Semiclassical treatment of logarithmic perturbation theory

I V Dobrovolska and R S Tutik†

Department of Physics, Dniepropetrovsk State University, Dniepropetrovsk, UA-320625, Ukraine

Abstract. The explicit semiclassical treatment of logarithmic perturbation theory for the nonrelativistic bound states problem is developed. Based upon $\hbar$-expansions and suitable quantization conditions a new procedure for deriving perturbation expansions for the one-dimensional anharmonic oscillator 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 harmonic oscillator perturbed by λx^6 are considered.

1. Introduction

Logarithmic perturbation theory [1–8] is one of the principal approximation techniques in theoretical and mathematical physics. Within the framework of this theory, the conventional way to solve a quantum-mechanical bound-state problem consists in changing from the wavefunction to its logarithmic derivative and converting the time-independent Schrödinger equation into the nonlinear Riccati equation. Such a procedure leads to handy recursion relations in the case of ground states, but becomes extremely cumbersome in the description of radial excitations when nodes of wavefunctions are taken into account. Although several attempts have been made to improve the method in the latter case [9–11], they have not resulted in a desirable simple algorithm.

On the other hand, it is well known, that the radial quantum number, n, most conveniently and naturally is introduced into consideration by means of quantization conditions, as in the Wentzel–Kramers–Brillouin (WKB) approximation [12–14]. However, the WKB approach is more suitable for obtaining energy eigenvalues in the limiting case of large quantum numbers, whereas the perturbation theory deals with low-lying levels. Usually, the perturbation results are obtained within the framework of the WKB method by recasting the WKB expansions [15–19].

The objective of this paper is to develop an explicit semiclassical treatment of logarithmic perturbation theory and to describe a straightforward semiclassical procedure for obtaining the perturbation corrections through handy recursion formulae, having the same form both for ground and excited states.

For the sake of simplicity, we restrict ourselves to the consideration of the bound-state problem for the one-dimensional anharmonic oscillator. The generalization to the three-dimensional problem requires including the quantization conditions for orbital momentum and will be published elsewhere.

† Author to whom all correspondence should be addressed. E-mail address: `tutik@ff.dsu.dp.ua`

2. Method

The system to be treated is described by the Schrödinger equation

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

where the potential function, $V(x)$, has a simple minimum and hence can be given by the expression

$$V(x) = \tfrac{1}{2}m\omega^2 x^2 + \sum_{i \geqslant 1} f_i x^{i+2}. \tag{2}$$

With changing the scale of the variable, $x \rightarrow \sqrt{\hbar}\,x$, it becomes obvious that the coupling constants, f_i, appear in common with powers of Planck's constant, $\hbar$. Therefore, the perturbation series must be semiclassical $\hbar$-expansions, too. Although well known in the folk wisdom of theoretical physics, this assertion was, nevertheless, proved not so long ago [20]. It has been argued that the energy eigenvalues under consideration should be concentrated near the minimum of the potential and should behave as

$$E = \hbar\omega\left(n + \tfrac{1}{2}\right) + \sum_{i \geqslant 2} E_i(\omega, n)\,\hbar^i. \tag{3}$$

To our knowledge, there are only a few procedures for computing the coefficients $E_i(\omega, n)$. They involve, in particular, applying the methods of the comparison equation [21] and complex 'sprout' [22]; an analytic continuation in the $\hbar$-plane [23]; various approaches within the framework of the WKB approximation [15–19]; quantization using the methods of classical mechanics [17, 24]; and, lastly, expansions in the $\hbar^{1/2}$-series [25]. However, all of these methods have some disadvantages.

Here we propose a new, simpler and more straightforward semiclassical technique. Being explicitly opposed to the WKB approach, it is based on different quantization conditions which are more appropriate for describing the solution of the bound-state problem in the vicinity of a potential minimum.

Following usual practice, we apply the substitution, $C(x) = \hbar U'(x)/U(x)$, accepted in the logarithmic perturbation theory and go over from the Schrödinger equation (1) to the Riccati equation

$$\hbar C'(x) + C^2(x) = 2m[V(x) - E]. \tag{4}$$

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

$$E = \sum_{k=0}^{\infty} E_k \hbar^k \qquad C(x) = \sum_{k=0}^{\infty} C_k(x)\,\hbar^k \tag{5}$$

that result in the system

$$
\begin{aligned}
&C_0^2 = 2m[V(x) - E_0] \\
&C_0' + 2C_0(x)\,C_1(x) = -2mE_1 \\
&\ \vdots \\
&C_{k-1}'(x) + \sum_{i=0}^{k} C_i(x)\,C_{k-i}(x) = -2mE_k.
\end{aligned}
\tag{6}
$$

In the case of ground states, this system coincides with one derived by means of the standard technique and can be solved straightforwardly. However, complications of the logarithmic perturbation theory arise in the description of radial excitations when the nodes of

wavefunctions are included in some separate factor. We intend to circumvent these difficulties by making use of the quantization conditions. The matter of the latter consists in applying the principle of argument, known from the analysis of complex variables, to the logarithmic derivative, $C(x)$.

