

# Perturbation theory and variation principle in quantum mechanics

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A nonstandard perturbation theory (PT) is developed in many-dimensional quantum mechanics; in this theory knowledge of the entire spectrum of the unperturbed problem is not required, and only the characteristics of the level for which corrections are to be determined must be known. In the one-dimensional case this theory reduces to the PT proposed by Zel'dovich. It is shown that the problem of constructing the PT in the  $k$ -dimensional case is equivalent to that of  $k$ -dimensional electrostatics with a variable dielectric constant. The relation between the variational principle and PT is found, and it is shown that the PT developed here makes it possible to estimate the accuracy of variational calculations and to improve this accuracy by using an iteration method. A recipe is formulated for constructing an unperturbed problem so as to get converging PT series. A theorem on the uniqueness of PT series is proved. Examples considered are the ground states in the potentials  $x^{2n}$  ( $n = 2, 3, 4$ ) and  $m^2x^2 + gx^4$ ; it is shown that the first two or three approximations are enough to calculate the energy to an accuracy of  $10^{-3}$ – $10^{-5}$  (for arbitrary  $g$ ). For the two-dimensional anharmonic oscillator calculations are made of the first several coefficients of the PT series in powers of the coupling constant.

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## 1. INTRODUCTION

One of the problems most frequently encountered in quantum mechanics is that of finding the energies of bound states. It is analyzed in detail in practically all books on quantum mechanics (cf., e.g., Ref. 1). Its importance is due to the fact that many phenomena in various fields of physics can be described by means of potentials, so that frequently an investigation reduces to the solution of the Schrödinger equation with some particular potential. The main difficulty in almost all cases is that the Schrödinger equation with a potential that describes an actual physical phenomenon is almost always incapable of exact integration. This makes necessary the use of various approximate methods. Here it must be stressed that the present possibilities for numerical integration of the Schrödinger equation are rather limited: It can be used successfully only for one-dimensional problems, and is practically helpless even in two-dimensional quantum-mechanical problems (see the discussion in Ref. 2). For this reason, in dealing with many-dimensional problems or studying the analytic properties of solutions of the Schrödinger equation one has to use approximate methods.

The most frequently used approximate methods are the Rayleigh-Schrödinger perturbation theory and the Rayleigh-Ritz variation principle. Let us examine each of them in more detail. To construct the Rayleigh-Schrödinger perturbation theory (PT) it is necessary

to know the entire spectrum of the unperturbed problem or, equivalently, its Green's function, since the corrections to the wave function and the energy are expressed as sums over intermediate states or integrals containing the Green's function. This means that the unperturbed problem must be exactly soluble. Up to now the number of exactly solved problems is rather limited. A typical situation is that of a perturbation potential that is more singular than that of the unperturbed problem, or, in other words, is large compared with it. This is the main cause of the divergence of PT series in physically interesting cases. Consequences are the difficulties with coupling constants of the order of unity and with strong-coupling cases (see the discussion in an earlier paper<sup>3</sup>). Besides this, the use of the Schrödinger-Rayleigh PT gives rise to technical difficulties with calculating matrix elements and finding multiple sums over intermediate states. These difficulties are especially marked in attempts to deal with many-dimensional problems.

The Rayleigh-Ritz variation method and other variational methods of the Hartree-Fock type are practically the only tool for investigating the spectra of many-dimensional problems. However, when this tool is used it is a very complicated problem to estimate the accuracy of the results (see, e.g., Ref. 4). There are other difficulties with variational calculations; in particular it is rather complicated to construct a one-parameter family of test functions. All of these difficulties of the two approaches, those of principle and

those less profound, often lead to great complications in finding the spectrum and frequently make it impossible to carry out any reasonable investigation of a solvable problem.

The present paper expounds a method which allows us to combine PT and the variation method in a single approach. This method is free of such essential difficulty as the necessity of knowing the entire spectrum of the unperturbed problem, and makes it possible to make estimates of the accuracy of variational calculations. The essence of the method lies in a "nonlinearization" procedure,<sup>5,6</sup> which consists in changing from the Schrödinger equation to a nonlinear equation and then developing a PT for the latter. Furthermore, the problem of constructing the PT is linear and turns out to be equivalent to the problem of electrostatics with a variable dielectric constant. This approach does not require knowing the entire spectrum of the unperturbed problem; it is enough to know the wave function of the unperturbed level for which one is seeking the correction. This leads to a most powerful flexibility, that of freedom in choosing the potential of the unperturbed problem, and consequently it becomes possible to construct a converging PT series. This is one of the main virtues of this method. It is worth emphasizing that for one-dimensional problems and some many-dimensional problems all of the corrections can be obtained in explicit form, in terms of quadratures. In cases where the solution cannot be written out explicitly, it can be obtained by numerical methods.

We give some attention to the history of the question,<sup>1</sup> since this approach is nonstandard and not well known. A pioneering paper by Zel'dovich<sup>7</sup> (see also Ref. 8, Secs. 4 and 5) gave the first statement of the assertion that the construction of a PT does not require knowing the entire spectrum, or else the Green's function, of the unperturbed problem, and that it suffices to know merely the wave function of the state for which corrections are sought. This paper was the first to write out explicitly formulas for the first correction to the wave function and the second correction to the energy and to show how to find subsequent corrections. The formulas derived did not contain sums over intermediate states, but were in the form of quadratures.

