Perturbation theory for sextic doubly anharmonic oscillator

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A simple method for the calculation of higher orders of the logarithmic perturbation theory for bound states of the spherical anharmonic oscillator is developed. The structure of the perturbation series for energy eigenvalues of the sextic doubly anharmonic oscillator is investigated. The recursion technique for deriving renormalized perturbation expansions is offered.

1. INTRODUCTION

The problem of the quantum anharmonic oscillator has been the subject of much discussion for decades because of its importance in quant-field theory, molecular physics, and solid-state and statistical physics. However, while very extensive literature has been devoted to the one-dimensional consideration, relatively less attention has been given to physically more interesting but more complicated three-dimensional case. This applies to the doubly anharmonic oscillator of the type

\[ V(r) = \frac{1}{2} \omega^2 r^2 + \lambda r^4 + \mu r^6, \quad \mu > 0 \]  

as well. In the one-dimensional space, there has been some interest in this theory both in its own right \[1, 2\], and in the corresponding scalar field theory in 2+1 dimensions \[3, 4\]. Besides double perturbation expansions in terms of the two coupling constants \(\lambda\) and \(\mu\) \[4, 5\], this problem has been studied using the theory of continued fraction \[6\], too.

In the three-dimensional space, only exact solutions for the case when the parameters satisfy certain relations have been obtained by a number of authors \[7, 8, 9, 10, 11\] and first four eigenvalues have been calculated with the Hill determinant approach \[12\].

The main tool for studying energy eigenvalues and eigenfunctions of the bound-state problem within the framework of the Schrödinger equation is the logarithmic perturbation

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theory (for references see \[5, 13\]). But the nonconvergence of obtained expansions compels
us to resort to modern procedures of summation of divergent series, such as various ver-
sions of the renormalization technique \[5\]. However, to provide a reasonable accuracy these
procedures need to know high orders of the perturbation series. Unfortunately, with the
standard approach to the logarithmic perturbation theory we can easily obtain the higher
order corrections only for the ground states, because the description of radially excited states
becomes extremely cumbersome.

Recently, a new procedure based on the specific quantization conditions has been pro-
posed to get series of the logarithmic perturbation theory via the $\hbar$-expansions within the
framework of the one-dimensional Schrödinger equation \[13\]. Avoiding disadvantage of the
standard approach, this straightforward semiclassical procedure results in the new handy
recursion formulae with the same simple form both for ground and excited states. Moreover,
these formulae can be easily applied to any renormalization scheme of improving the
convergence of expansions \[5\].

The object of this paper is to extend the above mentioned formalism to the bound-state
problem for the spherical anharmonic oscillator with its subsequent applying to the doubly
anharmonic oscillator.

\section{The Method}

At the beginning we shall concentrate our attention on the bound-state problem for a non-
relativistic particle moving in a central potential of anharmonic oscillator of a general form
admitted bounded eigenfunctions and having in consequence a discrete energy spectrum.
This potential has a single simple minimum at the origin and is given by the symmetric
function

$$V(r) = \frac{1}{2}m\omega^2 r^2 + \sum_{i \geq 1} v_i r^{2i+2}. \quad (2)$$

Then after separating the angular part, the reduced radial part of the Schrödinger equation
takes the form

$$-\frac{\hbar^2}{2m} U''(r) + \left( \frac{\hbar^2 l(l + 1)}{2mr^2} + V(r) \right) U(r) = EU(r). \quad (3)$$

With applying the substitution, $C(r) = \hbar U'(r)/U(r)$, accepted in the logarithmic per-
turbation theory, we go over from the Schrödinger equation to the Riccati one

\[ \hbar C'(r) + C^2(r) = \frac{\hbar^2 l(l+1)}{r^2} + 2mV(r) - 2mE. \]  

We attempt to solve it in a semiclassical manner with series expansions in the Planck constant

\[ E = \sum_{k=0}^{\infty} E_k \hbar^k, \quad C(r) = \sum_{k=0}^{\infty} C_k(r) \hbar^k. \]  

In the complex plane, the number of zeros \( N \) of a wave function inside the closed contour is defined by its logarithmic derivative, \( C(r) \), through the relation

\[ \frac{1}{2\pi i} \oint C(r) \, \frac{\, dr}{r} = \frac{1}{2\pi i} \sum_{k=0}^{\infty} \hbar^k \oint C_k(r) \, \frac{\, dr}{r} = \hbar N. \]  

This quantization condition is exact and is widely used for deriving higher-order corrections to the WKB-approach \([14, 15]\) and the \(1/N\)-expansions \([16, 17, 18]\). There is, however, one important point to note. Because the radial and orbital quantum numbers, \( n \) and \( l \), correspondingly, are specific quantum notions, the quantization condition \([6]\) must be supplemented with a rule of achieving a classical limit for these quantities. It is this rule that stipulates the kind of the semiclassical approximation.

