SEMICLASSICAL APPROACH TO PERTURBATION THEORY

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The problem of constructing approximate solution methods and finding convenient recurrent algorithms for the study of bound states of quantum mechanical equations is one of the central problems of modern theoretical physics. In this paper an explicit semiclassical treatment of perturbation theory for non-relativistic bound states based on $\hbar$-expansions and corresponding quantization conditions of one-dimensional problems is developed. The wave functions are chosen in the same way as in the logarithmic perturbation theory. Due to the introduction of new quantization conditions, this method made it possible to obtain recurrent relations, which are convenient for finding the energy eigenvalues and wave functions of bound states in the case when nodes of wave functions are taken into account. Avoiding the flaws of the standard approach, the obtained recurrent relations have the same form both for the ground and perturbed states.

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1. Introduction

Since 1926, when Schrödinger suggested his well-known equation, and up to now, many different methods of its solution have been developed, including those for finding the eigenstates of various quantum mechanical systems. The existence of small class of problems that have exact solutions gave impulse to the development of various theoretical approaches. The exact solution of the Schrödinger equation, which determines the energy of stationary states of systems, is possible only for some simple potential fields corresponding to idealized systems. When studying real systems, one has to resort to approximate methods of calculation eigenvalues and eigenfunctions of Hamiltonian operators.

Currently, in non-relativistic quantum mechanics there are many solution methods for problems that are not solved exactly [1,2]. The Rayleigh–Schrödinger perturbation theory is one of the best known and widely-accepted techniques [3]. For its application, it is necessary to know the entire spectrum for an unperturbed problem. In this way, it is practically possible to find only a first approximation to the exact solution of the problem. The practical implementation of the Rayleigh–Schrödinger perturbation theory method is very limited, because even when calculating the first order of approximation for the wave function (for the second order for energy), an infinite sum appears in the recurrent relations, which makes it impossible to calculate numerically the exact value.

Logarithmic perturbation theory is a technique of approximate calculation in theoretical and mathematical physics [4, 5]. This theory is based on a method for solving quantum-mechanical problems, which involves substituting the wave functions by their logarithmic derivatives and going from the stationary Schrödinger equation to the nonlinear Riccati equation [6]. In this connection, there is no need to know the spectrum for an unperturbed problem, but the recurrent formulas have a convenient form only for the ground states.

The Wentzel–Kramers–Brillouin approximation has a sufficiently restricted application area, being usually valid for strongly perturbed states, which correspond to rapidly oscillating wave functions, although modifications of the WKB method have extended the potential of its application [7]. To study lower states, it is necessary to utilize higher orders of quasi-classical approximation, finding of which is associated with great difficulties. It should be noted that quasi-classical approximation is developed in detail only for one-dimensional and spherically symmetric cases.

The $1/N$-expansion method is based on the consideration of the classical motion of a particle located at the potential well bottom, formed by the effective potential of the radial Schrödinger equation, with further accounting for quantum fluctuations and anharmonicity effects as a perturbation series in small parameter, which determines the inverse value of the space size [8, 9]. The main advantage of this approach is that calculations in the case of ground states are carried out according to simple recurrent relations [10–12].

Semiclassical treatment of logarithmic perturbation theory reduces the linear Schrödinger equation to the nonlinear Riccati equation. But in contrast to the logarithmic perturbation theory, solving the obtained Riccati equation is based on expanding energies and functions $F(x) = \hbar\frac{\Psi'(x)}{\Psi(x)}$ in powers of $\hbar$, hereafter $\Psi(x)$ are wave functions. While using this method, the difficulties of standard approach are eliminated, and obtained recurrent relations have a simple form both for the ground and perturbed states and provide, in principle, the calculation of perturbative corrections of arbitrary orders not only analytically, but also numerically.

2. Modification of semiclassical approach to perturbation theory

The purpose of this work is to investigate the possibilities of constructing a modified semiclassical perturbation theory with the choice of a wave function in the same form as in the standard logarithmic perturbation theory. This could make it possible to take into account the nodes of the wave function easily and obtain recurrent relations which have a simple form both for the ground and perturbed states.

For simplicity, we consider only the bound state problem for a one-dimensional anharmonic oscillator.

Let our system be described by the Schrödinger equation

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

where the potential-energy function $V(x)$ has a simple minimum and can be given in the following form

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

that fulfils the condition for minimum of the function ($V'(x) = 0$, $V''(x) > 0$). If we perform the rescaling of the coordinate x, $x \to \sqrt{\hbar}x$, it becomes apparent that couplings f_i are shared in common with powers of Planck's constant $\hbar$. Thereby, the perturbation series should also be semiclassical $\hbar$-expansions. However, this statement, well known in theoretical physics, was proved quite recently [13].

It was stated that energy eigenvalues under consideration should be clustered around the potential minimum and represented as

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

At the moment, there are only a few procedures for calculating the coefficients $E_i(\omega, n)$. They include, in particular, applying the methods for equation comparing; analytical continuation to the $\hbar$-plane; different approaches within the WKB approximation; quantization by methods of classical mechanics [14, 15], and, finally, expansion into $\hbar^{1/2}$-series [16]. But all these methods

have a variety of disadvantages.

