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Higher-order semiclassical energy expansions for potentials with non-integer powers

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Abstract. In this paper, we present a semiclassical eigenenergy expansion for the potential $|x|^\alpha$ when α is a positive rational number of the form $2n/m$ (n is a positive integer and m is an odd positive integer). Remarkably, this expansion is found to be identical to the WKB expansion obtained for the potential x^N (N-even), if $2n/m$ is replaced by N. Taking the limit $m \to 2$ of the above expansion, we obtain an explicit asymptotic energy expansion of symmetric odd power potentials $|x|^{2j+1}$ (j-positive integer). We then show how to develop approximate semiclassical expansions for potentials $|x|^\alpha$ when α is any positive real number.

Keywords. Eigenenergies; asymptotic; WKB; polynomial potentials.

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1. Introduction

In the last several years, many studies have been carried out to understand the transition from classical mechanics to quantum mechanics. These studies are motivated by the so-called quantum chaos [1–3]. In the context of quantum chaos, systematic study of the global behavior of eigenfunctions and energy spectra of quantum mechanical systems are very important. In a recent paper [4], it was reported that chaotic signatures are present in the spectrum of the one-dimensional quantum double-well and demonstrated the importance of studying 1D systems analytically. Analytical expressions of energy spectra provide analytical insight into the global behavior of quantum mechanical systems. In addition to the perturbative and variational methods, semiclassical approximations are the most widely used approximation methods in quantum mechanics to obtain analytic expansions.

Towards achieving better understanding of the transition between classical mechanics and quantum mechanics, we have recently developed an asymptotic energy expansion method (AEE in short) [5], providing a powerful tool for obtaining analytic expressions of quantum systems for which usual WKB methods can not be used directly. It is important to note that WKB expansions are power series expansions in the Planck constant $\hbar$

while AEE are power series expansions of energy. They are the same for certain potentials but entirely different for other potentials [5]. However, the evaluation of integrals in AEE is quite straight-forward compared to WKB and AEE integrals are independent of energy. Unlike in WKB expansion, parameters of the potential appear in the AEE expansion explicitly. All the integrals in AEE coefficients discussed here have the general form

$$\int_C \frac{x^p}{(1-x^q)^{\gamma+1/2}}\mathrm{d}x,$$

where p, q and r are positive integers and contour C encloses points $+1$ and -1 on the real axis. Also these integrals can be evaluated in terms of Γ functions. Please see ref. [5] for more details on the AEE method.

Detailed studies were carried out on 1-D systems such as x^N (N even) to obtain analytic eigenenergy expansions using WKB methods [6]. For some of these potentials WKB series were summed to all orders to obtain the exact solution [7].

In this paper, we analyse 1-D system $|x|^\alpha$ (α-real) for which we are able to obtain analytic eigenenergy expansions in terms of Γ functions. Important results presented in this paper are

1. Derivation of AEE which is a relationship between quantum number k and the power series expansion of energy for the potential $V(x) = x^{2n/m}$. These expansions are not only useful in obtaining approximate bound state energy eigenvalues but also provides analytic insight into the global behavior of energy spectra of a wide class of potentials.
2. The asymptotic energy expansion derived for $x^{2n/m}$ becomes the WKB expansion obtained for the potential x^N (N-even), if $2n/m$ is replaced by N.
3. Using the method introduced by Robnik *et al* [8], we obtain almost explicit formulae for AEE terms for the energy eigenvalues of the potential $V(x) = x^{2n/m}$.
4. Taking the limit $m \to 2$ of AEE of $V(x) = x^{2n/m}$, the energy expansions for the potential $|x|^{2j+1}$ (j-positive integer) is derived.
5. Choosing suitable n and m, we obtain approximate AEE for $|x|^\alpha$ where α is any positive real number. In other words, we present a single higher-order asymptotic energy expansion, which represents all forms of the potential $|x|^\alpha$ for any real positive α.

The outline of the paper is as follows: In §3, we derive recurrence relations and explicit AEE for the potential $x^{2n/m}$. We also obtain almost explicit formulae for AEE terms for this potential. The AEE for the potential $|x|^{2j+1}$ and discussion on potentials $|x|$ are given in §4. In §5, AEE of general power potential $|x|^\alpha$ is discussed.

