The eigenvalue spectrum in quantum mechanics and the nonlinearization procedure

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A new approach to the eigenvalue problem in quantum mechanics is proposed. This approach is based on three propositions: 1) a perturbation theory which does not require knowledge of the entire eigenvalue spectrum of the unperturbed problem and which uses a "nonlinearization" procedure (leaving some latitude in the choice of a zeroth order approximation); 2) a relationship between the perturbation theory and a variational principle, namely that any variational calculation is none other than the first two terms of some nontrivial perturbation theory which, when developed further, can reveal the accuracy of the variational calculations and can refine them by an iterative procedure; 3) "Dyson's argument," which serves as a criterion for the "reasonableness" of the choice of a zeroth order approximation (the unperturbed problem). The realization of this perturbation theory in a k-dimensional space is equivalent to the solution of a k-dimensional electrostatic problem with a variable dielectric permittivity. In the one-dimensional case and in cases which reduce to the one-dimensional case, all the corrections are written in quadratures. It is shown that the construction of an ordinary perturbation theory (in which the zeroth order approximation is an exactly solvable problem) within the framework of this perturbation theory is a purely algebraic procedure, which reduces to the solution of some simple recurrence relations. An approximation analogous to the leading logarithmic approximation of quantum field theory is constructed. Some standard problems of quantum mechanics—the anharmonic oscillator, the Zeeman effect, and the Stark effect—are treated as examples. It is shown that this new approach makes it possible to develop systematically a theory for strong coupling and large perturbations.

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1. INTRODUCTION

Since Schrödinger wrote his celebrated equation back in 1926, many different methods have been developed to solve it, in particular to find the eigenstates of various quantum mechanical systems. This effort continues today. The existence of a few exactly solvable problems stimulated the development of various perturbation-theory approaches. This work led in turn to the problem of large perturbations, or, in other terms, the problem of strong coupling, since real physics usually involves the region of large perturbations. One of the most important and most common manifestations of the difficulties which arise is the zero convergence radius of the perturbation theory series.

The strong coupling problem is a central problem in many of the physical sciences. Essentially wherever it has been found possible to go into the region of strong coupling, some nontrivial phenomena have been discovered. It is thus an important and timely problem to develop regular methods for studying the large-perturbation region. From this standpoint we will attempt to evaluate the present state of affairs in quantum mechanics and quantum field theory. For

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the discussion below it is more natural to begin with quantum field theory.

One of the methods which has been worked out in most detail for studying field theory problems which are not exactly solvable is a standard technique based on the use of Feynman diagrams. This approach uses the theory of the free field as a zeroth order approximation and usually makes it possible to study the region of weak coupling and small interaction constants. This approach is not effective in the region of large perturbations, since in addition to the purely technical difficulties which arise in attempts to evaluate multiloop diagrams there is trouble of a fundamental nature: a zero convergence radius for the resulting perturbation theory series in the coupling constant for quantities of physical importance. The qualitative explanation of this phenomenon is quite simple and is based on "Dyson's argument"[1]: In strong fields the Lagrangian of the interaction becomes "greater" than that of a free field, regardless of the particular dependence on the interaction constant. To get to the heart of this difficulty, we pose a question which is by no means of purely academic interest: Has the problem been solved if we know an arbitrary n-term of the perturbation theory series? As surprising and slightly paradoxical as it may sound, the answer is no, the problem has not been solved! Even if we know an arbitrary term of the series in the coupling constant, we still have to deal with the problem of how to sum this series. Since its coefficients increase factorially with the index, and the sum has a zero convergence radius, the problem of carrying out this summation is extremely ambiguous. Roughly speaking, any answer can be generated for a given coupling constant. In order to decide which method to use to sum the resulting series, we must study the structure of the singularities of the function of interest near the zero of the interaction constant. One possible way to solve this problem is to study the analytic structure of such a nontrivial construction as a functional integral. Just how complicated this structure can be has been demonstrated by Bender and Wu[2,3] and Simon[4] in an example from a one-dimensional field theory: the anharmonic oscillator $V(x) = m^2x^2 + gx^4$. The correct summation method in this example turns out to be Borel's method.[5] The terms presenting the greatest danger in the summation are those which may be nonanalytic in the perturbation parameter and which make vanishing contributions to the coefficients of the perturbation theory series. At the moment there are rather few problems for which the correct summation method is known.

