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Asymptotic Energy Expansion for Rational Power Polynomial Potentials

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Asymptotic Energy Expansion for Rational Power Polynomial Potentials

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Abstract *Asymptotic energy expansion method is extended for polynomial potentials having rational powers. New types of recurrence relations are derived for the potentials of the form* $V(x) = x^{2n/m} + b_1 x^{n1/m1} + b_2 x^{n2/m2} + \cdots + b_N x^{n_N/m_N}$ *where* $n, m, n_1, m_1, \ldots, n_N, m_N$ *are positive integers while coefficients* $b_k \in \mathbb{C}$*. As in the case of even degree polynomial potentials with integer powers, all the integrals in the expansion can be evaluated analytically in terms of* Γ *functions. With the help of two examples, we demonstrate the usefulness of these expansions in getting analytic insight into the quantum systems having rational power polynomial potentials.*

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1 Introduction

The algebraic form of eigenenergy spectra of Schrödinger equation provides a way to have analytic insight into the system of interest. The exact analytic expressions of eigenspectra can only be obtained for very few potentials such as the Coulomb potential, the Morse potential, the Poeschl–Teller potential, the square-well potential, and the Harmonic oscillator potential. For certain systems such as $V(x) = x^{2N}$, WKB methods can be utilized to obtain analytic semiclassical expressions for asymptotic eigenspectra. However, when the potential contains additional powers such as in the case of $V(x) = x^{2N} + ax^2$, the integrals involved in higher order WKB method[1] become almost impossible to evaluate analytically. Moreover, finding approximate eigenvalue expressions for polynomial potentials having non integer powers is a challenging task especially when coefficients of the potential are not real. When the coefficients of the potential are not real, solution along the real axis does not satisfy the boundary conditions at $\pm\infty$ and integration has to be performed along specialized curves in the complex x plane.[2] Although PT symmetric single term potentials such as $V(x) = x^2(\mathrm{i}x)^\epsilon$ with non-integer ϵ have been studied intensively,[3–6] when they involve multiple terms of non-integer powers, it is even difficult to obtain the first order WKB eigenenergy expressions analytically.

On the other hand, Asymptotic Energy Expansion (AEE) method provides an analytic expression for the quantum action variable J in terms of Gamma functions and hence one can obtain asymptotic energies by applying the quantization condition to J. Recently, AEE method which was developed for polynomial potentials with integer powers has also been utilized for obtaining isospectral Hermitian equivalence of non-Hermitian Hamiltonians.[7]

In this paper we show how to extend the Asymptotic Energy Expansion (AEE) method which was developed for polynomial potentials with integer powers[8–10] to obtain analytic energy expansions for the polynomial potentials with non-integer powers such as $V(x) = x^{2n/m} + a_1 x^{n_1/m_1}$ for $n, m, n_1, m_1 \in \mathbb{N}^+$. One of the main advantages of AEE is that all the non-zero integrals involved in the series are of the form $\int [x^n/(1-x^{2N})^{m+1/2}]\mathrm{d}x$ and can be evaluated analytically in terms of Γ functions.[8–11] The AEE expansion and the higher order WKB expansion are identical for $V(x) = x^{2N}$ while they are completely different for $V(x) = x^{2N} + ax^2$.[9] Another advantage of obtaining AEE expansion is that with few terms of the expansion, one can find analytically, how the parameters of the potential affect the behavior of eigenvalues and the level spacing or density of states for large energies or large quantum numbers.[9,12]

Outline of the paper is as follows. In Sec. 2, AEE method is extended and new recurrence relations for rational power polynomial potentials of the type

$$V(x) = x^{2n/m} + b_1 x^{n_1/m_1} + b_2 x^{n_2/m_2} + \cdots + b_N x^{n_N/m_N}$$

are derived. As illustrations, explicit algebraic expressions for AEE's are obtained for the potentials with two rational power terms in Sec. 3. Further, asymptotic eigenenergies and expressions for density of states are obtained. Concluding remarks are made in Sec. 4.

