\,dx, \tag{9}$$

where γ_y encloses the two branch points of $\sqrt{1 - V_0(y)}$. The Asymptotic Energy Expansion (AEE) can be obtained as

$$J(E) = \sum_{m=0}^{\infty}b_m E^{\frac{-(m-m_0-1)}{2m_0}}, \tag{10}$$

where

$$b_m = \frac{1}{2\pi}\int_{\gamma_y}a_m(y)\,dy. \tag{11}$$

2.2. Odd degree potentials

When n_0 is odd, the system has boundstates for certain $V_k\ (y)$, especially when they are PT symmetric. Let $n_0 = 2m_0 + 1$ for some $m_0 \in N$. Let $\epsilon = E^{-1/(4m_0+2)}$ and $y = i\epsilon^2 x$. Then (5) becomes, after simplification,

$$\hbar\epsilon^{4m_0+4}\frac{\partial P(y,\epsilon)}{\partial y} + \epsilon^{4m_0+2}P^2(y,\epsilon) = 1 - V_0(y) - \sum_{k=1}^{N}i^{-n_k}\epsilon^{4m_0+2-2n_k}V_k(y). \tag{12}$$

Now we expand $P(y,\epsilon)$ as a power series in ϵ,

$$P(y,\epsilon) = \epsilon^s\sum_{n=0}^{\infty}a_n(y)\epsilon^n. \tag{13}$$

Substituting (13) in (12) and equating coefficients of ϵ^n, we obtain $s = -(2m_0+1)$, $a_0 = \sqrt{1 - V_0(y)}$ and

$$a_n = \frac{-1}{2a_0}\left[\sum_{i=1}^{n-1} a_i a_{n-i} + \hbar \frac{da_{n-2m_0-3}}{dy} + \sum_{k=1}^{N} i^{-n_k} V_k \ (y)\delta_{4m_0+2-2n_k,n}\right]. \tag{14}$$

In the above formula $a_n = 0 \ \forall n < 0$.

The Asymptotic Energy Expansion (AEE) can be obtained as

$$J\,(E) = \sum_{k=0}^{\infty} b_m E^{\frac{-(m-2m_0-3)}{4m_0+2}}, \tag{15}$$

where

$$b_m = \frac{1}{2i\pi}\int_{\gamma_y} a_m\,(y)\,dy. \tag{16}$$

where γ_y encloses the two branch points of $\sqrt{1 - V_0(y)}$.

For both cases of even degree and of odd degree, γ_y will depend on $V_0(y)$ and Eqs. (11) and (16) can be evaluated analytically. In the next section we introduce Padé approximants to improve the accuracy of AEE energy especially for the ground state and lower eigenstates.

3. The Padé approximants

The Padé approximant is one of the standard tools in theoretical physics to overcome problems with slowly convergent or divergent power series. Consequently, there is a large number of publications on the mathematical properties of Padé approximants as well as on their applications in theoretical physics [17]. A Padé approximant is a rational function [18], i.e. a function expressed as a fraction whose numerator and denominator are both polynomials, whose power series expansion agrees with a given power series to the highest possible order. The primary application of Padé approximants is for problems where it is possible to derive the solution formally as a power series expansion in some parameter. The corresponding Padé approximants often turn out to be much more useful than the power series itself. In this study we apply Padé approximation to AEE.

For a given AEE expansion

$$J(E) = \sum_{k=0}^{\infty} b_k E^k \tag{17}$$

the $[L, M]$ Padé approximant $R_{L,M}(E)$ is defined by

$$R_{L,M}(E) = \frac{\sum_{k=0}^{L} p_k E^k}{1 + \sum_{k=1}^{M} q_k E^k} \tag{18}$$

such that

$$J(E) - R_{L,M}(E) = O(E^{L+M+1}), \tag{19}$$

i.e. the first $L+M+1$ terms of the power series of $R_{L,M}(E)$ match the first $L+M+1$ terms of the power series of $J(E)$.

Equations for the coefficients $p_k,\ k=0,\ldots,L$ and $q_k,\ k=1,\ldots,M$, can be obtained by multiplying (18) by the denominator of $R_{L,M}(E)$ and equating coefficients of E^k for $k=0,\ldots,L+M$. The result is M simultaneous equations for the $q_k,\ k=1,\ldots,M$,

$$\sum_{k=1}^{\min(r,M)} q_k b_{r-k} = -b_r, \qquad r=L+1,\ldots,L+M, \tag{20}$$

and $L+1$ expressions for the $p_k,\ k=0,\ldots,L$,

$$p_k = b_k + \sum_{s=1}^{\min(k,M)} q_s b_{k-s}, \qquad k=0,\ldots,L. \tag{21}$$

In many cases it is convenient to consider only 'diagonal' Padé approximants with $L=M$.