2. Derivation of recurrence relations and AEE for *V(x)=x*$^{2n/m}$

In this section we derive recurrence relations of the asymptotic energy expansion of the potential $V(x) = x^{2n/m}$ where n is a positive integer and m is an odd integer. The Schrödinger equation for a 1-D analytic potential $V(x)$ is given by

$$-\hbar^2\frac{\partial^2 U(x,E)}{\partial x^2} + V(x)U(x,E) = EU(x,E). \tag{1}$$

Substituting $P(x,E) \equiv (\hbar/i)((\partial U(x,E)/\partial x)/U(x,E))$ in eq. (1), we obtain

$$\frac{\hbar}{i}\frac{\partial P(x,E)}{\partial x} + P^2(x,E) = E - x^{2n/m}. \tag{2}$$

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

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

with the quantization condition $J(E) = \kappa\hbar$. The contour γ encloses two physical turning points of $E - x^{2n/m}$.

The turning points x_k for this potential is given by

$$x_k = E^{m/2n}\mathrm{e}^{i\pi km/n}.$$

After the transformation carried out on eq. (2) and the contour integral (3), the choice of the turning points, that is enclosed by the contour, becomes very clear.

Let us make the substitution $\varepsilon = E^{-(1/2n)}$ and $y = \varepsilon x^{1/m}$ in (2). The turning points now become

$$y_k = \mathrm{e}^{i\pi km/n}.$$

The turning points now lie in the unit circle in the complex plane and two turning points $+1$ and -1 lie on the real axis. We now choose these two branch points for the contour integration. In the new variables ε and y, eqs (2) and (3) become

$$\frac{\hbar}{im}\frac{\varepsilon^{2n+m}}{y^{m-1}}\frac{\partial P(y,E)}{\partial y} + \varepsilon^{2n}P^2(y,E) = 1 - y^{2n} \tag{4}$$

and

$$J(\varepsilon) = \frac{m}{2\pi\varepsilon^m}\int_{\gamma_y} y^{m-1}P(y,\varepsilon)\mathrm{d}y, \tag{5}$$

where γ_y encloses two branch points $+1$ and -1 of $\sqrt{1-y^{2n}}$. We now expand $P(y,\varepsilon)$ as a power series in ε,

$$P(y,\varepsilon) = \varepsilon^S \sum_{k=0} a_k(y)\varepsilon^k, \tag{6}$$

where s is determined below. Substituting (6) in (4) and equating coefficients of ε^0, we get $s = -n$ and $a_0 = \sqrt{1-x^{2n}}$. Equation (4) becomes

$$\sum_{k=0}^{\infty}\frac{\hbar}{im}\frac{\mathrm{d}a_k}{\mathrm{d}y}\frac{1}{y^{m-1}}\varepsilon^{k+n+m} + \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} a_i a_j \varepsilon^{i+j} = 1 - y^{2n}. \tag{7}$$

Equating coefficients of ε^k for arbitrary k produces recurrence relations

$$a_k = 0, \qquad \text{if } 0 < k \le n+m$$
$$a_k = -\frac{1}{2a_0}\left\{\sum_{i=1}^{k-1} a_i a_{k-i} + \frac{\hbar}{im}\frac{1}{y^{m-1}}\frac{\mathrm{d}a_{k-n-m}}{\mathrm{d}y}\right\}, \qquad \text{if } k > n+m \tag{8}$$

with

$$J(E) = \sum_{k=0} \alpha_k(n,m) E^{((k-n-m)/2n)}, \tag{9}$$

where

$$\alpha_k(n,m) = \frac{m}{2\pi}\int_{\gamma_y} y^{m-1} a_k(y)\mathrm{d}y. \tag{10}$$

Starting with $a_0 = \sqrt{1-x^{2n}}$ and using eqs (8)–(10), asymptotic energy expansion can be obtained. As stated before, the contour γ_y encloses two branch points $+1$ and -1 of $\sqrt{1-y^{2n}}$. Any computer algebra package can be used to do the integrals in (10) and non-zero $\alpha_k(n,m)$ can be expressed in terms of Γ functions.

By observing non-zero terms generated by the recurrence relations (8) for arbitrary n and m and then performing the contour integral (10), we obtain AEE for the potential $x^{2n/m}$. It is

$$J(E) = -\frac{\hbar}{2} + \sum_{k=0}^{\infty} b_k(n,m) E^{-(((2k-1)(n+m))/2n)} \tag{11}$$

with

$$b_k(n,m) = \frac{(-1)^k \hbar^{2k}\Gamma\left[\frac{(2n+m-2km)}{2n}\right]\beta_k(n,m)}{\sqrt{\pi}\Gamma\left[\frac{(3n+m-2k(n-m))}{2n}\right](2k+2)!\,2^{k-1}}, \tag{12}$$

where $\beta_k(n,m)$ are polynomials in n and m and the first five are given as

$$\beta_0(n,m) = 1,$$
$$\beta_1(n,m) = \frac{2(2n-m)}{m},$$
$$\beta_2(n,m) = \frac{(m-2n)(3m-2n)(3m+4n)}{m^3},$$
$$\beta_3(n,m) = \frac{-4(m-2n)(5m-2n)(139m^3+234m^2n-88mn^2-192n^3)}{9m^5},$$
$$\beta_4(n,m) = \frac{1}{3m^7}((m-2n)(7m-2n)(12961m^5+29432m^4n-6484m^3n^2 -41504m^2n^3-4800mn^4+13824n^5)). \tag{13}$$