In particular, within the framework of the WKB-method the passage to the classical limit is implemented using the rule

\[ \hbar \to 0, \quad n \to \infty, \quad l \to \infty, \quad \hbar n = \text{const}, \quad \hbar l = \text{const}, \]  

whereas the \(1/N\)-expansion requires the condition \([16, 17, 18]\)

\[ \hbar \to 0, \quad n = \text{const}, \quad l \to \infty, \quad \hbar n \to 0, \quad \hbar l = \text{const}. \]  

The semiclassical treatment of the logarithmic perturbation theory proved to involve the alternative possibility:

\[ \hbar \to 0, \quad n = \text{const}, \quad l = \text{const}, \quad \hbar n \to 0, \quad \hbar l \to 0. \]  

Let us consider the latter rule from the physical point of view. Since \( \hbar l \to 0 \) as \( \hbar \to 0 \), the centrifugal term, \( \hbar^2 l(l+1)/r^2 \), has the second order in \( \hbar \) and disappears in the classical limit that corresponds to falling a particle into the center. This means that a particle drops into the bottom of a potential well as \( \hbar \to 0 \) and its classical energy becomes \( E_0 = \)
min \, V(r) = 0. It appears from this that the series expansion in the Planck constant for the energy eigenvalues must now read as 
\[ E = \sum_{k=1}^{\infty} E_k h^k. \]

Upon inserting the \( h \)-expansions for \( E \) and \( C(r) \) into the Riccati equation (4) and collecting coefficients of equal powers of \( h \), we obtain the following hierarchy of equations:

\[
C_0^2(r) = 2 \, mV(r),
\]

\[
C_0'(r) + 2 \, C_0(r) C_1(r) = -2 \, mE_1,
\]

\[
C_1'(r) + 2 \, C_0(r) C_2(r) + C_1^2(r) = \frac{l(l + 1)}{r^2} - 2 \, mE_2,
\]

\[
\ldots
\]

\[
C_{k-1}'(r) + \sum_{i=0}^{k} C_i(r) C_{k-i}(r) = -2 \, mE_k, \quad k > 2.
\]

In the case of ground states, the recurrence system at hand coincides with one derived by means of the standard technique and can be solved straightforwardly. For excited states, however, it is necessary to take into account the nodes of the wave function, that we intend to do by making use of the quantization condition (6).

It should be stressed that our approach is quite distinguished from the WKB method not only in the rule of achieving a classical limit but also in the choice of a contour of integration in complex plane. With a view to elucidating the last difference let us now sketch out the WKB treatment of the bound-state problem for the spherical anharmonic oscillator. In the complex plane, because the potential is described by the symmetric function (2), this problem has two pairs of turning points, i.e., zeros of the classical momentum. Therefore we have two cuts between these points: in the region \( r > 0 \) as well as in the region \( r < 0 \). In spite of only one cut lies in the physical region \( r > 0 \), the contour of integration in the WKB quantization condition has to encircle both cuts for the correct result for harmonic oscillator to be obtained (19).

In our approach, when a particle is dropping into the bottom of a potential well, these four turning points are drawing nearer and, at last, are joining all together at the origin. Hence, all nodes of the wave function are now removed from both positive and negative sides of the real axis into the origin and our contour of integration must enclose only this point and no other singularities. Further, let us count the multiplicity of zero formed at \( r = 0 \). For the regular solution of the equation (3), the behaviour \( r^{l+1} \) as \( r \to 0 \) brings the value \( l + 1 \). The number of nodes of eigenfunction in the region \( r > 0 \) is equal to radial quantum
number \( n \). But because the potential (2) is a symmetric function the same number of zeros must be in the region \( r < 0 \), too. Then the total number of zeros inside the contour becomes equal to \( N = 2n + l + 1 \).