In this work, we propose a new, simpler and clearer procedure. Let's take the wave function Ψ in the form

$$\Psi(x,\hbar) = \Omega(x,\hbar)e^{-\frac{1}{\hbar}\int D(x)dx}. \tag{3}$$

Finding the first and second derivatives of the wave function Ψ, we obtain

$$\Psi'(x,\hbar) = e^{-\frac{1}{\hbar}\int D(x)dx}\left(\Omega'(x,\hbar) - \frac{1}{\hbar}\Omega(x,\hbar)D(x)\right);$$

$$\Psi''(x,\hbar) = e^{-\frac{1}{\hbar}\int D(x)dx}\left(\Omega''(x,\hbar) - \frac{2}{\hbar}\Omega'(x,\hbar)D(x) + \frac{1}{\hbar^2}\Omega(x,\hbar)D^2(x) - \frac{1}{\hbar}\Omega(x,\hbar)D'(x)\right)$$

where sign $'$ denotes derivative with respect to the variable x. Substituting these values into the Schrödinger equation (1), we get the following differential equation

$$\frac{\hbar^2}{2m}\left(\Omega''(x,\hbar) - \frac{2}{\hbar}\Omega'(x,\hbar)D(x) + \frac{1}{\hbar^2}\Omega(x,\hbar)D^2(x) - \frac{1}{\hbar}\Omega(x,\hbar)D'(x)\right) = \\ = (V(x) - E)\,\Omega(x,\hbar). \tag{4}$$

Equating the coefficients at powers of $\hbar$ equal to 0 and taking into account the fact that the expansion of E in a series in $\hbar$ can be written as

$$E = \hbar\sum_{k=0}^{\infty} E_k\hbar^k, \tag{5}$$

and also owing to expansion of the functions $\Omega(x,\hbar)$, $\Omega'(x,\hbar)$, $\Omega''(x,\hbar)$ in series in powers of $\hbar$

$$\Omega(x,\hbar) = \sum_{k=0}^{\infty}\Omega_k\hbar^k, \quad \Omega'(x,\hbar) = \sum_{k=0}^{\infty}\Omega'_k\hbar^k, \quad \Omega''(x,\hbar) = \sum_{k=0}^{\infty}\Omega''_k\hbar^k,$$

we get

$$-\frac{1}{2m}\Omega(x,\hbar)D^2(x) + V(x)\Omega(x,\hbar) = 0,$$

which defines the integral function in the expression (3) as

$$D(x) = \left[2mV(x)\right]^{1/2}. \tag{6}$$

After this substitution, the equation (4) takes the form

$$-\frac{\hbar}{2m}\Omega''(x,\hbar) + \left(\frac{D(x)}{m} + \frac{D'(x)}{2m}\right)\Omega'(x,\hbar) = \frac{1}{\hbar}E\Omega(x,\hbar). \tag{7}$$

In this case, it is convenient to put $2m = 1$, as well as consider the formulas (5) and (6) and the fact that $D'(x) = \frac{V'(x)}{2\sqrt{V(x)}}$. We rearrange the equation (7) to the following form

$$-\hbar\sum_{k=0}^{\infty}\Omega''_k\hbar^k + 2\sqrt{V(x)}\sum_{k=0}^{\infty}\Omega'_k\hbar^k + \frac{V'(x)}{2\sqrt{V(x)}}\sum_{k=0}^{\infty}\Omega_k\hbar^k = \sum_{k=0}^{\infty}\hbar^k\sum_{i=0}^{k}E_i\Omega_{k-i}. \tag{8}$$

As a result, we get a system of n equations with $2n$ unknowns. Considering the equation (8) for the case $k = 0$, we obtain the relation

$$4V(x)\Omega_0' + \left(V'(x) - 2\sqrt{V(x)}E_0\right)\Omega_0 = 0; \tag{9}$$

for the case $k \geqslant 1$ we find an expression

$$4V(x)\Omega_k' + \left(V'(x) - 2\sqrt{V(x)}E_0\right)\Omega_k - 2\sqrt{V(x)}\Omega_{k-1}'' = 2\sqrt{V(x)}\sum_{i=1}^{k} E_i\Omega_{k-i}. \tag{10}$$

Considering that the wave function Ψ has n real zeros by oscillation theorem, then according to the residue theorem, we may write

$$\oint_\Gamma \left(\frac{\Omega'(x,\hbar)}{\Omega(x,\hbar)} + D(x)\right)dx = 2\pi i n.$$

Since the function $D(x)$ is regular in the region Γ, the last integral can be written as follows

$$\frac{1}{2\pi i}\oint_\Gamma \frac{\Omega'(x,\hbar)}{\Omega(x,\hbar)}dx = \frac{1}{2\pi i}\oint_\Gamma \frac{d}{dx}\ln\Omega(x,\hbar)dx = n. \tag{11}$$

Let's expand the logarithm function into a Taylor series in powers of $\hbar$:

$$\ln\Omega(x,\hbar) = \ln\Omega + \sum_{k=1}^{\infty}\left(\frac{\Omega_k}{\Omega_0} + O(k)\right)\hbar^k,$$

where $O(k)$ is a new function which contains the sum of ratios of the functions Ω_k and Ω_k'.