In practice we usually know only a finite number of terms of the perturbation theory series, although in some cases this number may be quite large. To go beyond the range of applicability of perturbation theory use is made of one of various approximation methods: Pade approximants, a refined perturbation theory, the Pade-Borel method, conformal transformations, etc. [See Refs. 6 and 7, for example. These methods have recently been refined substantially following the studies by Lipatov (Ref. 8; see also the review by Bogomolny *et al.*[9]), who proposed a method for finding the asymptotic behavior of the coefficients of the perturbation theory series.] When such methods are used, however, it is almost never clear at the outset whether they will converge to the correct results.[1)]

In nonrelativistic quantum mechanics the situation is slightly better, if still far from satisfactory. Below we will discuss the situation in the case of bound states, so we will briefly review the methods which are ordinarily used in solving problems of this type, focusing on their shortcomings under the assumption that their merits are well known.

1) The Rayleigh-Schrödinger perturbation theory.[2)] This approach is one of the best known and the most widely used. In order to take this approach one needs to know the entire eigenvalue spectrum of the unperturbed problem and all the matrix elements. The zeroth order approximation is thus an exactly solvable problem. One usually has to deal with divergent perturbation theory series and all the problems discussed above.

2) The variational principle and its various modifications (the Hartree method, the Hartree–Fock method, etc.). The variational approach is the only tool we have for solving multidimensional problems of any degree of complexity at all, in particular, problems of atomic physics. The basic shortcoming of this approach is that we have no way of estimating the accuracy of the results. All possible lower bound estimates on the accuracy of variational calculations, such as Temple's estimate (see Ref. 12, for example), are usually very crude. To refine them is a complicated problem. Furthermore, we have no really rigorous criteria for choosing trial wave functions which would lead to the necessary accuracy in the shortest possible time. Yet another difficulty is that, since the energy of a state is a rather crude characteristic of a system, a high accuracy in terms of the energy does not guarantee accuracy in terms of other, more subtle characteristics. Serious difficulties can arise in the construction of trial wave functions for excited states (the orthogonality problem).

3) The semiclassical approximation (the WKB method). This approach has a rather restricted range of applicability (usually, highly excited states), although this range has been expanded significantly by, for example, the modification of this method proposed by Marinov and Popov.[13] In order to study low-lying states it is necessary to appeal to higher orders of the semiclassical approximation, which can be found only with serious difficulty (see Ref. 14, for example). We might add that the semiclassical approximation has been worked out in detail only for one-dimensional and spherically symmetric cases.

4) Numerical methods. Although many people have the impression that any problem can be solved on a decent computer, this is far from being the case. In the realm of eigenvalue problems, numerical calculations have so far provided reliable results only in the one-dimensional case. Even the two-dimensional problem is very complicated for numerical calculations, and as a result contradictory results have been found (more on this below).

This ends our brief review of the standard and familiar approaches to the solution of the steady-state Schrödinger

[1)] See Refs. 10 for an example in which the Pade approximants converge to an incorrect limit.
[2)] See, for example, Ch. 6 in Ref. 11.

equation. The mathematical side of the matter and some other subtleties are described in the monographs by Morse and Feshbach[15] and Courant and Hilbert,[16] among other places. Many modifications of these approaches have of course been developed although we have not mentioned them here; some of these modifications are quite general, while others are suitable for the solution of a specific problem.

Before we take up the approach which is the subject of this review, we will take a brief look at the present state of affairs in several standard quantum-mechanical problems—problems which are mentioned in essentially any text on quantum mechanics and which we will be discussing below as examples of the application of the approach described here.

a) The hydrogen atom in a static electric field (the Stark effect). In this problem the region of strong coupling begins at fields $\mathscr{F} \sim 0.1$ a.u. in the case of the ground state. Several calculations of the energy and width of the ground state in the region of strong fields have been reported: both numerical calculations and calculations by the approach described in this review. Essentially none of the numerical calculations for $\mathscr{F} \gtrsim 0.15$ a.u. have yielded the same results (see Ref. 17 and the bibliography there), and in some cases the results differ in order of magnitude.

b) The hydrogen atom in a static magnetic field (the Zeeman effect). The problem of classifying the states has not been resolved for this problem.[3)] In principle, the problem is simpler than that of the Stark effect, since there is no tunneling. A rather large number of calculations have been reported (see Ref. 18 and the bibliography there), restricted to the few lowest-lying states. The energies calculated for the fields of 10^{11}–10^{12} G which are encountered in astrophysics and semiconductor physics differ by several orders of magnitude.

c) The hydrogen atom in crossed fields. Again in this case, the states have not been classified. Actually, we have only a qualitative theory.[19,20] In the strong coupling region we do not even know the first cross term of the perturbation theory, of the order of $\mathscr{F}^2\mathscr{H}^2$, for the ground state.

