A new approach to the logarithmic perturbation theory for the spherical anharmonic oscillator

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Abstract. The explicit semiclassical treatment of the logarithmic perturbation theory for the bound-state problem for the spherical anharmonic oscillator is developed. Based upon the $\hbar$-expansions and suitable quantization conditions a new procedure for deriving perturbation expansions is offered. Avoiding disadvantages of the standard approach, new handy recursion formulae with the same simple form both for ground and excited states have been obtained. As an example, the perturbation expansions for the energy eigenvalues of the quartic anharmonic oscillator are considered.

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1. Introduction

The main task in application of the quantum mechanics is to solve the Schrödinger equations with different potentials. Unfortunately, realistic physical problems can practically never be solved exactly. Then one has to resort to some approximations. Most widely used among them is the perturbation theory. However, the explicit calculation with the Rayleigh–Schrödinger perturbation theory, described in most quantum mechanics textbooks, runs into the difficulty of the summation over all intermediate unperturbed eigenstates. To avoid this difficulty, alternative perturbation procedures have been proposed. They are Sternheimer’s method [1, 2], the Dalgarno–Lewis technique [3–6], the method developed by Zel’dovich [7–9] and the logarithmic perturbation theory [10–17].

It must be stressed that in both the Steinheimer method and the Dalgarno–Lewis technique one has to solve inhomogeneous differential equations. In solving the Schrödinger equation with the Zel’dovich method, for avoiding the summation over intermediate states the Lagrange condition of the theory of differential equations is used.

The logarithmic perturbation theory is more straightforward in the sense that it does not require solving any equation or involving any additional condition. Within the framework of this approach, the conventional way to solve a quantum-mechanical bound-state problem consists in changing from the wave function to its logarithmic derivative and converting the time-independent Schrödinger equation into the nonlinear Riccati equation.

In the case of ground states, the consequent expansion in a small parameter leads to handy recursion relations that permit us to derive easily the corrections to the energy as well as to the wave function for each order. Notice that the obtained series are typically divergent and the evaluation of perturbation terms of large orders is needed for applying the modern procedures of summation of divergent series. However, when radially excited states are considered, the standard technique of the logarithmic perturbation theory becomes extremely cumbersome and, practically, inapplicable for describing higher orders of expansions.

For this reason authors of the paper [9] conclude that in dealing with excited states the method developed by Zel’dovich has a remarkable advantage over the logarithmic perturbation theory. But in fact there is another approach to obtaining expansions of the logarithmic perturbation theory that describes excited states and the ground state exactly in the same manner by means of simple recursion formulae.

Indeed, the above mentioned disadvantage of the standard approach to the logarithmic perturbation theory is caused by factoring out zeros of the unperturbed wave functions with taking into account corrections to the positions of these nodes. On the other hand, the number of zeros of the wave function most conveniently and naturally is introduced in the consideration by means of quantization conditions for the logarithmic derivative of the wave function just as within the framework of the Wentzel–
Kramers–Brillouin (WKB) method [18–20]. However, since the WKB-approximation is more suitable for obtaining energy eigenvalues in the limiting case of large quantum numbers but the perturbation theory, on the contrary, deals with low-lying levels, the WKB quantization conditions need change.

Recently, a new procedure based on specific quantization conditions has been proposed to get series of the logarithmic perturbation theory via the \( \hbar \)-expansion technique within the framework of the one-dimensional Schrödinger equation [21]. Avoiding disadvantage of the standard approach, this straightforward semiclassical procedure results in new handy recursion formulae with the same simple form both for the ground state and excited states. Moreover, these formulae can be easily applied to any renormalization scheme of improving the convergence of expansions [22].

However, in most of the practical applications of quantum mechanics, one deals with the more complicated case involved the three-dimensional Schrödinger equation with the anharmonic oscillator potential or the screened Coulomb potential. The object of this paper is to extend the above mentioned formalism to the bound-state problem for the spherical anharmonic oscillator that has numerous applications in the theory of molecules and solid state physics. The another widely used bound-state problem for the three-dimensional Schrödinger equation with the potential, having the Coulomb singularity, will be published elsewhere.