2 Modified AEE Method

In this section we will modify the AEE method and derive recurrence relations for the one-dimensional Hamiltonian of the form

$$H(x,p) = p^2 + V(x)\,, \tag{1}$$

where

$$V(x) = x^{2n/m} + b_1 x^{n_1/m_1} + b_2 x^{n_2/m_2} + \cdots + b_N x^{n_N/m_N}\,,$$

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with n, $n_i m_i$, $N \in \mathbb{N}^+$ and $(2n/m) > (n_1/m_1) > n_2/m_2 \cdots > (n_N/m_N)$. As in the polynomial case,[9–10] the AEE quantization condition is

$$J(E) = \tilde{n}\hbar\,, \tag{2}$$

where $\tilde{n}$ is a positive integer and quantum action variable $J(E)$ is given by

$$J(E) = \frac{1}{2\pi}\int_\gamma P(x,E)\,\mathrm{d}x\,, \tag{3}$$

$P(x,E)$ satisfies the equation

$$\frac{\hbar}{\mathrm{i}}\frac{\partial P(x,E)}{\partial x} + P^2(x,E) = E - V(x) = P_c(x,E)\,, \tag{4}$$

and it is related to the wave function as $P(x,E) = (\hbar/\mathrm{i})[(\partial\Psi/\partial x)/\Psi]$. The contour γ in Eq. (3) encloses two physical turning points of $P_c(x,E)$. In order to obtains asymptotic energy expansion, first $P(x,E)$ is expanded in a series of powers of energy and subsequently obtains recurrence relations. For the above potential, Eq. (4) reads

$$\frac{\hbar}{\mathrm{i}}\frac{\partial P(x,E)}{\partial x} + P^2(x,E) = E - x^{2n/m} - b_1 x^{n_1/m_1} - b_2 x^{n_2/m_2} - \cdots - b_N x^{n_N/m_N}\,. \tag{5}$$

In the case of polynomial potentials with integer powers, the selection of the transformation needed for deriving AEE is straight forward (see Refs. [8–10] for details). However this method cannot be used when powers are non integers as integer powers of ϵ is necessary for the AEE expansion.

In order to obtain recurrence relations for polynomial potentials with non-integer powers, we assume that $\epsilon = E^{-1/(2nm_\alpha)}$ and $y^{mm_\alpha} = \epsilon^{mm_\alpha}x$ where $m_\alpha = \mathrm{hcp}(m, m_1, m_2, \ldots, m_{_N})$. (hcp is the highest common multiplier). These transformations ensure that all the terms in the right hand side of Eq. (5) will produce integer powers of ϵ so that AEE expansion can be made. With these transformations, Eq. (5) becomes

$$\frac{\hbar}{\mathrm{i}}\frac{\epsilon^{(2n+m)m_\alpha}}{mm_\alpha}y^{1-mm_\alpha}\frac{\partial P}{\partial y} + \epsilon^{2nm_\alpha}P^2 = 1 - y^{2nm_\alpha} - \sum_{l=1}^{N} b_l y^{mm_\alpha n_l/m_l}\epsilon^{(2n-mn_l/m_l)m_\alpha}\,. \tag{6}$$

Note that m_α/m_k is an integer for all $0 < k \le N$ as $m_\alpha = \mathrm{hcp}(m, m_1, m_2, \ldots, m_{_N})$ and $(2n/m) > (n_1/m_1) > (n_2/m_2) > \cdots > (n_N/m_{_N})$. Now we expand $P(y,\epsilon)$ as a power series in ϵ.

$$P(y,\epsilon) = \epsilon^s\sum_{k=0}^{\infty}a_k(y)\epsilon^k\,, \tag{7}$$

where a_k and k are determined below. Substituting Eq. (7) in Eq. (6) and equating coefficients of ϵ^0, we obtain $s = -nm_\alpha$ and $a_0 = \sqrt{1-y^{2nm_\alpha}}$ and Eq. (6) becomes

$$\frac{\hbar}{\mathrm{i}}\frac{1}{mm_\alpha}y^{1-mm_\alpha}\sum_{k=0}^{\infty}\epsilon^{k+(n+m)m_\alpha}\frac{\mathrm{d}a_k}{\mathrm{d}y} + \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}a_i a_j\epsilon^{i+j} = 1 - y^{2nm_\alpha} - \sum_{l=1}^{\bar{N}} b_l y^{mm_\alpha n_l/m_l}\epsilon^{(2n-mn_l/m_l)m_\alpha}\,, \tag{8}$$

and assuming $a_k = 0$ when $k < 0$ and rearranging terms, we obtain

$$\frac{\hbar}{\mathrm{i}}\frac{1}{mm_\alpha}y^{1-mm_\alpha}\sum_{k=(n+m)m_\alpha}^{\infty}\epsilon^k\frac{\mathrm{d}a_{k-(n+m)m_\alpha}}{\mathrm{d}y} + \sum_{k=1}^{\infty}\sum_{i=1}^{k-1}a_i a_{k-i}\epsilon^k + 2a_0\sum_{k=1}^{\infty}a_k\epsilon^k = 1 - y^{2nm_\alpha} - \sum_{l=1}^{N} b_l y^{mm_\alpha n_l/m_l}\epsilon^{(2n-mn_l/m_l)m_\alpha}\,. \tag{9}$$