Taking into account the first order in \( \hbar \) of the right-hand side, the quantization condition (10) is now rewritten as:

\[
\frac{1}{2\pi i} \oint C_1(r) \, r = 2n + l + 1, \quad \frac{1}{2\pi i} \oint C_k(r) \, r = 0, \quad k \neq 1. \tag{11}
\]

A subsequent application of the theorem of residues to the explicit form of functions \( C_k(r) \) easily solves the problem of description of the radially excited states. With that end in view let us consider the system (10) and investigate the behaviour of the function \( C_k(r) \).

From the first equation it is seen that \( C_0(r) \) can be written in the form

\[
C_0(r) = - [2mV(r)]^{1/2} = -m\omega r \left( 1 + \frac{2}{m\omega^2} \sum_{i=1}^{\infty} v_i r^{2i} \right)^{1/2} = r \sum_{i=0}^{\infty} C_0^i r^{2i}, \tag{12}
\]

where the minus sign is chosen from the boundary conditions and coefficients \( C_0^i \) are defined by parameters of the potential through the relations:

\[
C_0^0 = -m\omega, \quad C_i^0 = \frac{1}{2m\omega} \left( \sum_{p=1}^{i-1} C_p^0 C_{i-p}^0 - 2mv_i \right), \quad i \geq 1. \tag{13}
\]

From (12) we recognize that \( C_0(0) = 0 \) and, consequently, the function \( C_1(r) \) has a simple pole at the origin, while \( C_k(r) \) has a pole of the order of \( (2k - 1) \). Hence it appears that \( C_k(r) \) can be represented by the Laurent series:

\[
C_k(r) = r^{1-2k} \sum_{i=0}^{\infty} C_i^k r^{2i}, \quad k \geq 1. \tag{14}
\]

With definition of residues, this expansion permits us to express the quantization condition (11) explicitly in terms of the coefficients \( C_i^k \) as

\[
C_{k-1}^k = (2n + l + 1) \delta_{1,k}. \tag{15}
\]

It is this quantization condition that makes possible the common consideration of the ground and excited states and permits us to derive the simple recurrent formulae.
The substitution of the series (13) and (14) into the system (10) in the case \( i \neq k - 1 \) yields the recursion relation for obtaining the Laurent coefficients

\[
C_i^k = -\frac{1}{2C_0^0} \left[ (3 - 2k + 2i)C_i^{k-1} + \sum_{j=1}^{k-1} \sum_{p=0}^{i} C_j^p C_i^{k-j} \right. \\
+ \left. 2 \sum_{p=1}^{i} C_0^p C_i^{k-p} + l(l+1)\delta_{2,k}\delta_{0,i} \right].
\]  

(16)

If \( i = k - 1 \), by equating the explicit expression for \( C_{k-1}^k \) to the quantization condition (15) we arrive at the recursion formulae for the energy eigenvalues

\[
2mE_k = -C_{k-1}^{k-1} - \sum_{j=0}^{k} \sum_{p=0}^{k-1} C_j^p C_{k-1-p}^{k-j}.
\]  

(17)

Thus, the problem of obtaining the energy eigenvalues and eigenfunctions for the bound-state problem for anharmonic oscillator can be considered solved. The equations (16) and (17) have the same simple form both for ground and excited states and define a useful procedure of the successive calculation of higher orders of the logarithmic perturbation theory.

III. PERTURBATION CORRECTIONS TO ENERGY EIGENVALUES

On applying the recursion relations obtained, analytical expressions for first corrections to the energy eigenvalues of the sextic doubly anharmonic oscillator (1) are found to be
equal to:

\[
E_1 = \frac{1 + 2 N}{2} \omega,
E_2 = \frac{(3 - 2 L + 6 \eta)}{4 \omega^2} \lambda,
E_3 = \frac{1 + 2 N}{8 \omega^5} \left((-21 + 9 L - 17 \eta) \lambda^2 + (15 - 6 L + 10 \eta) \omega^2 \mu\right),
E_4 = \frac{1}{16 \omega^8} \left((333 + 11 L^2 - 3 L (67 + 86 \eta) + 3 \eta (347 + 125 \eta)) \lambda^3
- 6 \left(60 + 3 (-13 + L) L + 175 \eta - 42 L \eta + 55 \eta^2\right) \omega^2 \lambda \mu \right),
E_5 = -\frac{1 + 2 N}{128 \omega^{11}} \times \left((30885 + 909 L^2 - 27 L (613 + 330 \eta) + \eta (49927 + 10689 \eta)) \lambda^4
- 4 \left(11220 + 393 L^2 - 6 L (1011 + 475 \eta) + \eta (16342 + 3129 \eta)\right) \omega^2 \lambda^2 \mu
+ 2 \left(3495 + 138 L^2 + 4538 \eta + 786 \eta^2 - 30 L (63 + 26 \eta)\right) \omega^4 \mu^2 \right),
\]