The layout of the paper is as follows: in the next section we summarize the main ideas of our approach concerning the construction of new quantization conditions which are more suitable for the semiclassical treatment of the logarithmic perturbation theory. In section 3 the quantization conditions obtained are used for deriving new simple recursion relations for the calculation of perturbation expansions, which have the same simple form both for the ground state and excited states. Section 4 demonstrates that in the case of the harmonic oscillator potential the described approach restores the exact results for the energy eigenvalues and eigenfunctions. Here we illustrate our method by applying it to the example of the quartic anharmonic oscillator, as well. The paper ends with a brief summary.

2. The classical limit and the quantization rule

We study the bound-state problem for a non-relativistic particle moving in a central potential of an anharmonic oscillator 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 a symmetric function \( V(r) \) which can be written as

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

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

\[
-\frac{\hbar^2}{2m} U''(r) + \left( \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) \right) U(r) = EU(r).
\] (2)
Following usual practice, we apply the substitution, $C(r) = \frac{\bar{h}U'(r)}{U(r)}$, accepted in the logarithmic perturbation theory and go over from the Schrödinger equation (2) to the Riccati equation

$$\hbar C'(r) + C^2(r) = \frac{\hbar^2 l(l + 1)}{r^2} + 2mV(r) - 2mE.$$ \hfill (3)

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

$$E = \sum_{k=0}^{\infty} E_k \hbar^k \quad C(r) = \sum_{k=0}^{\infty} C_k(r) \hbar^k.$$ \hfill (4)

The $\hbar$-expansions under discussion simplify the problem of taking into account the nodes of wave functions for excited states, allowing the use of the quantization condition and the formalism of the theory of functions of a complex variable.

In the complex plane, a number of zeros $N$ of a wave function inside the closed contour is defined by the principle of argument known from the analysis of complex variables. Being applied to the logarithmic derivative, $C(r)$, it means that

$$\frac{1}{2\pi i} \oint C(r) \, dr = \frac{1}{2\pi i} \sum_{k=0}^{\infty} \hbar^k \oint C_k(r) \, dr = \hbar N.$$ \hfill (5)

This quantization condition is exact and is widely used for deriving higher-order corrections to the WKB-approximation [23, 24] and the $1/N$-expansions [25–27]. 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 (5) 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-approach the passage to the classical limit is implemented using the rule

$$\hbar \to 0 \quad n \to \infty \quad l \to \infty \quad \hbar n = \text{const} \quad \hbar l = \text{const}.$$ \hfill (6)

whereas the $1/N$-expansion requires the condition [25–27]

$$\hbar \to 0 \quad n = \text{const} \quad l \to \infty \quad \hbar n \to 0 \quad \hbar l = \text{const}.$$ \hfill (7)

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

$$\hbar \to 0 \quad n = \text{const} \quad l = \text{const} \quad \hbar n \to 0 \quad \hbar l \to 0.$$ \hfill (8)

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 the 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 $E = \sum_{k=1}^{\infty} E_k \hbar^k$. 

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

\[
C_0^2(r) = 2mV(r)
\]
\[
C_0'(r) + 2C_0(r)C_1(r) = -2mE_1
\]
\[
C_1'(r) + 2C_0(r)C_2(r) + C_0^2(r) = \frac{l(l+1)}{r^2} - 2mE_2
\]
\[
\cdots
\]
\[
C_{k-1}'(r) + \sum_{i=0}^{k} C_i(r)C_{k-i}(r) = -2mE_k \quad k > 2.
\]

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.

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 the 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 case of the spherical anharmonic oscillator. In the complex plane, because the potential is described by the symmetric function, 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 the harmonic oscillator to be obtained.