Then coefficients a_ks are given by

$$a_k = \frac{-1}{2a_0}\left[\begin{array}{l}\dfrac{\hbar}{\mathrm{i}}\dfrac{1}{mm_\alpha}y^{1-mm_\alpha}\dfrac{\mathrm{d}a_{k-(n+m)m_\alpha}}{\mathrm{d}y} + \displaystyle\sum_{i=1}^{k-1}a_i a_{k-i} \\ \displaystyle\sum_{l=1}^{N} b_l y^{mm_\alpha n_l/m_l}\delta\Big[k, \Big(2n - \frac{mn_l}{m_l}\Big)m_\alpha\Big]\end{array}\right]. \tag{10}$$

In the above formula $a_k = 0\ \forall k < 0$. Now J can be written as

$$J(E) = \sum_{k=0}^{\infty}c_k E^{-(k-(n+m)m_\alpha)/2nm_\alpha}\,, \tag{11}$$

where $c_k = (1/2\pi)\int_\gamma a_k\,\mathrm{d}y$ and can be determined analytically in terms of the coefficient of the potential $b_1, b_2, \ldots, b_{_N}$. The contour γ encloses the two branch points of $\sqrt{1-y^{2nm_\alpha}}$ (i.e. $+1$ and -1) on the real axis. The quantization condition $J(E) = \tilde{n}\hbar$ determines the eigenenergies of $V(x) = x^{2n/m} + b_1 x^{n_1/m_1} + b_2 x^{n_2/m_2} + \cdots + b_N x^{n_N/m_N}$.

For polynomial potentials with integer powers, all the integrals $\int_\gamma a_k\,\mathrm{d}y$ have the general form either $\int x^n(1-x^{2N})^{m+1/2}\mathrm{d}x$ or $\int x^n/(1-x^{2N})^m\mathrm{d}x$ where $n \in N^+$ and $m \in N$. However, the second integral, in general, does not contribute to J except when $m = 1$. On the other hand, for polynomial potentials with non-integer powers, in addition to the above two forms, there is an integral of the form $\int[1/x^l(1-x^{2N})^{m+1/2}]\mathrm{d}x$, with l as a positive integer contributes to the J. Importantly, all the above integral forms can be evaluated in terms of Gamma functions analytically.

3 Illustrations

In this section we present two simple illustrations for polynomial potentials with non integer powers. The first potential has the leading power less than unity while for

the other it is greater than unity. The method described in this paper can be applied to general potentials of the form $V(x) = x^{2n/m} + b_1 x^{n_1/m_1} + b_2 x^{n_2/m_2} + \cdots + b_N x^{n_N/m_N}$. with $n,\ n_i\ m_i, N \in \mathbb{N}^+$ and $(2n/m) > (n_1/m_1) > (n_2/m_2) > \cdots > (n_N/m_N)$. AEE expansion is more accurate for large eigenvalues and therefore, it is suitable for investigating asymptotic behavior of eigenvalues. It is convenient to use a computer algebra package such as *MATHEMATICA* for deriving the AEE series. Using *MATHEMATICA* 8.0,[13] the recurrence relation (10) was implemented with $a_0 = \sqrt{1 - y^{2nm_\alpha}}$, for the two potentials. Results are given below.

3.1 $V(x) = x^{2/3} + ax^{1/3}$

In order for this potential to be real for all $-\infty < x < \infty$ we define $V(x)$ as

$$V(x) = (x^2)^{1/3} + a(x^2)^{1/6}\,. \tag{12}$$

For the potential in Eq. (12), $m_\alpha = 3$ and Eq. (11) becomes

$$J(E) = \sum_{k=0}^{\infty} c_k E^{-(k-12)/6}\,. \tag{13}$$

It is found that $c_k = 0\ \forall k > 12$ non zero $c_k' s$ are $c_0 = 3/8$, $c_6 = 9a^2/16$ and $c_{12} = 15a^4/128 - \hbar/2$ and the AEE expansion is

$$J(E) = \frac{3}{8}E^2 + \frac{9a^2}{16}E + \frac{15a^4}{128} - \frac{\hbar}{2}\,. \tag{14}$$

Applying quantization condition $J(E) = \tilde{n}\hbar$, $\tilde{n} = 0, 1, 2, \ldots$ the eigenenergies are obtained. The asymptotic eigenvalues for this potential are given by

$$E_{\tilde{n}} = \frac{2\sqrt{3}\sqrt{3a^4 + 16\hbar + 32\tilde{n}\hbar} - 9a^2}{12}\,. \tag{15}$$

For comparison purposes, the Schrodinger equation for the above potential is solved numerically as well. Eigenenergies are shown in Table 1.