Analogous equations were given independently by Kirzhnits,<sup>9</sup> who by their use was able to find the correction to the Hartree-Fock approximation in calculations on two-electron atoms. One of the possible types of such PT's was constructed by Polikanov,<sup>10</sup> who used for this purpose a change from the Schrödinger equation to a Riccati equation. Another type of PT, closer to that considered in the present paper, was described in a paper by Pekar,<sup>11</sup> and then repeatedly rediscovered in other papers.<sup>13-16</sup> All of these papers<sup>7-16</sup> on this approach to PT showed its superiority to the standard method. For example, in a paper by Sakhnovskii<sup>12</sup> a problem on diffusion of electrons was solved by such a method. In the framework of this method Dolgov and Popov,<sup>13</sup> and also Hikami and Brézin,<sup>14</sup> carried out studies of the PT series in the coupling constant for the

anharmonic oscillator. Moreover, Dolgov and Popov<sup>13</sup> constructed a concrete example of a rapidly converging iteration scheme for dealing with the anharmonic oscillator. It can be shown<sup>5</sup> that this scheme reduces to the new PT. A detailed study of this approach was also contained in Refs. 15 and 16, and in Ref. 16 a general recipe was formulated for securing convergence of the PT series. As an example, rapidly converging PT series were constructed for the lowest states in potentials  $x^{2n}$ , which gave accuracies of the order of one percent by including only the first two orders. The problem of the Stark effect of the hydrogen atom in arbitrary fields was solved in the framework of this approach in a paper by Dolgov and the writer.<sup>17</sup>

A many-dimensional generalization of this approach was formulated in Ref. 5. The connection of PT with the variation principle was described in Ref. 6. It was shown that the results of variational calculations comprise the first two coefficients of the PT series, and therefore the calculation of the subsequent coefficients (if the PT series converges) makes it possible in principle to estimate the accuracy of the variational calculation. Moreover, it was found in this paper that the recipe for securing the convergence of the PT series formulated earlier<sup>5,16</sup> is nothing other than the usual requirements, on the basis of which one constructs the class of comparison functions used in variational calculations. In particular, it should be mentioned that the recipe proposed by Dolgov and Popov<sup>13</sup> is a special case of the general recipe; it is valid only for nonnegative potentials that increase to infinity.

The present paper is devoted to a detailed exposition of the method and its further development in the many-dimensional case. The main attention will be given to the treatment of the lowest state in various potentials. We shall try to demonstrate the superiority of our approach over others. A separate paper will be devoted to the study of excited states.

The organization of the paper is as follows. Section 2 explains the essentials of the method; the procedure of linearization is described, the PT is constructed for the ground and excited states, and the connection with the usual Rayleigh-Schrödinger PT is discussed. In Sec. 3 the connection of PT with the variation method is demonstrated and questions about the convergence of the PT series are discussed. A theorem on convergence is proved. The rest of the paper is devoted to a detailed examination of various special cases: one-dimensional problems are discussed in Sec. 4, and many-dimensional problems are studied in Sec. 5 with the example of the two-dimensional anharmonic oscillator. Conclusions and a discussion of the method are contained in Sec. 6.

## 2. DESCRIPTION OF THE METHOD

We proceed to describe the method. Its main point lies in a transformation procedure, which we shall call the *nonlinearization* procedure, applied to the Schrödinger equation, which is a homogeneous linear equation of the second order

$$\Delta\psi + (E - V)\psi = 0, \quad (1)$$

to give a nonlinear first-order equation with an explicitly known right-hand side, followed by the development of a PT applicable to this nonlinear equation. The transformation which realizes this procedure is of the form<sup>5,6</sup>

$$\mathbf{y} = -\nabla\psi/\psi = -\nabla \ln \psi, \quad (2)$$

where  $\Delta$  and  $\nabla$  are the usual  $k$ -dimensional Laplace operator and gradient.<sup>2)</sup> Using Eqs. (1) and (2), we get the following nonlinear equation for the vector field  $\mathbf{y}$ :

$$\operatorname{div} \mathbf{y} - \mathbf{y}^2 = E - V, \quad (3)$$

which is equivalent to the original Schrödinger equation provided that  $\mathbf{y}$  is a potential field, i.e., that

$$\mathbf{y} = \nabla\varphi \quad (4)$$

(with  $\varphi$  a scalar function), or, in other words, the skew derivative must be equal to zero,

$$\partial_i y_j - \partial_j y_i = 0. \quad (4')$$

Equation (3) with the condition (4) or (4') is the fundamental equation of our work, on which the method to be developed is based. In the one-dimensional case it is the well known Riccati equation. We shall discuss the question of boundary conditions for Eq. (3) later.

We shall now begin the construction of the PT, first making the following preliminary remark. It is obvious that the potential  $V$  in question can always be expressed as a sum  $V = V_0 + \lambda V_1$ , where  $\lambda$  is a formal parameter introduced for convenience, such that the equation

$$\Delta\psi_0 + (E_0 - V_0)\psi_0 = 0 \quad (5)$$

can be solved exactly. In other words, this can be stated thus: For any sufficiently smooth function  $\psi_0 \in L_2(\mathbb{R}^k)$  we can find a corresponding potential  $V_0$ , and then the potential  $V_1$  will be equal to the difference  $V - V_0$ . It should be noted that

$$\mathbf{y}_0 = -\nabla\psi_0/\psi_0. \quad (5')$$

After this remark we proceed to the construction of the PT for the ground state.

*The ground state.* It is well known that if the potential considered is sufficiently smooth the wave function of the ground state is nowhere equal to zero. This means that the vector function  $\mathbf{y}$  [see the definition (2)] has no pole singularities for real values<sup>3)</sup> of  $x$ . We now write the expansions of  $\mathbf{y}$  and  $E$  in Taylor series in the parameter  $\lambda$ :

$$\mathbf{y} = \mathbf{y}_0 + \lambda \mathbf{y}_1 + \lambda^2 \mathbf{y}_2 + \dots = \sum_n \lambda^n \mathbf{y}_n, \quad (6)$$