where \( N = 2 n + l + 1, \eta = N (N + 1), L = l(l + 1), m = 1. \)

As it is seen, that obtained expansion is the expansion in powers of the coupling constants. It is also evident that for the energy eigenvalues, when \( k = 1 \), we readily have the oscillator approximation \[20\]

\[
E_1 = \left(2n + l + \frac{3}{2}\right) \omega.
\]

As a check of the obtained formulae we calculate the energy eigenvalue for the ground state of the anharmonic potential

\[
V(r) = a r^2 + \frac{b}{3} r^4 + \frac{c}{9} r^6
\]

admitted the quasi-exact solution \[11\]. In this case the expression for first corrections to the
energy eigenvalue with: \( n = 0, \ l = 1 \) take the form:

\[
\begin{align*}
E_1 &= \frac{5 \sqrt{a}}{\sqrt{2}}, \\
E_2 &= \frac{35b}{24a}, \\
E_3 &= \frac{35 (-5b^2 + 6ac)}{96 \sqrt{2a^5}}, \\
E_4 &= \frac{35 (475b^3 - 864abc)}{6912a^4}, \\
E_5 &= \frac{-35 (27565b^4 - 67488ab^2c + 17688a^2c^2)}{110592 \sqrt{2a^{11}}}, \\
E_6 &= \frac{35 (1451815b^5 - 4482360ab^3c + 2489328a^2bc^2)}{2654208a^7}.
\end{align*}
\]  

Under the constraints

\[ b = \sqrt{2c} (2a + \frac{7}{3} \sqrt{2c})^{1/2} \]  

we arrive at the analytical expression (with \( \hbar = m = 1 \))

\[
E_{0,1} = \frac{5}{2} (2a + \frac{7}{3} \sqrt{2c})^{1/2}
\]  

derived with the supersymmetric consideration in [11].

Just as it was expected, the obtained series [18] for the sextic doubly anharmonic oscillator is divergent that compels us to resort to modern procedures of summation of divergent series. One of the most common among them are various versions of the renormalization procedures intended to reorganize a given series into another one with better convergence properties.

It was found that the proposed technique is easily adapted to any renormalization scheme. Now we consider the case of the renormalization of a frequency. For this purpose it is enough to think of the harmonic oscillator frequency incoming in the potential as a function of Plank’s constant variable, with subsequent its expansion in an \( \hbar \)-series. However, for later use it is more convenient to take

\[
\omega^2 = \sum_{k=0}^{\infty} \omega_k^2 \hbar^k.
\]  

(24)
The relations for the coefficients $C_i^k$ then reads

\begin{align*}
C_0^0 &= -m\omega_0, \quad C_i^0 = \frac{1}{2m\omega_0} \left( \sum_{p=1}^{i-1} C_p^0 C_{i-p}^0 - 2mv_i \right), \quad i \geq 1, \\
C_i^k &= -\frac{1}{2C_0^0} \left[ -m^2\omega_k^2 \delta_{i,k} + (3 - 2k + 2i)C_i^{k-1} - \sum_{j=1}^{k-1} \sum_{p=0}^{i} C_p^j C_{i-p}^{k-j} + 2 \sum_{p=1}^{i} C_p^0 C_{i-p}^k + l(l+1)\delta_{2,k}\delta_{0,i} \right], \quad k \geq 1,
\end{align*}

but the recursion system for the energy eigenvalues does not change.

The coefficients $\omega_k^2$ are defined by the chosen version of renormalization. In practice, the one-parameter schemes are usually used. They are obtained with the truncation of the series (24) as

\begin{equation}
\omega^2 = \omega_0^2 + \omega_k^2 \hbar^k,
\end{equation}

where $\omega_0$ is a trial frequency and an order in $\hbar$ of the remainder is determined by the anharmonic term in a potential. In the case of our potential (1), taking into account the order in $\hbar$ of the dimensionless parameter of the expansion, we must put $k = 1$.