Table 1 Some eigenvalues calculated with AEE for $V(x) = x^{2/3} + ax^{1/3}$ are compared with the numerical eigenvalues. The calculation is carried out for $a = 0.1$ and $a = 1.0$ and the results are shown up to six significant figures.

n	$a = 0.1$		$a = 1.0$	
	AEE	Numerical	AEE	Numerical
0	1.147 21	1.036 99	0.508 306	0.495 861
5	3.822 21	3.823 10	3.112 21	3.122 49
10	5.284 01	5.285 46	4.565 07	4.567 08
15	6.421 08	6.420 13	5.698 51	5.695 58
20	7.386 19	7.386 96	6.660 58	6.660 86
40	10.3848	10.3844	9.654 33	9.653 57
60	12.6942	12.6944	11.6915	11.6435
100	16.3632	16.3631	15.6283	15.6281
200	23.1154	23.1154	22.3783	22.3783

Although the eigenvalues obtained from numerical method are not exact, here we assume that they are at least accurate up to 6 significant figures. It is apparent from Table 1 that AEE method produced less accurate eigenvalues when $\tilde{n}$ is small. However, as $\tilde{n}$ increases, the AEE method has became more accurate. The analytic expression of $E_{\tilde{n}}$ presented in Eq. (15) for the above potential can be utilized to investigate the asymptotic behavior of eigenvalues analytically.

As an example one can find out whether it is possible to have zero energy ground states for the potentials of the form in Eq. (12). Since action the variable contains only positive powers of E, by making $E_0 = 0$ in Eq. (15), we find that when $a^4 \simeq 64/15$ this system has zero energy ground state. When $a = a_0$, $-a_0$, $\mathrm{i}a_0$ or $-\mathrm{i}a_0$ (where $a_0 = (64/15)^{1/4} \simeq 1.437\ 216\ 4$) this system has zero energy ground states. This a_0 is an approximate value and the exact value of a_0 is found to be 1.474 568 15 (for this a_0 ground state energy found to be less than 10^{-10}). Further, we can find out whether the eigenvalues of Eq. (12) are real when Hamiltonian is PT symmetric (i.e. $a = \mathrm{i}b$ for real b). Equation (15) clearly indicates that the potential has the same energy spectra for both a and $-a$ and energy spectrum is real even when a is pure imaginary.

Next we determine the density of states and the asymptotic level spacings for the system in Eq. (12). Density of states ρ is given by

$$\rho(E) = \frac{\partial J}{\partial E}\,. \tag{16}$$

For the first potential $V(x) = x^{2/3} + ax^{1/3}$, from Eq. (14), we have

$$\rho(E) = \frac{3}{4}E + \frac{9a^2}{16}\,. \tag{17}$$

For large E, the density of states increases linearly with the energy. Consequently, by the relation

$$\Delta E \approx \frac{1}{(\partial J/\partial E)}\,, \tag{18}$$

the asymptotically level spacing becomes $\Delta E \approx 4/3E - a^2/E^2$.

This implies that for large energies level spacings will decrease as the parameter $|a|$ increases. On the other hand, when a is pure imaginary or the system is PT symmetric, the level spacings is $\Delta E \approx 4/3E + a^2/E^2$ and increases as the parameter $|a|$ increases.