Since the wavefunction of the nth radially excited state has n real zeros we have

$$\frac{1}{2\pi i} \oint C(x)\,dx = \frac{1}{2\pi i} \sum_{k=0}^{\infty} \hbar^k \oint C_k(x)\,dx = \hbar n. \tag{7}$$

There is, however, one important point to note. In the WKB approach, this condition is supplemented by the following rule of achieving a classical limit:

$$\hbar \to 0 \qquad n \to \infty \qquad \hbar n = \text{constant} \tag{8}$$

accompanied by the equality of the quantum energy to the classical one.

In contrast to this, our method, dealing with low-lying states and being complementary to the WKB approach, involves the alternative possibility

$$\hbar \to 0 \qquad n = \text{constant} \qquad \hbar n \to 0 \tag{9}$$

which was formerly applied in deriving coefficients of the $1/N$ expansions [26–29]. In the limiting case, as $\hbar \to 0$, a particle is now lowered to the bottom of a potential well and its classical energy becomes $E_{\text{cl}} = \min V(x)$, which equals zero in our case.

Thus, in view of the rule (9), the quantization conditions (7) become

$$\frac{1}{2\pi i} \oint C_1(x)\,dx = n \qquad \frac{1}{2\pi i} \oint C_k(x)\,dx = 0 \qquad k > 1. \tag{10}$$

A further application of the theorem of residues to the explicit form of functions $C_k(x)$ easily solves the problem of taking into account nodes of the wavefunctions.

3. Recursion formulae

Let us consider the system (6) and investigate the behaviour of the functions $C_k(x)$. From the first equation it is seen that

$$C_0(x) = -[2mV(x)]^{1/2} = -m\omega x \left(1 + \frac{2}{m\omega^2} \sum_{i \geqslant 1} f_i x^i\right)^{1/2} = x \sum_{i=0}^{\infty} C_i^0 x^i \tag{11}$$

where the minus sign is chosen from boundary conditions, and coefficients C_i^0 are defined by parameters of the potential as

$$C_0^0 = -m\omega \qquad C_i^0 = \frac{1}{2m\omega}\left(\sum_{p=1}^{i-1} C_p^0 C_{i-p}^0 - 2mf_i\right) \qquad i \geqslant 1. \tag{12}$$

Because the point $x = 0$ is a simple zero for the function $C_0(x)$, the function $C_k(x)$ has a pole of the order of $(2k - 1)$ at this point and consequently can be represented by a Laurent series

$$C_k(x) = x^{1-2k} \sum_{i=0}^{\infty} C_i^k x^i \qquad k \geqslant 1. \tag{13}$$

Then, according to the theorem of residues, the quantization conditions (10), expressed in terms of the Laurent series coefficients, take an especially simple form

$$C_{2k-2}^k = n\delta_{1,k} \tag{14}$$

where the symbol $\delta_{1,k}$ is the Kronecker delta.

Substituting the expansions (11) and (13) into (6) and equating coefficients of equal powers of x, we derive

$$(3 - 2k + i)C_i^{k-1} + \sum_{j=0}^{k}\sum_{p=0}^{i} C_p^j C_{i-p}^{k-j} = -2mE_k\delta_{i,2k-2}. \tag{15}$$

Sorting out the case of $i \neq 2k - 2$ yields the recursion relation for obtaining the coefficients C_i^k:

$$C_i^k = -\frac{1}{2C_0^0}\left[(3 - 2k + i)C_i^{k-1} + \sum_{j=1}^{k-1}\sum_{p=0}^{i} C_p^j C_{i-p}^{k-j} + 2\sum_{p=1}^{i} C_p^0 C_{i-p}^k\right] \tag{16}$$

whereas putting $i = 2k - 2$ we would find the recursion formula for the energy eigenvalues

$$2mE_k = -C_{2k-2}^{k-1} - \sum_{j=0}^{k}\sum_{p=0}^{2k-2} C_p^j C_{2k-2-p}^{k-j}. \tag{17}$$

Thus, equations (16) and (17) determine coefficients of perturbation expansions of energy eigenvalues and eigenfunctions in the same simple form both for the ground and excited states.

It should be noted that just conditions (9), represented in the form (14) simplify the consideration of the perturbation theory by means of semiclassical expansions. It becomes more evident under comparison of our technique with the rescaled version of the WKB approach [17–19], where the order of the energy is taken into account by the equality $E = \hbar\varepsilon$. In this case, the coefficients $C_k(\varepsilon, x)$ in equation (7) have poles, too. The WKB quantization condition (8) then reads as

$$\sum_{k=0}^{\infty} \hbar^{k-1} \operatorname{Res} C_k(\varepsilon, x) = n \tag{18}$$

with the residues being polynomial with respect to ε. By truncating the series in the left-hand side we arrive at the equation for determination of approximations to the energy eigenvalues ε, and only after subsequent re-expanding, can we restore the results of perturbation theory [17–19].