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots = \sum_n \lambda^n E_n, \quad (7)$$

where  $E_0$  and  $\mathbf{y}_0$  are given by Eqs. (5) and (5'), respectively. Substituting the expressions (6) and (7) in Eq. (3) and collecting the terms in  $\lambda^n$ , we get the following equation for  $E_n$  and  $\mathbf{y}_n$ :

$$\operatorname{div}(\psi_0^2 \mathbf{y}_n) = (E_n - Q_n)\psi_0^2. \quad (8)$$

This equation can also be written in a different form

$$\operatorname{div} \mathbf{y}_n - 2\mathbf{y}_0 \mathbf{y}_n = E_n - Q_n, \quad (8')$$

where the vector field  $\mathbf{y}_n$  must also satisfy the condition (4) or (4') for a vector with a potential. Here

$$Q_n = V_n, \quad Q_n = -\sum_{i=1}^{n-1} \mathbf{y}_i \mathbf{y}_{n-i}, \quad n > 1. \quad (9)$$

Equation (8), along with the condition (4) or (4') for the gradient character of the field  $\mathbf{y}_n$ , is the equation of ordinary  $k$ -dimensional electrostatics, in which  $\psi_0^2$  and  $\mathbf{y}_n$  play the respective roles of the dielectric constant and the field strength and  $(E_n - Q_n)\psi_0^2$  is the charge density.

Let us now go on to discuss the question of boundary conditions. Since we are confining ourselves to the consideration of a discrete spectrum only, it is entirely natural to require that the vector field  $\mathbf{y}$  not increase at large values of  $x$  more rapidly than a power of  $x$ . This requirement can be written in the form

$$|\mathbf{y}_n \psi_0^2| \rightarrow 0 \quad \text{as} \quad |x| \rightarrow \infty. \quad (10)$$

The condition (10) can be converted immediately into information about the corrections  $E_n$ . To do so we integrate Eq. (8) over all space and transform the integral on the left-hand side into a surface with the theorem of Gauss and Ostrogradskii.<sup>7</sup> Then, using the condition (10), we get<sup>5</sup>

$$E_n = \int Q_n \psi_0^2 d^k x / \int \psi_0^2 d^k x. \quad (11)$$

This expression gives the value of the  $n$ -th correction to the energy level of the ground state of the unperturbed problem. We note that the first correction  $E_1$  is identical with the standard correction of the Rayleigh-Schrödinger PT,<sup>1</sup> and the second correction  $E_2$  is always negative, as it must be.<sup>1</sup>

To calculate the various corrections  $E_n (n > 1)$  it is necessary to solve the electrostatic problem (8), which is equivalent to the solution of the general elliptic equation<sup>4)</sup>

$$\operatorname{div}(\psi_0^2 \nabla \varphi_n) = (E_n - Q_n)\psi_0^2 \quad (12)$$

with the boundary condition (10), where  $\mathbf{y}_n = \nabla \varphi_n$  and  $E_n$  is given by the expression (11). This problem is no longer an eigenvalue problem, since  $E_n$  and  $Q_n$  are taken as known from the previous iterations [cf. Eqs. (9), (11)]. For this reason Eq. (12) is much simpler from the point of view of numerical calculation than the original Schrödinger equation.<sup>1</sup>

Let us discuss the question of finding the corrections  $\mathbf{y}_n$  in more detail. In the general case the solution of the equation (8) with the supplementary condition (4) or (4') is of the following form:

$$\psi_0^2 \mathbf{y}_n = \int \mathbf{G}_k(x, x') (E_n - Q_n)\psi_0^2(x') d^k x', \quad (13)$$

where  $\mathbf{G}_k(x, x')$  is the Green's function of Eq. (8) with the supplementary condition (4) or (4'). In the general case, when  $\psi_0^2$  is an arbitrary function which decreases exponentially at infinity, the solution is not known and it is evidently impossible to construct it. However, in some special cases this can be done. First, in the case of spherically symmetric  $\psi_0^2$  and  $Q_n$  the Green's function is

$$G_k(x, x') = \frac{1}{\sigma_k} \frac{(x-x')}{|x-x'|^k}, \quad (14)$$

where  $\sigma_k = 2\pi^{k/2}/\Gamma(k/2)$  is the area of a unit sphere in  $k$  dimensions. In this case the solution (13) becomes

$$\psi_0^2 y_n = \frac{1}{\sigma_k} \int \frac{x-x'}{|x-x'|^k} (E_n - Q_n) \psi_0^2(x') d^k x'. \quad (15)$$

We note that the general solution of an arbitrary one-dimensional problem is also given by Eq. (15).

Second, when the dielectric constant is Gaussian<sup>5)</sup>

$$\psi_0^2 = a \exp\{-\alpha x^2\},$$

the general solution of Eq. (8) is given by the formula

$$y_n = \frac{1}{2\pi^{k/2}} \int d^k x' [E_n - Q_n(x')] \int_0^\infty \frac{dt}{t^k} (t+\alpha)^{(k-2)/2} \times \exp\{-(t^k x - (t+\alpha)^k x')^2\} \{t^k x - (t+\alpha)^k x'\}. \quad (16)$$

**Excited states.** We now proceed to the consideration of excited states. There are several reasons that a separate treatment of excited states is necessary. First, in the integrals (11) nonintegrable singularities appear, since the zeroes of the wave function are transformed into pole singularities of the vector function  $y$ , and the integrals (11) depend on the  $Q_n$ , which are quadratic forms in the  $y_i$ . In the one-dimensional case it has been shown in papers by Polikanov<sup>11</sup> that correct results can be obtained by shifting the path of integration into the complex plane. We propose a somewhat different recipe. Second, the question of excited states in the many-dimensional case has not been studied very much, and we shall point out some difficulties.

It is quite obvious that if we consider a sufficiently smooth potential, the wave function of any excited state is characterized by some set  $S$  on which it vanishes. It is entirely clear that such a wave function can be represented in the form

$$\psi(x) = f(x) \exp\{-L(x)\}, \quad (17)$$

where  $f(x)$  and  $L(x)$  have no singularities for finite  $x$ , and  $f(x)$  does not increase faster than a power of  $x$  as  $x \rightarrow \infty$ , while  $f(x) = 0$  and  $\nabla f(x) \neq 0$  for<sup>6)</sup>  $x \in S$ . We now introduce the following vector  $g$ , such that

$$y = -\nabla \psi / \psi = g - \nabla f / f, \quad (18)$$

where  $g = \nabla L$ .