4. Illustrations

In general, the AEE method does not produce accurate eigenvalues for low eigenstates when parameters of the not leading term of the potential are large. In this section we study the AEE of two simple systems and test the accuracy of the AEE with Padé approximant.

The first system we study is the Hamiltonian

$$H = p^2 + x^4 + ax^2, \tag{22}$$

where $a \in \mathbb{C}$. The AEE of this system is obtained as

$$J(E) = n\hbar \approx -\frac{\hbar}{2} + E^{3/4}\sum_{k=0}^{\infty} b_k E^{-k/4}. \tag{23}$$

The first eight nonzero b_k are

$$b_0 = \frac{\Gamma\left[\frac{1}{4}\right]}{3\sqrt{\pi}\,\Gamma\left[\frac{3}{4}\right]}, \tag{24}$$

$$b_2 = -\frac{a\ \Gamma\left[\frac{3}{4}\right]}{\sqrt{\pi}\ \Gamma\left[\frac{1}{4}\right]}, \tag{25}$$

$$b_4 = \frac{a^2\ \Gamma\left[\frac{1}{4}\right]}{32\sqrt{\pi}\ \Gamma\left[\frac{3}{4}\right]}, \tag{26}$$

$$b_6 = -\frac{(a^3+8\hbar^2)\ \Gamma\left[\frac{3}{4}\right]}{32\sqrt{\pi}\ \Gamma\left[\frac{1}{4}\right]}, \tag{27}$$

$$b_8 = -\frac{a(5a^3 + 32\hbar^2)\ \Gamma\left[\frac{1}{4}\right]}{6144\sqrt{\pi}\ \Gamma\left[\frac{3}{4}\right]}, \tag{28}$$

$$b_{10} = \frac{a^2(21a^3 + 400\hbar^2)\ \Gamma\left[\frac{3}{4}\right]}{10240\sqrt{\pi}\ \Gamma\left[\frac{1}{4}\right]}, \tag{29}$$

$$b_{12} = \frac{(15a^6 + 480a^3\hbar^2 + 1408\hbar^4)\ \Gamma\left[\frac{1}{4}\right]}{196608\sqrt{\pi}\ \Gamma\left[\frac{3}{4}\right]}, \tag{30}$$

$$b_{14} = -\frac{7a(11a^6 + 520a^3\hbar^2 + 3200\hbar^4)\ \Gamma\left[\frac{3}{4}\right]}{327680\sqrt{\pi}\ \Gamma\left[\frac{1}{4}\right]}. \tag{31}$$

Since $J(E)$ is expanded as an infinite power series in terms of the reciprocal of eigenenergy E, the resulting series is divergent for small values of E. Now the Padé approximant technique is applied to sum the divergent series $\sum_{k=0}^{\infty} b_k E^{-k/4}$. It was found that by this method, the summation of AEE and hence the accuracy of the lowest eigenvalues are improved. Numerical eigenvalues determined with the matrix diagonalization method and the proposed method are compared in Table 1. It is clearly evident that the ground state energies improved significantly by the Padé and AEE energies for large parameter values became accurate.

Table 1. Comparison between calculated eigenvalues by AEE, AEE with Padé and exact which are obtained by the matrix diagonalization method for the Hamiltonian $H = p^2 + x^4 + ax^2$. The calculation was carried out for $\hbar = 1.0$.

a	n	E_{AEE}	$E_{\text{AEE+Padé}}$	E_{Exact}
1.0	0	1.5474951	1.3538472	1.3923516
	1	4.6504891	4.6504604	4.6488127
	2	8.6549860	8.6549867	8.6550499
	3	13.156806	13.156806	13.156804
5.0	0	3.5690620	2.3682205	2.3682396
	1	7.3332368	7.3322127	7.3322123
	2	12.707509	12.707622	12.707622
	3	18.424311	18.424327	18.424327
10.0	0	6.6616853	3.2313136	3.2335697
	1	10.278051	9.8340666	9.8341133
	2	16.642090	16.688358	16.688362
	3	23.716931	23.773018	23.773018