The derived AEE is valid for any positive integer values of n and any odd positive values of m. Since m is odd, $((2n+m-2km)/2n)$ is a non-integer and hence $\Gamma[((2n+m-2km)/2n)]$ in (12) is finite for all positive integer values of k,n, and odd positive values of m. Consequently, $b_k(n,m)$s are finite. However, for some even m values, $((2n+m-2km)/2n)$ becomes a negative integer and $\Gamma[((2n+m-2km)/2n)]$ becomes infinite.

The energy eigenvalues obtained from the above AEE for various values of n and m were compared with the exact energies calculated with numerical integration of the Schrödinger equation and with the truncated matrix representation of (1) in harmonic oscillator basis functions. It is found that higher AEE eigenvalues agrees very well with the exact energies (see Appendix 1 for illustrations).

It was shown in [5] that, the AEE of the potential x^N (N even positive integer) is the same as the WKB expansion of the same potential. It is obvious that when $m = 1$, AEE in (11) will become WKB expansion of x^N with the substitution $N = 2n$. Remarkably, it turns out that AEE for the potential $x^{2n/m}$ given above in (11), can simply be obtained by replacing N with $2n/m$ in WKB expansion of x^N (N even). Recently, Robnik *et al* [8] derived almost explicit formulae for the WKB terms for the energy eigenvalues for the potential x^N (N even positive integer). The corresponding explicit formulae for $b_k(n,m)$ of the potential $x^{2n/m}$ are

$$\begin{aligned} b_k(n,m) = {} & \frac{m\hbar^{2k}}{4n\sqrt{\pi}(6k-3)!!}\frac{\Gamma\left[\frac{(2n+m-2km)}{2n}\right]}{\Gamma\left[\frac{(3n+m-2k(n-m))}{2n}\right]} \\ & \times \left(A_{2k-1,0}\prod_{s=1}^{2k-1}\left(\frac{3-2k}{2}+\frac{m(1-2k)}{2n}-s\right)\right. \\ & + \sum_{i=1}^{2k-1} A_{2k-i-1,i}\prod_{s=1}^{i}\left(s+\frac{m(1-2k)}{2n}\right) \\ & \left.\times \prod_{s=1}^{2k-i-1}\left(\frac{3-2k}{2}+\frac{m(1-2k)}{2n}-s\right)\right), \end{aligned} \tag{14}$$

where $k \geq 1$ and $A_{2k-i-1,i}$ are computed according to the following recurrence relations

$$\begin{aligned} A_{s,l} = {} & \frac{1}{2}\sum_{i=0}^{2}\sum_{j=0}^{l-1} A_{i,j}A_{s-i,l-1-j} + \frac{l(n+m)+(3n+m)s-n}{2m}A_{s,l-1} \\ & + \frac{(2n-m)l+2n-ms}{2m}A_{s-1,l} \end{aligned} \tag{15}$$

with

$$A_{0,0} = \frac{n}{2m} \quad \text{and} \quad A_{\alpha,\beta} = 0 \quad \text{if} \quad \alpha < 0 \quad \text{or} \quad \beta < 0$$

and

$$b_0(n,m) = \frac{\Gamma\left[\frac{2n+m}{2n}\right]}{\sqrt{\pi}\Gamma\left[\frac{3n+m}{2n}\right]}.$$

Note that the above equations are obtained by manipulating Robnik's formulae. Also note that WKB expansions are power series expansions of the Planck constant $\hbar$ while asymptotic energy expansions (AEE) are power series expansions of energy E.

3. Explicit asymptotic energy expansions of $|x|^{2j+1}$ type potentials

Anharmonic potentials of the form $V(x) = x^{2j}$ (j-positive integer) always possess infinitely many bound states. Whereas odd power potentials $V(x) = x^{2j+1}$ have no bound states for any positive integer values of j. On the other hand, symmetric form $|x|^{2j+1}$ of the odd power potentials have bound states for all positive integer values of j as in the case of even power potentials. AEEs for the even power case $(V(x) = x^{2j})$ are given by eqs (11)–(13) as a special case of the potential $x^{2n/m}$ when m is unity. In this section we derive asymptotic energy expansions for the symmetric odd power potentials $V(x) = |x|^{2j+1}$ by manipulating the formulae (11)–(13).