Thus we have separated off explicitly the part of the vector field  $y$  that contains singularities. Substituting Eq. (18) in Eq. (3) and multiplying the resulting equation by  $f$ , we arrive at the following result:

$$f \nabla g - f g^2 - \Delta f + 2g \nabla f = (E - V)f. \quad (19)$$

Now set  $V = V_0 + \lambda V_1$  and let  $\psi_0$  be the solution of Eq. (5), where the set  $S_0$  on which  $S_0$  vanishes is given by the condition  $f_0(x) = 0$  [see Eq. (17)]. We now develop the perturbation theory in the parameter  $\lambda$ , expanding in series not only  $E$  and  $g$  [see Eqs. (6) and (7)] but also the function  $f$  which characterizes the set of zeroes<sup>7)</sup>

$$f = f_0 + \lambda f_1 + \lambda^2 f_2 + \dots = \sum \lambda^n f_n. \quad (20)$$

Collecting terms of order  $\lambda^n$  and then doing simple mathematical transformations, we get the equation

$$\operatorname{div}(\psi_0^2 \nabla(\varphi_n - f_n/f_0)) = (E_n - \bar{Q}_n) \psi_0^2, \quad \nabla \varphi_n = g_n, \quad (21)$$

$$\bar{Q}_n = -\sum_{i=1}^{n-1} g_i g_{n-i} - \frac{1}{f_0} \sum_{k=1}^{n-1} f_k \left( \sum_{i=0}^{n-k} g_i g_{n-k-i} - \nabla g_{n-k} + E_{n-k} \right) + \frac{2}{f_0} \sum_{i=1}^{n-1} g_i \nabla f_{n-i} + V_1 \frac{f_{n-1}}{f_0}, \quad n \geq 2, \quad (22)$$

$$\bar{Q}_1 = V_1.$$

The correction to the energy,  $E_n$ , takes the form, analogous to Eq. (11):

$$E_n = \int \bar{Q}_n \psi_0^2 d^k x / \int \psi_0^2 d^k x. \quad (23)$$

We note that just as in the case of the ground state the problem of finding the corrections reduces to the solution of an electrostatic problem. The role of electric field-strength vector is played here by the quantity

$$g_n - \nabla(f_n/f_0).$$

Let us now discuss the connection between this PT and the standard Rayleigh-Schrödinger theory. This is easily traced if we compare the expansion of the wave function in the usual approach

$$\psi = \psi_0 + \lambda \psi_1 + \lambda^2 \psi_2 + \dots = \sum_n \lambda^n \psi_n \quad (24)$$

with that described here<sup>8)</sup>

$$\psi = \exp\{-(L_0 + \lambda L_1 + \lambda^2 L_2 + \dots)\} = \prod_n \exp(-\lambda^n L_n(x)), \quad (25)$$

where  $\nabla L_n = y_n$ .

Let us now recall the expressions for  $\psi_n$  and  $E_n$  in the usual approach (see, for example, Ref. 1, Sec. 38) and compare it with the corresponding expressions in our present approach [for this we must expand the exponential function in Eq. (25) in series]. We then get two families of sum rules; for brevity we give one example of each:

$$\psi_1^{(n)} = \sum_m \frac{\langle m | V_1 | n \rangle}{E_0^{(n)} - E_0^{(m)}} \psi_0^{(m)} = -L_1 \psi_0^{(n)}, \quad (26)$$

$$E_2^{(n)} = \sum_m \frac{|\langle m | V_1 | n \rangle|^2}{E_0^{(n)} - E_0^{(m)}} = \int Q_2 \{\psi_0^{(n)}\}^2 d^k x / \int \{\psi_0^{(n)}\}^2 d^k x, \quad (27)$$

where the lower index is the number of the correction and the superscript is the number of the level. The fact that such sum rules appear has been noted in many papers.<sup>5,10,13,15,16</sup> In Refs. 5 and 15 they were constructed explicitly for the one-dimensional case, and in particular, in Ref. 15 a direct proof of Eq. (27) was carried out. In conclusion we point out that the study of these rules gives information about the spectrum of the unperturbed problem.

### 3. THE VARIATION PRINCIPLE AND PERTURBATION THEORY. CONDITIONS FOR CONVERGENCE OF THE METHOD

In the preceding section we have constructed a procedure for finding the eigenvalues of the Schrödinger operator without needing to know the entire spectrum of the unperturbed problem. Accordingly we have

available to us a great deal of freedom in the choice of the potential in the unperturbed problem. This allows us to choose almost arbitrarily the way we represent the given potential  $V$  in the form of a sum  $V_0 + V_1$ , and consequently offers a possibility for obtaining converging PT series. However, before discussing questions about the construction of converging PT series, we shall establish the connection between perturbation theory and the variation principle.

We begin the discussion with an obvious statement: Any sufficiently smooth function  $\psi_0 \in L_2(R^k)$  is an eigenfunction in a potential  $V_0$  given by

$$V_0 - E_0 = \Delta \psi_0 / \psi_0, \quad (28)$$

where  $E_0$  is the energy of the state. We now suppose that we wish to find the position of some level in a potential  $V$  by means of the Rayleigh-Ritz variation principle and have constructed for this purpose a class of normalized comparison functions  $\psi_0$ . By means of Eq. (26) we can see what the potentials  $V_0$  are to which the comparison functions  $\psi_0$  correspond.