4. Discussion and examples

From equation (17) it is readily seen that for the energy eigenvalues, when $k = 1$, we immediately have the oscillator approximation

$$E_1 = \omega\left(n + \tfrac{1}{2}\right) \tag{19}$$

and with $k = 2$ one obtains the form familiar from standard textbooks [15]

$$E_2 = -\frac{15f_1^2}{4m^3\omega^4}\left(n^2 + n + \tfrac{11}{30}\right) + \frac{3f_2}{2m^2\omega^2}\left(n^2 + n + \tfrac{1}{2}\right). \tag{20}$$

It is easy to demonstrate that in the case of the harmonic oscillator our technique restores the exact solution for the wavefunctions as well.

Putting, for simplicity, $\hbar = m = \omega = 1$, from equations (12), (13) and (16) we find

$$C_0(x) = -x \qquad C_k(x) = d_k x^{1-2k} \qquad k > 0 \tag{21}$$

where

$$2d_k = (3 - 2k)d_{k-1} + \sum_{j=1}^{k-1} d_j d_{k-j} \qquad k > 1 \tag{22}$$

$$d_1 = n.$$

Carrying out the integration of the function $C_0(x)$ we obtain the exponential factor of the eigenfunction. Its remaining part is a polynomial that satisfies the equation

$$P_n'/P_n = \sum_{k=1}^{\infty} d_k x^{1-2k} \tag{23}$$

and, consequently, has the form

$$P_n(x) = x^{\sigma} \sum_{i=0}^{m_0} a_i x^{2i} \qquad \sigma = 0 \quad \text{or} \quad 1 \qquad n = 2m_0 + \sigma. \tag{24}$$

On the basis of equation (23), the polynomial coefficients, a_i, are determined by the system

$$(n - 2m - \sigma)a_m + d_2 a_{m+1} + \cdots + d_{m_0-m+1} a_{m_0} = 0. \tag{25}$$

The combination of these equations, multiplied by a suitable d_j with a view to taking into account equation (22), arrives at the following relation between two consecutive coefficients:

$$a_m = -a_{m+1} \frac{(2m + \sigma + 2)(2m + \sigma + 1)}{4(m_0 - m)} \tag{26}$$

that is the recursion formula for the Hermite polynomials (see, for instance [30]).

And at last, as an example, we consider the anharmonic oscillator with the potential

$$V(x) = \tfrac{1}{2}x^2 + \tfrac{1}{2}\lambda x^6. \tag{27}$$

Though this oscillator is widely discussed in the scientific literature [31–33], the analytical expressions for the perturbation expansions of energy eigenvalues presented in [31] are incorrect. The correct expansion coefficients obtained by means of formulae (16) and (17) have the form

$$E_1 = n + \tfrac{1}{2}$$
$$E_3 = 5\lambda 2^{-4}\left(4n^3 + 6n^2 + 8n + 3\right)$$
$$E_5 = -\lambda^2 2^{-8}\left(1572n^5 + 3930n^4 + 12\,220n^3 + 14\,400n^2 + 11\,528n + 3495\right)$$
$$E_7 = 5\lambda^3 2^{-11}\left(23\,592n^7 + 82\,572n^6 + 418\,236n^5 + 839\,160n^4 + 1\,523\,968n^3\right.$$
$$\left. + 1\,488\,078n^2 + 939\,884n + 247\,935\right)$$
$$E_9 = -\lambda^4 2^{-16}\left(45\,804\,660n^9 + 206\,120\,970n^8 + 1\,471\,569\,960n^7 + 4\,188\,597\,000n^6\right.$$
$$+ 12\,317\,818\,548n^5 + 20\,804\,002\,800n^4 + 29\,394\,281\,120n^3$$
$$\left. + 25\,244\,303\,400n^2 + 13\,898\,196\,592n + 3\,342\,323\,355\right)$$
$$E_{11} = 5\lambda^5 2^{-19}\left(1\,023\,655\,464n^{11} + 5\,630\,105\,052n^{10} + 52\,379\,661\,180n^9\right.$$
$$+ 193\,482\,687\,420n^8 + 801\,071\,289\,576n^7 + 1\,940\,241\,040\,920n^6$$
$$+ 4\,424\,265\,058\,200n^5 + 6\,633\,369\,121\,920n^4 + 8\,108\,461\,519\,360n^3$$
$$\left. + 6\,378\,900\,376\,878n^2 + 3\,214\,574\,914\,460n + 725\,076\,383\,025\right). \tag{28}$$

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 an anharmonic oscillator within the framework of the one-dimensional Schrödinger equation have been obtained. Avoiding the disadvantages of the standard approach these formulae have the same simple form both for ground and excited states and provide, in principle, the calculation of the perturbation corrections up to an arbitrary order in the analytical or numerical form. The extension on the three-dimensional case and the relativistic equations will be published elsewhere.

Acknowledgment

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