4.1. $V(x) = ix^3 + bx$

For this potential, the Hamiltonian is

$$H = p^2 + ix^3 + bx, \tag{32}$$

where $m_0 = 1$. The AEE can be obtained as

$$J(E) = n\hbar \approx -\frac{\hbar}{2} + E^{5/6} \sum_{k=0}^{\infty} b_k E^{-k/6}. \tag{33}$$

The first eight nonzero b_k are

$$b_0 = \frac{\Gamma\left[\frac{1}{6}\right]}{5\sqrt{\pi}\,\Gamma\left[\frac{2}{3}\right]}, \tag{34}$$

$$b_4 = \frac{i\ b\ \Gamma\left[\frac{5}{6}\right]}{\sqrt{\pi}\ \Gamma\left[\frac{1}{3}\right]}, \tag{35}$$

$$b_{10} = -\frac{\hbar^2\ \Gamma\left[\frac{5}{6}\right]}{12\sqrt{\pi}\ \Gamma\left[\frac{1}{3}\right]}, \tag{36}$$

$$b_{12} = -\frac{ib^3\ \Gamma\left[\frac{1}{6}\right]}{648\sqrt{\pi}\ \Gamma\left[\frac{2}{3}\right]}, \tag{37}$$

$$b_{16} = \frac{5b^4\ \Gamma\left[\frac{5}{6}\right]}{1296\sqrt{\pi}\ \Gamma\left[\frac{1}{3}\right]}, \tag{38}$$

$$b_{18} = -\frac{7b^2\hbar^2\ \Gamma\left[\frac{1}{6}\right]}{2592\sqrt{\pi}\ \Gamma\left[\frac{2}{3}\right]}, \tag{39}$$

$$b_{22} = -\frac{55ib^3\hbar^2\ \Gamma\left[\frac{5}{6}\right]}{3888\sqrt{\pi}\ \Gamma\left[\frac{1}{3}\right]}, \tag{40}$$

$$b_{24} = \frac{91b(2b^5 + 189i\hbar^4)\ \Gamma\left[\frac{1}{6}\right]}{4199040\sqrt{\pi}\ \Gamma\left[\frac{2}{3}\right]}. \tag{41}$$

As in the previous case, the resulting series is divergent for small values of E. The Padé approximant technique is applied to sum the divergent series $\sum_{k=0}^{\infty} b_k E^{-k/3}$. The accuracies of eigenvalues determined with the proposed method are compared with numerical values obtained with matrix diagonalization method. The results are shown in Table 2.

5. Summary and concluding remarks

The AEE method is valuable for obtaining eigenenergies of polynomial type potentials. Usually the method is very accurate for higher eigenvalues. However, AEE

Table 2. Comparison between calculated eigenvalues by AEE, AEE with Padé and exact which are obtained by the matrix diagonalization method for the Hamiltonian $H = p^2 + ix^3 + bx$. The calculation was carried out for $\hbar = 1.0$.

b	n	E_{AEE}	$E_{\text{AEE+Padé}}$	E_{Exact}
$1.0i$	0	1.8535247	1.8547864	1.8561108
	1	5.1500657	5.1501751	5.1501689
	2	8.8162193	8.8162452	8.8162452
	3	12.736488	12.736497	12.736497
$5.0i$	0	6.3057314	6.3134284	6.3136320
	1	10.462396	10.464588	10.464599
	2	14.792884	14.793760	14.793762
	3	19.272456	19.272882	19.272882
$10.0i$	0	14.801125	14.533973	14.534073
	1	19.502800	19.331313	19.331307
	2	24.354135	24.234597	24.234595
	3	29.322512	29.234310	29.234310

does not produce accurate eigenvalues for the ground state and lower eigenstates as well as when parameters of the nonleading terms of the polynomial type potentials are large. The AEE expansion of $J(E)$ is asymptotically divergent and Borel summable. In this paper we have shown that by applying the Padé approximation method, the accuracy of the divergent series of AEE can be significantly improved. Eigenenergies of low eigenstates including ground state as well as eigenenergies of potentials having large parameters can be accurately determined with the combined AEE method and Padé technique. With the help of two examples, we have demonstrated the accuracy of lowest eigenvalues for both small parameter values as well as for large parameter values of the potential. Therefore, we conclude that the AEE method with the Padé approximant technique can be used to determine the accurate energy eigenvalues of low eigenstates of the polynomial type Hamiltonians.

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