And now let us look at the variational calculation from the point of view of PT:

$$E_{\text{var}} = \min \int \psi_0 H \psi_0 = \min \left\{ E_0 + \int \psi_0 (V - V_0) \psi_0 d^k x \right\} = \min (E_0 + E_1); \quad (29)$$

where

$$H(H_0) = p^2 + V(V_0), \quad H_0 \psi_0 = E_0 \psi_0, \quad E_1 = \int \psi_0 (V - V_0) \psi_0 d^k x$$

$E_1$  is the first correction to the energy level when the perturbation potential  $V_1$  is equal to  $V - V_0$ . Thus we have found that the variational calculations give the first two terms of the PT series [cf. Eq. (7)], in which the perturbation potential is equal to the deviation of the original potential from that which corresponds to the function  $\psi_0$  [see Eq. (28)]. Calculating the next terms in the PT series (7), i.e.,  $E_2, E_3, \dots$ , we get a way to estimate the accuracy of the variational calculations. Besides this, by comparing the potentials  $V$  and  $V_0$  we can see how reasonably the class of comparison functions has been constructed. What we have in mind here will be explained presently.

We now go on to discuss the question of when the procedure we have described will be convergent, i.e., when the series (6) and (7) will converge. Before doing so we shall explain why PT series usually diverge.<sup>9)</sup> As an example we consider the anharmonic oscillator  $V = x^2 + \lambda x^4$  ( $V_0 = x^2, V_1 = x^4$ ). When  $\lambda > 0$  there are an infinite number of bound states in the potential, but for  $\lambda < 0$  (by no matter how little) a tunnelling effect appears; that is, the energy  $E(\lambda)$  of the level is no longer real, and acquires an imaginary part. This means that for  $\lambda = 0$  the function  $E(\lambda)$  has a singularity, and since the PT series is an expansion  $E(\lambda) = \sum a_k \lambda^k$  near this singularity it has zero radius of convergence, i.e., it diverges. A rigorous treatment of this phenomenon in the case of the anharmonic oscillator was first carried out by Vainshtein,<sup>19</sup> who showed that a cut begins at the point  $\lambda = 0$ , and calculated the discontinuity across this cut for  $\lambda \rightarrow -0$ .

It follows from all of this that the PT series becomes

divergent when the perturbation potential is more singular than the unperturbed potential. In this case there is a radical restructuring of the spectrum as the perturbation parameter is varied. The level can become quasi-stationary, as in the example just now discussed; it can pass into a continuous spectrum. Therefore the general recipe for choosing a zeroth approximation to obtain a convergent PT series runs as follows.<sup>5,16</sup>

*Recipe.* We shall construct the zeroth-order wave function in such a way that the corresponding potential  $V_0$  [see Eq. (27)] will reproduce as much as possible of the characteristic features as the potential  $V$  to be studied. In particular, it is especially important that it should reproduce all of the singularities of the original potential and also its asymptotic behavior.<sup>10)</sup>

In the language of wave functions this means that  $\psi_0$  must include as many as possible of the properties of the true wave function: Its behavior at infinity, at zero, near singularities of the potential, information about its zeroes, and so on. It is easy to see that this recipe is practically identical with the procedure used in constructing the class of comparison functions in the Rayleigh-Ritz variational method.

We now return to the discussion of the question of convergence and prove the following theorem about convergence.<sup>11)</sup>

*Theorem.* If the first correction  $y_1$  is a bounded vector function, i.e., if 1)  $|y_1| \leq a_1$ , and also

$$2) |\psi_0^{-2}| \int |G_\lambda(x, x') \psi_0^2 d^k x'| \leq A,$$

with 3)  $a_1 A < 1/8$ , then the series (6) and (7) converge.

*Proof.* The proof will consist of the construction of a majorizing sequence. To begin with, let us verify that the corrections  $y_n$  are also bounded vector functions. Using the method of induction and the conditions 1) and 2), we see at once that

$$|y_n| \leq 2A \sum_{i=1}^{n-1} a_i a_{n-i} = a_n, \quad n \geq 2, \quad (30)$$

together with

$$|E_n| \leq \sum_{i=1}^{n-1} a_i a_{n-i}. \quad (31)$$

To find the region of convergence of the series (6) and (7), we use the following approach<sup>12)</sup>: We calculate the value of the sum

$$S = \sum_{i=1}^{\infty} a_i. \quad (32)$$

By means of Eq. (30) it is easy to show that

$$2AS^2 + a_1 = S. \quad (33)$$

The solution of Eq. (33) that we need is

$$S = [1 - (1 - 8Aa_1)^{1/2}] / 4A. \quad (34)$$

Accordingly, we have succeeded in constructing a majorizing series for  $y_n$  and  $E_n$  that converges for

$$8Aa_1 \leq 1, \quad (35)$$

and the theorem is proved. It is completely clear that this theorem is rather weak and can be considerably

strengthened. It seems almost obvious that the validity of the conditions 1) and 2) is sufficient for the convergence of the series (6) and (7). It may be mentioned that a similar theorem can be proved also for the general case of excited states.

#### 4. THE ONE-DIMENSIONAL CASE

We now proceed to the consideration of one-dimensional problems (and those reducible to one-dimensional cases). As examples we shall find the ground states in the potentials  $V(x) = x^{2n}$ ,  $n = 2, 3, 4$  (A), and  $V(x) = m^2 x^2 + gx^4$  (B).

In the one-dimensional case the equation (3) reduces to the well known Riccati equation, and the condition (4) or (4') is satisfied identically. It is easy to show that the solution of Eq. (8) is given by Eq. (15), which can be reduced to the form<sup>7-9,11,13,15,16</sup> (cf. Ref. 10)

$$y_n(x) = \psi_0^{-2}(x) \int_{-\infty}^x (E_n - Q_n) \psi_0^2(x') dx', \quad (36)$$

where  $Q_n$  is given by Eq. (9). The corrections  $E_n$  to the energy are given as before by Eq. (11).