It has been recognized that for three-dimensional sextic doubly anharmonic oscillator the schemes of both the minimal difference, $E_N(\omega_0) = 0$, and the minimal sensitivity, $(d/d\omega_0)E_N(\omega_0) = 0$, appear to give approximately an equal accuracy in vast range of values of the anharmonic parameters.

Typical results of the calculation are presented in the Table where the sequences of the partial sums of $N$ renormalized corrections to the energy eigenvalues of the spherical anharmonic oscillator with the potential $V(r) = \frac{1}{2}r^2 + \lambda r^4 + \mu r^6$ is compared with the results, $E_{num}$, obtained by the numerical integration for the values $\lambda = \mu$, ($\hbar = m = \omega = 1$). The free parameter $\omega_0$ in the one-parameter scheme (26) is defined order by order from the equation of minimal sensitivity, $(d/d\omega_0)E_N(\omega_0) = 0$, with choosing such the root that obeys the condition of the flattest extremum [21].

From the Table it is seen that the one-parameter renormalization procedure gives the accuracy which is quite sufficient for practical purposes.

In conclusion, a new useful technique for deriving results of the logarithmic perturbation theory has been developed. Based upon the $\hbar$-expansions and suitable quantization conditions, new handy recursion relations for solving the bound-state problem for a spherical
TABLE I: The sequences of the partial sums of $N$ renormalized corrections.

| $N$ | $n = 0, \ l = 0$ | $n = 1, \ l = 0$ | $n = 1, \ l = 1$ |
|-----|----------------|----------------|----------------|
|     | $\lambda = 0.01$ | $\lambda = 10$ | $\lambda = 0.01$ | $\lambda = 10$ |
| 2   | 1.535791        | 5.382133       | 3.670797        | 15.99931        |
|     | 4.765971        | 22.01213       | 5.545735        | 26.18935        |
| 5   | 1.616383        | 6.042488       | 4.144668        | 18.75063        |
|     | 5.614234        | 26.67913       | 5.545735        | 26.18935        |
| 10  | 1.620603        | 6.097330       | 4.184985        | 19.07378        |
|     | 5.614234        | 26.67913       | 5.614234        | 26.67913        |
| 15  | 1.621682        | 6.125723       | 4.193532        | 19.15066        |
|     | 5.629195        | 26.79595       | 5.629195        | 26.79595        |
| 20  | 1.621688        | 6.126339       | 4.223470        | 19.57157        |
|     | 5.683960        | 26.84757       | 5.683960        | 26.84757        |
| 25  | 1.621689        | 6.126361       | 4.223784        | 19.57557        |
|     | 5.684735        | 26.87657       | 5.684735        | 26.87657        |
| 30  | 1.621690        | 6.126367       | 4.223822        | 19.57838        |
|     | 5.685455        | 27.40164       | 5.685455        | 27.40164        |
| 35  | 1.621690        | 6.126369       | 4.223840        | 19.57880        |
|     | 5.685520        | 27.39683       | 5.685520        | 27.39683        |
| 40  | 1.621690        | 6.126370       | 4.223842        | 19.57928        |
|     | 5.685545        | 27.39740       | 5.685545        | 27.39740        |
| $E_{num}$ | 1.621690 | 6.126371 | 4.223843 | 19.57939 | 5.685575 | 27.39812 |

Anharmonic oscillator have been obtained. These relations can be applied to excited states exactly in the same manner as to the ground states providing, in principle, the calculation of the perturbation corrections of large orders in the analytic or numerical form. Besides this remarkable advantage over the standard approach to the logarithmic perturbation theory, our method does not imply knowledge of the exact solution for zero approximation, which is obtained automatically. And at last, the recursion formulae at hand are easily adapted to the use of any renormalization scheme for improving the convergence of obtained series.

The proposed technique has been applied for investigation of the bound-state problem of the three-dimensional sextic doubly anharmonic oscillator. It has been observed that the perturbation series of the logarithmic perturbation theory are divergent but the use of the one-parameter renormalization procedure gives the accuracy which is quite sufficient for practical purposes.
Acknowledgments

This research was supported by a grant N 0103U000539 from the Ministry of Education and Science of Ukraine which is gratefully acknowledged.

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