3.2 $V(x) = x^{6/5} + ax^{1/3}$

The second illustration is for

$$V(x) = x^{6/5} + ax^{1/3}\,. \tag{19}$$

For this potential $m_\alpha = 3$ and AEE expansion is

$$J(E) = \sum_{k=0}^{\infty} b_k E^{-(k-24)/18}\,. \tag{20}$$

Here $b_k = 0\ \forall$ odd k. First six non zero $b_k' s$ are

$$b_0 = \frac{15\Gamma[5/6]}{8\sqrt{\pi}\Gamma[1/3]}\,, \qquad b_{24} = -\frac{\hbar}{2}\,,$$

$$b_{26} = \frac{35a^2\Gamma[7/18]}{216\sqrt{\pi}\Gamma[28/9]}, \qquad b_{48} = \frac{\hbar^2\Gamma[1/6]}{180\sqrt{\pi}\Gamma[2/3]},$$
$$b_{52} = -\frac{425a^4\Gamma[17/18]}{23328\sqrt{\pi}\Gamma[4/9]}, \quad b_{74} = \frac{238a^2\hbar^2\Gamma[13/18]}{3645\sqrt{\pi}\Gamma[2/9]}.$$

Table 2 Some eigenvalues calculated with AEE method for $V(x) = x^{6/5} + ax^{1/3}$ are compared with numerical eigenvalues. The calculation was carried out for $a = 0.5$ and $a = 1.0$ and the results are shown up to six significant figures.

n	$a = 0.5$		$a = 1.0$	
	AEE	Numerical	AEE	Numerical
0	0.868+0.1287i	0.912 08	0.241-0.803i	0.651 704
5	6.547 37	6.547 86	6.440 98	6.432 46
10	10.6638	10.6654	10.5783	10.5755
15	14.2947	14.2931	14.2197	14.2227
20	17.6378	17.6389	17.5695	17.5691
40	29.4114	29.4113	29.3570	29.3571
60	39.7499	39.7496	39.7023	39.7019
100	58.1725	58.1725	58.1323	58.1323
200	97.6633	97.6633	97.6315	97.6315

As in the first illustration, the eigenvalues calculated with AEE method become more accurate for large n. Very low eigenvalues do not agree with the numerical eigenvalues. However, when $n > 15$ the eigenvalues agree well with the numerically calculated values as shown above. For general polynomial potentials $V(x) = x^{2n/m} + b_1x^{n_1/m_1} + b_2x^{n_2/m_2} + \cdots + b_Nx^{n_N/m_N}$, with n, n_i $m_i, N \in \mathbb{N}^+$ and $(2n/m) > (n_1/m_1) > n_2/m_2 > \cdots > (n_N/m_N)$, AEE method can be utilized to obtain eigenenergies as well as asymptotic behavior of the eigenvalues analytically.

As in the pervious system, for the potential $V(x) = x^{6/5} + ax^{1/3}$, the density of states ρ and asymptotic level spacings ΔE are given by

$$\rho(E) \approx \frac{5\Gamma[5/6]}{2\sqrt{\pi}\Gamma[1/3]}E^{1/3} - \frac{35a^2\Gamma[7/18]}{1944\sqrt{\pi}\Gamma[28/9]}E^{10/9}, \quad (21)$$

and

$$\Delta E \approx \frac{2\sqrt{\pi}\Gamma[1/3]}{5\Gamma[5/6]}E^{-1/3}.$$

We can also find how the asymptotic eigenenergies vary with the parameter a from AEE expansion.

$$\Delta E_a \approx \frac{1}{(\partial J/\partial a)}\Delta a. \quad (22)$$

For the first potential ΔE_a is approximated as

$$\Delta E_a \approx \frac{8}{9aE}\Delta a, \quad (23)$$

and for the second potential it is

$$\Delta E_a \approx \frac{108\sqrt{\pi}\Gamma[28/9]}{35a\Gamma[7/18]}E^{1/9}\Delta a. \quad (24)$$

It is evident from Eqs. (23) and (24) that for higher eigenstates of the first potential $V(x) = x^{2/3} + ax^{1/3}$, the eigenenergies are less sensitive to small changes in the parameter a as $|8/9aE|$ is small. On the other hand, the eigenstates of $V(x) = x^{6/5} + ax^{1/3}$ become more sensitive to small changes in parameter a for higher eigenstates.

4 Concluding Remarks

In this paper, we have obtained AEEs for the polynomial potentials with rational powers $V(x) = x^{2n/m} + b_1x^{n_1/m_1} + b_2x^{n_2/m_2} + \cdots + b_Nx^{n_N/m_N}$. Since AEE has been developed only for polynomial potentials with integer powers, it cannot directly be applied to the polynomial systems with rational powers. In this paper new types of recurrence relations are derived for such potentials and applied them to the above general polynomial potential to obtain expressions for J in terms of E and the parameters of the potential. These expansions are power series in energy and coefficients of the series contain parameters $b_1, b_2, \ldots, b_N$ explicitly. We demonstrate how to use AEE to obtain potentials with zero ground states and behavior of density of states as the parameters of the potential varies.

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