In the case of excited states the solution of Eq. (21) can be converted to the following form

$$g_n(x) = \psi_0^{-2}(x) \int_{-\infty}^x (E_n - \tilde{Q}_n) \psi_0^2(x') dx' + \left( \frac{f_n}{f_0} \right)', \quad (37)$$

while the deformation  $f_n$  of the set of the zeroes is given by

$$f_n(x_i^0) = \int_{-\infty}^{x_i^0} (E_n - \tilde{Q}_n) \psi_0^2 dx' / f_0'(x_i^0) \exp[2L_0(x_i^0)]; \quad x_i^0 \in S_0, \quad i=1, 2, \dots, l, \quad (38)$$

where  $l$  is the number of the level considered. Accordingly, the problem reduces to the determination of the coefficients of a polynomial  $P_n^l(x)$  of degree  $l$ , which is given at the points<sup>13</sup>  $x_i^0 [P_n^l(x_i^0) = f_n(x_i^0)]$ .

We note that  $g_n(x)$  has no singularities on the real axis. We emphasize that when the first excited level is considered, Eqs. (36)–(38) are actually identical with those given in Ref. 15. When a many-dimensional spherically symmetric problem is to be solved, Eqs. (36)–(38) are modified in an obvious way. In the case of the ground state they are given in a number of papers.<sup>7-9,13,14</sup>

Let us now consider the examples A and B. One of the simplest ground-state wave functions satisfying the requirements of Sec. 3 is

$$\psi_0^{(0)} = \exp \left\{ -\frac{ax^2}{2} - \frac{g^h}{n+1} |x|^{n+1} \right\}. \quad (39)$$

This comparison function is the wave function of the ground state in the potential

$$V_0^{(0)}(x) = -[g^h n |x|^{n-1} - 2ag^h |x|^{n+1}] + a^2 x^2 + gx^{2n}, \quad E_0^{(0)} = a. \quad (40)$$

Here  $a$  is a parameter; superscripts give the number of the level, subscripts, the number of the approximation.

*A. The potential  $V(x) = x^{2n}$ .* In Eqs. (39) and (40) we set the parameter  $g$  equal to 1 and emphasize the im-

TABLE I. Ground-state energies in various potentials.

Approximation		$V(x) = x^4$		$V(x) = x^6$		$V(x) = x^8$	
0	$E_0 = a$ $\begin{cases} a=1 \\ a_{\min} \end{cases}$	1	0.47	1	0.85	1	1.14
1	$\begin{cases} E_1 \\ E_0 + E_1 \end{cases}$	0.13359	0.598448	0.158409	0.302627	0.234760	0.089720
2	$\begin{cases} -E_2 \\ E_0 + E_1 + E_2 \end{cases}$	1.13359	1.068448	1.158409	1.152627	1.234760	1.229720
3	$\begin{cases} -E_3 \\ E_0 + E_1 + E_2 + E_3 \\ E^* \\ \text{exact} \end{cases}$	0.04841	0.007720	0.010936	0.007319	0.009164	0.003632
		1.08518	1.060728	1.147473	1.145308	1.225596	1.226088
		0.01542	0.000304	0.002033	0.000406	0.000226	0.000223
		1.06976	1.060424	1.145440	1.144902	1.225822	1.225865
			1.060362		1.14480246		1.22582010

\* $E_{\text{exact}}$  was obtained by M. S. Marinov and V. E. Shestopal by numerical integration of the Schrödinger equations.

portant fact that the potential (40) with  $g=1$  reproduces the behavior of the given potential at infinity. The perturbation potential is

$$V_1^{(0)}(x) = [n|x|^{n-1} - 2a|x|^{n+1}] - a^2 x^2. \quad (41)$$

Now, substituting Eqs. (39) and (41) in Eqs. (11) and (36), we calculate the corrections  $y_n$  and  $E_n$ . Table I shows the values of  $E_n$  calculated in this way for the case  $a=1$  and  $n=2, 3, 4$  (see Refs. 5 and 16). We see that the convergence of the method is rather good, especially for the potentials  $x^6$  and  $x^8$ , and use of the corrections to and including the third order gives accuracies better than or of the order of 1 percent as compared with the exact values.

And now we carry out the minimization of the expression  $E_0 + E_2$  (see Sec. 3) with respect to the parameter 3. The result is the variational value of the ground-state energy with the comparison function (39). After calculating  $E_2$  we find that we have succeeded in getting the energies correct to four places to the right of the decimal point.

*B. The anharmonic oscillator  $V(x) = m^2 x^2 + gx^4$ .* The problem of the anharmonic oscillator (AO) is one of the oldest problems in quantum mechanics; it has been studied by many authors even in recent times (see, for example, Refs. 2, 5, 6, 13, 14, 19–25). The most complete and detailed study of the one-dimensional AO has been made by Bender and Wu.<sup>20</sup> One of the reasons for the increased present interest in this problem is that the AO is a one-dimensional field theory<sup>20</sup> which contains many problems essential for relativistic many-dimensional field-theoretic models. Therefore it is interesting to study these problems with this simple model as an example. The AO also has important applications in various branches of physics, in atomic, molecular, and solid-state physics.

In a number of papers<sup>19-22</sup> quasiclassical methods have been used to study in detail the structure of the PT series in terms of the coupling constant  $g$  for various types of AO, and also the analytic structure of the ground-state energy as a function of the coupling constant  $g$ . Besides this, in Ref. 20 computed values of the coefficients of 75 terms of the PT series, in powers of  $g$ , were found. It was shown in Refs. 13, 14, and 23 that the change from the Schrödinger equation to the Riccati equation simplifies the calculation of these coefficients and the study of the structure of the PT series. In particular, in Ref. 13 a convergent

TABLE II. Ground-state energies of the anharmonic oscillator.