Now we rewrite the integral (11) as

$$\oint_\Gamma \frac{\Omega'(x,\hbar)}{\Omega(x,\hbar)}dx = \oint_\Gamma \frac{\Omega_0'}{\Omega_0}dx + \oint_\Gamma \sum_{k=1}^{\infty}\frac{d}{dx}\left(\frac{\Omega_k}{\Omega_0} + O(k)\right)\hbar^k dx = 2\pi i n. \tag{12}$$

In the formula (12), we change from the integral around the loop to the residue. At the same time, we equate the coefficients at the same powers of $\hbar$ on the left and right sides of equality. We obtain the expressions

$$\oint_\Gamma \frac{\Omega_0'}{\Omega_0}dx = 2\pi i n \;\Rightarrow\; Res\left(\frac{\Omega_0'}{\Omega_0}\right) = n, \tag{13}$$

$$\oint_\Gamma \frac{d}{dx}\left(\frac{\Omega_k}{\Omega_0} + O(k)\right)dx = 0 \;\Rightarrow\; Res\left[\frac{d}{dx}\left(\frac{\Omega_k}{\Omega_0} + O(k)\right)\right] = 0,\; k \geqslant 1. \tag{14}$$

3. Recurrent formula for energies

Due to the fact that $\Omega = \Omega(k,\hbar)$ is a bivariate function, the coefficients of expansion of this function into a series in powers of $\hbar$ can be developed as a Laurent series in x.

We also take into account that the function $O(k)$ changes into a certain Laurent series

when replacing the functions Ω_k with the corresponding Laurent series in powers of x, i. e. the function $O(k)$ can be written as:

$$O(k) = \sum_{i=-\infty}^{\infty} O_i(k) x^k.$$

After finding the x-derivative of the $O(k)$ function, the series on the right-hand side loses the term $1/x$, that is, the $O(k)$ function will not contribute to the residue. Considering this, the formula (14) can be presented in the form

$$Res\left[\frac{d}{dx}\left(\frac{\Omega_k}{\Omega_0}\right)\right] = 0,\ k \geqslant 1. \tag{15}$$

It follows from the formula (13) that the function Ω_0 should be given by

$$\Omega_0 = x^n \sum_{i=0}^{\infty} \Omega_i^0 x^i \tag{16}$$

where Ω_i^0 are the coefficients of expansion of the function Ω_0 in the power series in x. From the formula (15), we obtain the general form of the function Ω_k

$$\Omega_k = x^{n-2k} \sum_{i=0}^{\infty} \Omega_i^k x^i. \tag{17}$$

For the convenience of further calculations, we introduce such a notation

$$\mu = \sqrt{V} = x \sum_{i=0}^{\infty} \mu_i x^i \ \Rightarrow\ \mu' = \sum_{i=0}^{\infty} (i+1) \mu_i x^i. \tag{18}$$

Finding the corresponding derivatives of the functions (16) and (17), we substitute them into the set of equations (9-10), considering formula (18). As a result, we get

$$\begin{aligned} E_k \Omega_0^0 = b_{2k} \Omega_{2k}^{k-1} + \sum_{j=0}^{2k} \left(2a_{2k-j} + 1 + j\right) \mu_j \Omega_{2k-j}^k - \\ - \sum_{p=1}^{k-1} E_p \Omega_{2(k-p)}^{k-p} \sum_{i=0}^{2k} \left(b_i \Omega_i^{k-1} + \sum_{j=0}^{i} \left(2a_{i-j} + 1 + j\right) \mu_j \Omega_{i-j}^k \right) - \sum_{p=1}^{k-1} \sum_{i=p}^{2k} E_p \Omega_i^{k-p} \end{aligned} \tag{19}$$

where $a_i = i + n - 2k$, $b_i = a_i + 2$.

4. Conclusions

Considering the convenient recurrent algorithm development for study of bound states of quantum mechanical equations, we studied the possibility of constructing a modified semiclassical perturbation theory with the choice of a wave function in the same form as in the standard logarithmic perturbation theory. Within the framework of the modified logarithmic perturbation theory, a new approach to the construction of recurrent relations was developed. Based on $\hbar$-expansions, we obtained new convenient relations for solving the problem of the

bound state for an anharmonic oscillator in terms of the one-dimensional Schrödinger equation.

The developed procedure completely eliminates the limitations of the standard approach. The formulas take the same simple form both for the ground and perturbed states and provide, in principle, the computation of arbitrary order perturbation corrections in analytical, as well as in numerical form.

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