A new approach to determination of the energy levels of the bound states in quantum mechanics. Convergent perturbation theory

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(Submitted 20 July 1979)
Pis'ma Zh. Eksp. Teor. Fiz. **30**, No. 6, 379–383 (20 September 1979)

A perturbation theory (PT), each term of which is expressed in quadratures, is constructed. A procedure for selecting the zeroth approximation, which leads to a fast convergence of the PT series is formulated. As an example, the ground and first-excited states in the potential $V(x) = x^{2n}$ $(n = 2, 3, 4)$ are calculated.

PACS numbers: 03.65.Ge, 03.65.Db

At present, like many years ago, strong coupling is one of the central problems in quantum mechanics and quantum field theory. Thus far, there have been no reliable analytic methods available for investigation of the region of large coupling constants. Moreover, if this region can be investigated in one-dimensional quantum-mechanical systems by using numerical methods, then, on going over to problems that cannot be reduced to one-dimensional problems, even these methods are almost always ineffective. Let us discuss in detail the causes of this unsatisfactory situation in the search for the spectrum of the bound states in a quantum-mechanical system (these problems are now particularly urgent in the investigation of the physics of new particles). The standard Rayleigh-Schrödinger perturbation theory is usually used to solve such problems.[1] To use this method, however, the total spectrum of the unperturbed problem and its wave functions must be known, i.e., the unperturbed problem must be exactly solvable. Since the number of exactly solvable problems is rather limited, usually *the interaction potentials are more singular than the potentials of the unperturbed problems.* This in turn leads to a divergence of the PT series. Therefore, the information obtained from the PT series which is rather scanty, concerns principally the region of weak coupling.

In this paper we shall 1) formulate a PT for the one-dimensional case, in which each term is expressed in quadratures and which does not require a knowledge of the total spectrum of the unperturbed problem and 2) formulate a recipe for choosing the unperturbed problem, which will enable us to obtain a rapidly converging series of the PT.

Let us construct the PT. The unperturbed problem can be described by the Hamiltonian $H_0 = p^2 + V_0(x)$, and the interaction potential is equal to $\lambda V_1(x)$. The method involves going over from the *linear* Schrödinger equation by using the substitution $y = -\psi'/\psi$ (ψ is the wave function) to the *nonlinear* Riccati equation

$$y^1 - y^2 = E - V_0(x) - \lambda V_1(x) \tag{1}$$

and then constructing the PT in the parameter λ (in the Riccati equation) for y and E $[y = \Sigma_{n=0}^{\infty} \lambda^n y_n(x),\ E = \Sigma_{n=0}^{\infty} \lambda^n E_n]$. Thus, we must solve a first-order *linear* equa-

tion in order to calculate the nth term of the series of the PT if the preceding $(n-1)$ terms are known

$$\begin{aligned} y_1^1 - 2y_0 y_1 &= E_1 - V_1(x), \\ y_n^1 - 2y_0 y_n &= E_n + \sum_{i=1}^{n-1} y_i y_{n-i}, \qquad n \geqslant 2, \end{aligned} \tag{2}$$

where y_0 and E_0 correspond to any energy level of the unperturbed problem. Imposing the obvious boundary conditions $y_i(\pm\infty) = 0$, we obtain solutions of Eq. (2)

$$y_1 = \psi_0^{-2} \int_{-\infty}^{x} (E_1 - V_1(x))\psi_0^2\, dx, \qquad E_1 = \frac{\int_{-\infty}^{\infty} V_1(x)\psi_0^2\, dx}{\int_{-\infty}^{\infty} \psi_0^2\, dx}, \tag{3a}$$

$$y_n = \psi_0^{-2} \int_{-\infty}^{x} (E_n + \sum_{i=1}^{n-1} y_i y_{n-i})\psi_0^2\, dx, \qquad E_n = -\frac{\int_{-\infty}^{\infty} \sum_{i=1}^{n-1} y_i y_{n-1}\psi_0^2\, dx}{\int_{-\infty}^{\infty} \psi_0^2\, dx}, \tag{3b}$$

where ψ_0 is the wave function from which γ_0 and E_0 are constructed. We emphasize that E_1 coincides with the correction obtained by using the standard Rayleigh-Schrödinger PT. By expressing clearly the ψ_n corrections for the wave functions in terms of the y_n corrections and determining the integration constants properly, we can obtain the sum rules for the series in the conventional PT[1] in terms of the quadratures.[3] Thus, we need not necessarily know the total spectrum of the unperturbed problem in order to determine the location of any level.[1] It should be noted that Dolgov and Popov[2] noticed in studying the standard divergent PT for the anharmonic oscillator ($V_0 = x^2$ and $V_1 = x^{2n}$) that the Riccati equation is very suitable for calculating the terms of the PT series, since the $y_n(x)$ in this case are polynomials in x. This observation allowed them to easily duplicate the results of Bender and Wu,[3] after studying in detail the structure of the PT series.