$g'$	$a_{min}$	$E_1'$	$-\Delta E_2'$	$E_2'$	$E_{exact}'$
0.1	0.77	0.561738	0.002569	0.559169	0.559146
0.2	0.77	0.605769	0.003334	0.602435	0.602405
0.3	0.77	0.641838	0.003852	0.637986	0.637992
0.4	0.78	0.672984	0.004233	0.668751	0.668773
0.5	0.79	0.700687	0.004550	0.696137	0.696176
0.6	0.81	0.725803	0.004793	0.721010	0.721039
0.7	0.82	0.748892	0.005035	0.743857	0.743904
0.8	0.83	0.770336	0.005252	0.765084	0.765144
0.9	0.84	0.790411	0.005452	0.784959	0.785032
1	0.86	0.809320	0.005607	0.803713	0.803771
10	1.41	1.51622	0.001150	1.50472	1.50497
50	2.27	2.51864	0.01939	2.49925	2.49971
100	2.82	3.51516	0.02438	3.13078	3.13138
500	4.76	5.36040	0.04154	5.31886	5.31989
1000	5.98	6.74521	0.05230	6.69291	6.69422

\* $E_{exact}'$  taken from Ref. 2. Standardization of  $E$  and  $g$  as in Ref. 2. ( $E' = E/2$ ,  $g' = g/2$ ).

iteration procedure was proposed which, as can be proved,<sup>5</sup> is a special case of the approach developed in the latter paper, when the unperturbed potential is taken in the form  $V_0 = V - \frac{1}{2} V' V^{-1/2}$ , so that the perturbing potential is  $V_1 = \frac{1}{2} V' V^{-1/2}$ . Other kinds of converging PT series have been proposed in Refs. 5 and 24. We shall discuss the AO in the framework of the formalism developed above (cf. Ref. 5).

As our zeroth-order comparison function we take the function (39) with  $n=2$  (cf. Ref. 5), as in the case of example A. Then the perturbation potential is

$$V_1^{(0)}(x) = m^2 x^2 + 2[g^{1/2}|x| - ag^{1/2}|x|^3] - a^2 x^2. \quad (42)$$

We now develop the PT series, substituting (39) and (42) in Eqs. (36) and (11). We then get

$$E = E_0 + E_1 + \dots = a + \int_0^\infty [(m^2 - a^2)x^2 + 2g^{1/2}x(1 - ax^2)] \exp\left[-ax^2 - \frac{2g^{1/2}}{3}x^3\right] dx \times \left\{ \int_0^\infty \exp\left[-ax^2 - \frac{2g^{1/2}}{3}x^3\right] dx \right\}^{-1} + \dots \quad (43)$$

It is easy to see that Eq. (43) contains a cut in the  $g$  plane that goes from 0 to  $-\infty$ , and that for  $g \rightarrow 0$  the discontinuity across this cut is exponentially small, but is not the same as the semiclassical value.<sup>19-22</sup>

This situation is evidently typical of this approach and is not a disadvantage. One possible explanation of this phenomenon has been given by Dolgov and Popov.<sup>13</sup> If we now carry out a minimization with respect to the parameter  $a$ , calculate  $E_2$ , and compare with the results from numerical integration of the Schrödinger equation, it is found that our method gives such good accuracy that even with a very simple comparison function like (39) one can get several decimal places correct, both for large and for small values of the coupling constant  $g$  (see Table II and cf. Ref. 5). With this we conclude our discussion of one-dimensional problems.

## 5. SOME WORDS ABOUT THE MANY-DIMENSIONAL CASE

In this section we shall briefly discuss many-dimensional problems. It was shown in Sec. 3 that the realization of PT in the many-dimensional case is equivalent to the solution of an electrostatic problem with a variable dielectric constant. At present the

analytic solution of the problem is known for the case of a Gaussian dielectric constant, and in all other cases one must resort to numerical solution of the equations. However, in cases where it is possible to approximate a given potential with a spherically symmetric function in such a way that the deviations from sphericity are small, we may hope that the use of the Green's function (14) is justified and that the errors are small. We shall show how to construct the PT for a two-dimensional anharmonic oscillator in the case when the zeroth approximation is the harmonic oscillator.

Let us consider the ground state of a two-dimensional nonsymmetrical oscillator

$$V(x, y) = m^2(x^2 + y^2) + g(x^4 + y^4 + 2cx^2y^2), \quad (44)$$

where  $m$ ,  $g$ , and  $c$  are parameters. This is a complicated problem, which was first studied only recently.<sup>2,25</sup> It is quite obvious that finding the coefficients of the Rayleigh-Schrödinger PT series

$$E = \sum_k E_k g^k \quad (45)$$

is a rather complicated problem. In the framework of our approach this is done rather simply and reduces either to an algebraic problem or to the calculation of integrals of Gaussian type. We shall show how this can be done.

The zeroth approximation  $V_0 = m^2(x^2 + y^2)$  is given by

$$y_0 = mx, \quad E_0 = 2m \quad (\psi_0 = \exp(-1/2m(x^2 + y^2))), \quad (46)$$

where  $\psi_0$  is the zeroth-order wave function. To develop the PT we use Eq. (8'), not forgetting the gradient condition (4'), i.e., that  $y_n = \nabla\varphi_n$ . It is easily shown that the functions  $\varphi_n(x, y)$  that are solutions of Eq. (8') depend only on  $x^2$  and  $y^2$  and are invariant under the exchange  $x \leftrightarrow y$ . Their general form is

$$\varphi_n(x, y) = \sum_{k,l=0}^{n+1} a_{n,k,l} (x^2)^k (y^2)^l, \quad (47)$$

with

$$a_{n,k,l} = a_{n,l,k}, \\ a_{n,k,l} = 0 \quad \text{for } k+l > n+1.$$

Substituting (47) in Eq. (8'), we get a sequence of recurrence relations for the  $a_{n,k,l}$  (see Ref. 25), from which there follows the important relation

$$E_n = 2a_{n,1,0} + 2a_{n,0,1}. \quad (48)$$

This equation enables us to find the energy corrections in terms of the coefficients in the representation (47).