When n is odd (say $n = 2j+1$), the $\lim_{m\to 2}\Gamma[((2n+m-2km)/2n)]$ becomes infinite for some values of k. However, it is found that the rational part of $b_k(2j+1,m)$ are zero for such values and consequently, $\lim_{m\to 2} b_k(2j+1,m) = 0$. As $m \to 2$, the potential $V(x) = x^{(2(2j+1)/m)} \to V(x) = |x|^{2j+1}$. Hence AEE for the potential $|x|^{2j+1}$ is given by

$$J(E) = -\frac{\hbar}{2} + \sum_{k=0}^{\infty} b_k(j) E^{-((2k-1)(2j+3)/2(2j+1))} \tag{16}$$

with

$$b_k(j) = \frac{(-1)^k \hbar^{2k}\Gamma\left[\frac{(j+2-2k)}{2j+1}\right]\beta_k(j)}{\sqrt{\pi}\Gamma\left[\frac{(6j+5-2k(2j-1))}{2(2j+1)}\right](2k+2)!\,2^{k-1}}, \tag{17}$$

where $\beta_k(j)$ are polynomials in j and the first five are given as

$$\begin{aligned}
\beta_0(j) &= 1,\\
\beta_1(j) &= 4j,\\
\beta_2(j) &= 4j(j-1)(4j+5),\\
\beta_3(j) &= \frac{32j(j-2)(96j^3+188j^2-j-105)}{9},\\
\beta_4(j) &= \frac{16j(j-3)(3456j^5+7440j^4-4136j^3-14665j^2-1565j+5250)}{3}.
\end{aligned} \tag{18}$$

Explicit recurrence formulae can be found for the potential $|x|^{2j+1}$ similar to that in (14) and (15). Let us consider the potential $V(x) = |x|$. When $j = 0$, (16) and (17) become

$$J(E) = \sum_{k=0}^{\infty} b_k(0) E^{-(3(2k-1)/2)} \tag{19}$$

with

$$b_k(0) = \frac{(-1)^k \hbar^{2k}\Gamma[2-2k]\beta_k(0)}{\sqrt{\pi}\Gamma\left[\frac{5+2k}{2}\right](2k+2)!\,2^{k-1}}. \tag{20}$$

Note that $\Gamma(2-2k)$ in (20) is infinite when $k > 0$. However, $\beta_k(0)$ in (18) becomes zero for $j = 0$. Since $x\Gamma(x) \to 1$ as $x \to 0$ and apparently, as $j \to 0$, $\beta_k(j) \sim j * f(j)$ for some $f(j)$ with $f(0) \neq 0$, $b_k(0)$ becomes

$$b_k(0) = \frac{(-1)^k \hbar^{2k} \theta_k(0)}{\sqrt{\pi}\Gamma\left[\frac{5+2k}{2}\right](2k+2)!\,2^{k-1}},$$

where

$$\theta_0(0) = 1, \quad \theta_1(0) = 2, \quad \theta_2(0) = -10, \quad \theta_3(0) = \frac{1120}{3}, \quad \theta_4(0) = -42000. \tag{21}$$

Eigenenergies obtained from this formulae were tested with that of exact values obtained numerically. It was found that they are in good agreement, specially for higher eigenstate (see table 3 in Appendix 1 for an illustration).

4. Discussion on the potential $|x|^\alpha$ (α-real)

In this section we will discuss the validity of the asymptotic formulae given in (11)–(13) for a general symmetric potential $|x|^\alpha$ with real α. The formulae (11)–(13) are derived when m is an odd positive integer. When $m = 2$, in the previous section, we derived the asymptotic expansions for them. However, when m is even and greater than 2, it can be proved that there exists an integer $k_0 > 0$ such that the gamma function in the numerator of eq. (12) becomes infinite for all $k > k_0$ and the rational part of $b_k(n,m)$ is non-zero unlike when $m = 2$. Therefore formulae (11)–(13) are not valid for even m greater than 2. But we can get approximate asymptotic expansions for any real α as described below.

It can be proved that, for a given rational number a/b, the integers n and m (m odd) can be found such that $2n/m$ is arbitrarily close to a/b. Furthermore, since rational numbers are dense in real numbers, this result is valid for any real number α as well. In other words, for a given positive real number α and a positive real number δ, there exists a positive integer n and an odd integer m such that $|(2n/m) - \alpha| < \delta$. Hence by choosing appropriate n and m to satisfy the condition $|(2n/m) - \alpha| < \delta$, asymptotic expansion given in (11) and (12) can be approximated to be valid for the potentials $|x|^\alpha$ for real α up to any desired accuracy δ.