In our approach, when a particle is dropping into the bottom of the potential well these four turning points are drawing nearer and, at last, are joining 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 a zero formed at $r = 0$. For the regular solution of the equation, 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 the radial quantum number $n$. But because the potential 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 is now rewritten as

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

A subsequent application of the theorem of residues to the explicit form of functions $C_k(r)$ easily solves the problem of the description of the radially excited states.
3. Recursion formulae

Let us consider the system (9) 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

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

(11)

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

$$C_0^0 = -m\omega C_0^0, \quad C_0^i = \frac{1}{2m\omega} \left(\sum_{p=1}^{i-1} C_0^p C_0^{i-p} - 2mv_i\right), \quad i \geq 1.$$  

(12)

From (11) 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 order $(2k - 1)$. Thus $C_k(r)$ can be represented by the Laurent series

$$C_k(r) = r^{1-2k} \sum_{i=0}^{\infty} C_k^i r^{2i} \quad k \geq 1.$$  

(13)

With definition of residues, this expansion permits us to express the quantization condition (10) explicitly in terms of the coefficients $C_k^i$ as

$$C_k^k = (2n + l + 1) \delta_{1,k}.$$  

(14)

It is this quantization condition that makes possible the common consideration of the ground and excited states and permits us to derive the simple recursion formulae.

The substitution of the series (12) and (13) into the system (9) in the case $i \neq k - 1$ yields the recursion relation for obtaining the Laurent-series coefficients

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

(15)

If $i = k - 1$, by equating the explicit expression for $C_{k-1}^k$ to the quantization condition (14) we arrive at the recursion formulae defined the perturbation corrections to the energy eigenvalues

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

(16)

Thus, the problem of obtaining the energy eigenvalues and eigenfunctions for the bound-state problem for the anharmonic oscillator can be considered solved. The equations (15) and (16) have the same simple form both for the ground and excited states and define a useful procedure of the successive calculation of higher orders of the logarithmic perturbation theory.
4. Discussion and example of application

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

\[
E_1 = \frac{1 + 2N}{2} \omega \\
E_2 = \frac{(3 - 2L + 6\eta)}{4m^2\omega^2} \nu_1 \\
E_3 = \frac{1 + 2N}{8m^4\omega^5} \left( (-21 + 9L - 17\eta) \nu_1^2 + m \left( 15 - 6L + 10\eta \right) \omega^2 \nu_2 \right) \\
E_4 = \frac{1}{16m^6\omega^8} \left( (333 + 11L^2 - 3L(67 + 86\eta) + 3\eta(347 + 125\eta)) \nu_1^3 \\
- 6m \left( 60 + 3(-13 + L) + 175\eta - 42L\eta + 55\eta^2 \right) \omega^2 \nu_1 \nu_2 \\
+ m^2 \left( 6L^2 - 12L(6 + 5\eta) + 35(3 + 2\eta(4 + \eta)) \right) \omega^4 \nu_3 \right) \\
E_5 = -\frac{1 + 2N}{128m^8\omega^{11}} \left( (30885 + 909L^2 - 27L(613 + 330\eta) + \eta(49927 + 10689\eta)) \nu_1^4 \\
- 4m \left( 11220 + 393L^2 - 6L(1011 + 475\eta) + \eta(16342 + 3129\eta) \right) \omega^2 \nu_1^2 \nu_2 \\
+ 16m^2 \left( 33L^2 - L(501 + 190\eta) + 63(15 + \eta(19 + 3\eta)) \right) \omega^4 \nu_1 \nu_3 \\
+ 2m^2 \left( 3495 + 138L^2 + 4538\eta + 786\eta^2 - 30L(63 + 26\eta) \right) \omega^4 \nu_2^2 \\
- 4m^3 \left( 30L^2 - 20L(24 + 7\eta) + 63(15 + 2\eta(8 + \eta)) \right) \omega^6 \nu_4 \right)
\]

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

As it is seen, the obtained expansion is the expansion in powers of the Taylor-series coefficients for the potential function.

It is also evident that for the energy eigenvalues, when \( k = 1 \), we readily have the oscillator approximation [29]

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

Let us demonstrate that in the case of the isotropic harmonic oscillator our technique restores the exact solution for the wave functions, \( U(r) \), too.