We write out the first few corrections explicitly:

$$\varphi_1 = 1/8(x^4 + y^4) + (3/8 + 1/8c)(x^2 + y^2) + 1/8cx^2y^2, \\ \varphi_2 = -1/16(x^6 + y^6) - 1/16((1/4 + 3/8c + 1/12c^2)(x^4 + y^4) - 1/4((1/8 + 3/8c + 3/8c^2)(x^2 + y^2) - 1/24c(1 + 1/2c)x^2y^2(x^2 + y^2) - 1/8c(3/2 + c)x^2y^2), \quad (49)$$

$$E_1 = 3/2 + 1/2c, \quad E_2 = -(2/8 + 3/2c + 3/8c^2). \quad (50)$$

Equations (49) and (50) can be obtained in a different way, by means of Eqs. (11)-(13) and the use of the Green's function (16). We note that in particular cases when the variables can be separated, Eq. (50) agrees

with earlier results: For  $c=0$  with those of Bender and Wu,<sup>20</sup> and for  $c=1$  with those of Refs. 13 and 14, when the notations are matched. It is also worth pointing out that for some coefficients in the expansion (47) one can write closed expressions by using formulas derived in Ref. 13 for the one-dimensional case; in particular

$$a_{n,n+1,0} = a_{n,0,n+1} = \frac{(-1)^{n+1}}{2^{2n}} \frac{(2n-2)!}{(n+1)!(n-1)!}. \quad (51)$$

In conclusion we emphasize that many-dimensional PT can be obtained in a similar way in the case when the perturbation is in the form of a polynomial. Convergent PT for these cases, in particular for the potential (44), will be discussed soon in another paper.

## 6. CONCLUSION

In this paper we have expounded a point of view based on a nonstandard approach to perturbation theory. Its unusual features are as follows:

1. The construction of this PT does not require knowledge of the entire spectrum of the unperturbed problem; it is sufficient to know the characteristics of only the level for which corrections are sought. Thus it is possible to investigate one given level, without being concerned about what happens to the whole spectrum. This saves us from the problems associated with the degeneracy of levels.

2. The discovery of a connection with the variation principle makes it possible to estimate the accuracy of variational calculations and use an iteration method to improve the variational results. Furthermore, owing to the possibility of selecting the unperturbed problem, the PT can be made convergent.

3. This approach does not depend critically on the dimensionality of the space in which we are to deal with the Schrödinger equation. The problem of constructing the PT is equivalent to the solution of a problem in electrostatics with variable dielectric constant.

On the basis of all of these properties it can be asserted that there is a real possibility of investigating the strong-coupling region in quantum mechanics. This has been demonstrated with one-dimensional examples. In this paper we have dealt only briefly with many-dimensional problems, since the main purpose here was only to show how the method is constructed for the many-dimensional Schrödinger equation.

In conclusion we shall try to answer the question: Why is knowledge of the whole spectrum not required for the construction of PT? In the one-dimensional case the answer to this question is actually contained in the first papers on this subject,<sup>7-10</sup> and is as follows. If one solution of an ordinary second-order equation is known, a second linearly independent solution can be constructed by quadratures. Then, knowing two linearly independent solutions, one can construct the Green's function of the equation. When the Green's function is known, perturbation theory can be developed and all of the corrections can be expressed in quadratures, as shown in a number of papers.<sup>7-11,13,15,16</sup>

Unfortunately, with this method we can find the Green's function for only one fixed value of the energy of the unperturbed problem; otherwise, we would know the entire spectrum of the unperturbed problem, which is usually not the case (in the method we have developed, of course). In the many-dimensional case I do not know the answer to our question, but it seems that there must exist a procedure for obtaining the Green's function for a given energy in the many-dimensional case, analogous to the one just described for the one-dimensional case.

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<sup>1)</sup> It must be particularly emphasized that all such papers now known to me are devoted to the examination of one-dimensional problems or problems which can be reduced to the one-dimensional case.

<sup>2)</sup> As applied to the ground state this sort of transformation was proposed independently in a paper which appeared recently.<sup>26</sup>

<sup>3)</sup> From now on we write  $k$  for brevity, meaning a point in the space  $R_x$  with coordinates  $(x_1, x_2, \dots, x_k)$ .

<sup>4)</sup> We note that the operator on the left side of Eq. (12) is the Laplace operator in a curved space with a conformally flat metric, with  $\Psi_0^2$  playing the role of the determinant of the metric tensor. Accordingly, the problem reduces to finding the Green's function of the Laplace operator in a curved space. I am grateful to Ya. A. Smorodinskii for calling my attention to this fact.

<sup>5)</sup> This means that the zeroth-approximation potential is quadratic, i.e., the unperturbed problem is a harmonic oscillator.

<sup>6)</sup> At points of self-intersection, where branching occurs,  $\nabla^2 = 0$ .

<sup>7)</sup> In the one-dimensional case, as a consequence of the oscillation theorem, the set  $S$  is a finite point set, and  $f$  is a polynomial:

$$f(x) = \prod_{i=1}^m (x - \alpha_i),$$

where  $m$  is the number of zeroes. Therefore we can expand the positions  $\alpha_i$  of the zeroes directly in series in  $\lambda$ , i.e., write  $\alpha_i = \sum \alpha_{ik} \lambda^k$ , as was proposed in Refs. 10 and 15. However, this method cannot be extended to the many-dimensional case (see the further discussion), and therefore we proceed somewhat differently, as suggested in Ref. 6.

<sup>8)</sup> For simplicity we shall not give attention to the modifications that appear when we are to deal with excited states.

<sup>9)</sup> The ensuing discussion is usually called the "Dyson instability argument."<sup>18</sup>

<sup>10)</sup> We note that in a paper by Dolgov and Popov,<sup>13</sup> devoted to the study of the one-dimensional harmonic oscillator, a convergent PT was constructed in which the zeroth-approximation wave function chosen was one having the correct behavior at infinity and at zero (see the further discussion).

<sup>11)</sup> We confine ourselves to the case of the ground state and of excited states subject to the condition that  $f_n = 0$ .

<sup>12)</sup> I am grateful to A. D. Dolgov, who suggested this device.

<sup>13)</sup> I.e., the problem reduces to the solution of  $l$  linear equations with  $l$  unknowns.



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