Let us now consider the problem of choosing the zeroth approximation in the equation.[1] The recipe for choosing the zeroth approximation wave function for determining any level in the $V(x)$ potential must be such that the potential $V_0(x)$ corresponding to $\psi_0(x)$ [i.e., $V_0(x) - E_0 = \psi_0''(x)/\psi_0$] would contain *all* the singularities of the $V(x)$ potential. In this case the perturbation potential $\lambda V_1(x)$, which is equal to the difference between $V(x)$ and $V_0(x)$, is small compared to $V(x)$. It is clear that the PT series in this case is convergent.

Let us calculate, for example, the locations of the zero level and the first level in the potential $V(x) = x^{2n}$, $n = 2$, 3 and 4. The wave functions of zeroth approximation have the form

TABLE I. The quantity ΔE gives the value of the corresponding term of the PT. The numbers in parentheses indicate the relative deviation from the exact answer.

Potential		$V(x) = x^4$		$V(x) = x^6$		$V(x) = x^8$	
Approximation number		zero level	first level	zero level	first level	zero level	first level
0	E	1	3	1	3	1	3
	ΔE	1	3	1	3	1	3
1	E	1.13359(6.9%)	3.94939 (4%)	1.15841(1.2%)	4.35903(0.5%)	1.23476(0.73%)	4.87684(2.5%)
	ΔE	0.13359	0.94939	0.15841	1.35903	0.23476	1.87684
2	E	1.09519(2.3%)	3.84482(1.2%)	1.14747(0.2%)	4.33976(0.03%)	1.225595(0.02%)	4.75414(0.036%)
	ΔE	0.04841	0.10458	0.01094	0.01927	0.009165	0.122696
3	E	1.06976(0.9%)	–	–	–	–	–
	ΔE	0.01542	–	–	–	–	–
exact		1.06036211	3.79967315	1.14480246	4.33859882	1.22582010	4.75587451

$$ {}_n\psi_o^{(0)} = \exp\left\{-\frac{x^2}{2} - \frac{x^{n+1}}{n+1}\right\}, \qquad {}_n\psi_o^{(1)} = x\exp\left\{-\frac{x^2}{2} - \frac{x^{n+1}}{n+1}\right\}, \tag{4} $$

respectively. These wave functions correspond to the potentials and levels

$$ {}_nV_o^{(0)}(x) = -\{nx^{n-1} - 2x^{n+1} - x^2\} + x^{2n}, \quad {}_nE_o^{(0)} = 1, \tag{5a} $$

$$ {}_nV_o^{(1)}(x) = -\{(n+2)x^{n-1} - 2x^{n+1} - x^2\} + x^{2n}, \quad {}_nE_o^{(1)} = 3. \tag{5b} $$

The expressions in the braces in Eqs. (5a) and (5b) are $V_1(x)$.[2] Developing the PT described earlier and substituting Eqs. (4), (5a), and (5b) in Eqs. (3a) and (3b), we can calculate the locations of the levels. The results of the calculations in Table I are compared with the results of a numerical solution of the Schrödinger equation. It can be seen that a second approximation gives rather good accuracy. It is particularly worth noting that convergence of the PT series in this case can be proved by constructing a majorized sequence.[3]

In summary, we emphasize that in the one-dimensional quantum-mechanical problems the spectra of different potentials can be easily investigated and, in particular, the wave functions corresponding to these spectra can be calculated in the manner described above. This method apparently can be used to investigate the region of strong coupling. The next paper, in which the anharmonic oscillator and the potential with two minima are examined, will be devoted to this problem. Although it is quite trivial to generalize this method to include multidimensional problems with spherical symmetry, it is rather complicated to generalize it for problems without spherical symmetry, since the multidimensional analog of the equation (1) has a rather complex construction. Nonetheless, the entire program can be realized in the two-dimensional case. All the results will be published in the near future.

In conclusion, I consider it my duty to thank K. A. Ter-Martirosyan, B. L. Ioffe, and Yu. A. Simonov for useful discussions and interest in this work and also M. S. Marinov and V. E. Shestopal for the numerical calculations and solutions of the Schrödinger equation with the potential $V(x) = x^{2n}$.

[1)]The construction of the PT for the excited levels involves difficulties associated with the orthogonality of the wave functions of different states. These problems and their solutions will be examined in a detailed article.

[2)]In this case $\lambda = 1$.

[3)]The proof will be published in a detailed article. Here we only point out that there is no evidence of physical causes of the singularities at the finite points of the λ plane.

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