Putting, for simplicity, \( \hbar = m = \omega = 1 \), from equations (12), (13) and (15) we find that

\[
C_0(r) = -r \quad C_k(r) = d_k r^{1-2k} \quad k > 0
\]

where coefficients \( d_k \) obey the relations

\[
d_0 = -1 \\
d_1 = N \\
2d_2 = N^2 - N - l(l + 1) \\
\ldots \\
2d_k = (3 - 2k)d_{k-1} + \sum_{j=1}^{k-1} d_j d_{k-j} \quad k > 2.
\]
Due to the definition $C(r) = U'(r)/U(r)$, the straightforward integration of the function $C_0(r)$ and the part of the function $C_1(r)$ immediately gives factors $e^{-r^2/2}$ and $r^{l+1}$ in the eigenfunctions, $U(r)$, providing their correct behaviour at infinity and the origin. The remaining part is a polynomial $P_n(r) = \sum_{k=0}^{n} p_k r^{2k}$ that satisfies the equation

$$P'_n(r^2)/P_n(r^2) = \sum_{k=1}^{\infty} d_k r^{1-2k} - (l+1)r^{-1}.$$  

The polynomial coefficients, $p_k$, are determined by the system

$$2 p_m(n - m) + \sum_{j=m+1}^{n} p_j d_{j-m+1} = 0.$$  

The combination of these equations, multiplied by a suitable $d_j$ with a view to taking into account equation (20), arrives at the following relation between two consecutive coefficients:

$$\frac{p_{m-1}}{p_m} = \frac{m(m+l+1/2)}{m-n-1}$$  

that is the known recursion formula for the associated Laguerre polynomial, $L^{l+1/2}_n(r^2)$, of degree $n$ [30]. Thus, the described technique restores the exact result for the unnormalized wavefunctions of the harmonic oscillator [29], too.

As an example of application we examine excited states as well as the ground states of the quartic anharmonic oscillator with a potential

$$V(r) = m\omega^2 r^2/2 + \lambda r^4$$  

where $\lambda$ is a positive constant.

Equations (17) for the energy eigenvalues now are rewritten as

$$E_1 = \left(\frac{1}{2} + N\right) \omega$$
$$E_2 = \frac{(3 - 2L + 6\eta)}{4 m^2 \omega^2} \lambda$$
$$E_3 = \frac{-(1+2N) (21 - 9L + 17\eta) \lambda^2}{8 m^4 \omega^5}$$
$$E_4 = \frac{(333 + 11L^2 - 3L (67 + 86\eta) + 3\eta (347 + 125\eta)) \lambda^3}{16 m^6 \omega^8}$$
$$E_5 = \frac{-(1+2N) (30885 + 909L^2 - 27L (613 + 330\eta) + \eta (49927 + 10689\eta)) \lambda^4}{128 m^8 \omega^{11}}$$

We recall that here $N = 2n + l + 1$, $\eta = N(N+1)$, $L = l(l+1)$.

It is readily seen that the use of the $\hbar$-expansion technique does lead to the explicit perturbation expansion in powers of the small parameter $\lambda$.

In the case of ground states, obtained expansions for the energy eigenvalues coincide with those listed in [31]. In the case of excited states, our corrections coincide with corrections up to the second order which are just only calculated in [32].

Thus, we derive the recursion formulae for obtaining arbitrary order terms of the weak coupling power series for the bound-state problem of the anharmonic oscillator.
Unfortunately, as it is known, this series is asymptotic and diverges for any finite value of the parameter $\lambda$ that requires the use of some procedures of improving the convergence (for references see [33]). The most common among them are various versions of the renormalization technique, intended to reorganize a given series into another one with better convergence properties. In practice, these procedures involve quite a number of the perturbation terms and are stopped at a finite order approximation when the change of some eigenvalue with increasing order of approximation becomes less than the needed exactness. If the series begins diverge before achieving the needed exactness of the approximation, we must apply one of the methods of summation of divergent series.

It should be noted, that the proposed formalism of the logarithmic perturbation theory is easily adapted to the treatment of any renormalization scheme in terms of handy recursion relations within the framework of the united approach [22]. Besides, the described technique can be extended to the case of the screened Coulomb potential through the modification of the quantization conditions, that will be published elsewhere.

5. Summary

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 anharmonic oscillator have been obtained. These relations can be applied to excited states exactly in the same manner as to 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, having the same simple form both for the ground state and excited states, can be easily adapted to applying any renormalization scheme for improving the convergence of obtained series, as it is described in [22].

The another widely used case of the three-dimensional Schrödinger equation with the potential having the Coulomb singularity will be published elsewhere.

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