When α is real, eigenenergies obtained by approximate energy expansions were compared with the numerical eigenenergies, to find out the validity/accuracy of the expansions (see table 4 in Appendix 1 for illustrations). We found that AEE formulae in eqs (11)–(13) gave less accurate energy spectra when $\alpha \leq 0.6$. However, when $\alpha > 0.6$, the formulae gave correct and accurate energies, specially for higher eigenstates.

Appendix 1

In this appendix, we present four numerical illustrations to show the accuracy of the formulae derived in the paper. The following truncated series is used to calculate AEE energies while exact energies are obtained by matrix diagonalization method using 800 harmonic oscillator basis functions.

$$n\hbar = b_0 E^{((n+m)/2n)} - \frac{\hbar}{2} + b_1 E^{-((n+m)/2n)} + b_2 E^{-(3(n+m)/2n)}, \tag{A1}$$

where

$$b_0 = \frac{\Gamma\left[1+\frac{m}{2n}\right]}{\sqrt{\pi}\Gamma\left[\frac{3}{2}+\frac{m}{2n}\right]}, \quad b_1 = \frac{\hbar^2(m-2n)\Gamma\left[1-\frac{m}{2n}\right]}{12m\sqrt{\pi}\Gamma\left[\frac{1}{2}-\frac{m}{2n}\right]},$$

$$b_2 = -\frac{\hbar^4(m-2n)(3m+n)(9m^2+6mn-8n^2)\Gamma\left[1-\frac{3m}{2n}\right]}{2880m^3\sqrt{\pi}\Gamma\left[\frac{1}{2}-\frac{3m}{2n}\right]}. \tag{A2}$$

Using the above formulae, we calculate eigenenergies for the potentials $V_1(x) = x^6$, $V_2(x) = |x|^{6.5}$ and $V_4(x) = |x|^{\pi}$ and compare them with exact energies. For potentials V_1, n and m are taken to be $n = 3$ and $m = 1$ and for the potential V_2, n and m are chosen as $n = 1300000$ and $m = 399999$ such that $2n/m \approx 6.5$. Also for potential V_4, n and m are taken to be $n = 3141592$ and $m = 1999999$ such that $2n/m \approx \pi$. For the potential $V_3(x) = |x|^5$, we used eqs (16)–(18) with $j = 2$. Results are given in the tables 1–4 and it is evident from these tables that accuracy increases with the energy. Except for the first few low eigenenergies, for all the other energies, AEE energies agrees with exact eigenenergies to a high accuracy.

Table 1. $V_1(x) = x^6$.

k	AEE energy	Exact energy
0	1.0430200487	1.1448024719
1	4.3176474776	4.3385986805
2	9.0761250710	9.0730845916
5	29.299664105	29.299645892
10	77.127342451	77.127341454
20	210.28347235	210.28347229
30	381.57096047	381.57096047
40	583.83575048	583.83575045
50	812.89991691	812.89991690
100	2282.1182242	2282.1182242

Table 2. $V_2(x) = |x|^{6.5}$.

k	AEE energy	Exact energy
0	1.0783265816	1.2422935164
1	4.4222913847	4.4517611610
2	9.3999707880	9.3982725107
5	31.002443359	31.002484570
10	83.148924329	83.148923013
20	231.18469299	231.18469234
30	424.42041436	424.42041437
40	654.83372731	654.83372735
50	917.68754674	917.68754673
100	2628.9635352	2628.9635353

Table 3. $V_3(x) = |x|^5$.

k	AEE energy	Exact energy
0	0.9855914687	1.1043568386
1	4.0850505601	4.0888708666
2	8.3405395281	8.3433163809
5	25.535693803	25.534993201
10	64.225909928	64.225907960
20	166.96655929	166.96655300
30	294.50318307	294.50318314
40	441.58460731	441.58460733
50	605.22571728	605.22571726
100	1617.6092441	1617.6092441

Table 4. $V_4(x) = |x|^\pi$.

k	AEE energy	Exact energy
0	0.9487017397	1.0277098573
1	3.5170584685	3.5048010076
2	6.5358946682	6.5391345697
5	17.093213375	17.092886164
10	37.655018513	37.655073089
20	85.280834664	85.280833225
30	138.57923108	138.57923195
40	195.97202910	195.97202913
50	256.63001088	256.63001080
100	595.03066281	595.03066288

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