The approach which is the subject of this review is a combination of perturbation theory and a variational method. It may be classified as a variational-iterative method. From the perturbation theory standpoint it is an attempt to develop a regular method for studying the strong coupling region and large perturbations, and formally it contains no small parameter. The approach actually consists of three parts:

1) A perturbation theory which does not require knowledge of the complete spectrum of the unperturbed problem.

2) A representation of the variational calculations as the first two terms of some perturbation theory.

3) A comparison of the potentials of the original and unperturbed problems in the light of Dyson's argument.

An important technical point is that we speak in terms of potentials instead of wave functions on the basis of the trivial assertion that *any normalizable function is an eigenfunction of some state in some potential.* It thus becomes possible to assess the "quality" of the variational calculation (or, equivalently, of the unpertubed problem, in terms of a perturbation theory) by comparing the potential corresponding to the variational trial function with the potential of the original problem, in contrast with a comparison of a trial function with an implicit actual wave function. Here we have the physically meaningful criterion of reasonableness based on Dyson's argument.

A perturbation theory which does not require knowledge of the spectrum of the unperturbed problem was proposed a rather long time ago. It was apparently first worked out in 1954 by Price[22] and slightly later by Zel'dovich[23] (see also Ref. 24) for the ground state in the one-dimensional case. Price used a transformation from the Schrödinger equation to a Ricci equation, while Zel'dovich found the Green's function of the Schrödinger equation explicitly. All the corrections were expressed in the form of explicit quadratures. This perturbation theory was later rediscovered by Kirzhnits,[25,26] who used it to calculate the correction to the Hartree-Fock approximation in a calculation for two-electron atoms. Dalgarno, Lewis, and Steinhammer developed a slightly different approach to perturbation theory, which also yielded quadrature expressions.[27] These approaches and closed expressions for the perturbation theory corrections have subsequently been rederived repeatedly by various investigators,[28–32] who have demonstrated the advantages of these expressions over the standard expressions.[4)] In particular, Dolgov and Popov[30] constructed an example of a rapidly converging iterative scheme for solving the anharmonic-oscillator problem. As was shown later, this scheme also reduces to the perturbation theory which we are discussing here. A recipe for constructing converging perturbation theory series was first formulated in Ref. 32. As an example, a perturbation theory was constructed for the low-lying states in the potential $V(x) = x^{2n}$ This method was studied in detail in Ref. 33.

A generalization of the approach to the case of excited states in one dimension was proposed by Polikanov[34] and later by Aharonov and Au[31]; a generalization to the case of arbitrary states was made in Refs. 33 and 35.

A multidimensional generalization of this approach was formulated by Au and Aharonov[36] and, independently, by the present author.[37] The relationship between perturbation theory and the variational principle was described in Ref. 35. It was shown that the results of variational calculations are actually the first two coefficients of a perturbation theory series, so that calculation of the subsequent coefficients of this series reveals the accuracy of variational calculations and makes it possible to improve the accuracy by an iterative procedure. It was also found in this study that the recipe which had been given earlier[32] for constructing convergent perturbation theories is none other than a list of the usual requirements which must be met in order to construct a class of trial wave functions for variational calculations. In

[3)] Very recently, significant progress has been achieved in classifying highly excited states.[21]

[4)] This process of rediscovery continues today. After the present review was written, Imbo and Sukhatme[100] published a paper discussing the development of a new (!) and very convenient perturbation theory, which reduces to the perturbation theory which we are discussing here.

particular, the recipe proposed by Dolgov and Popov[30] is a particular case of the general recipe—one which applies only to non-negative potentials which are increasing at infinity. The approach was also generalized to excited states in the multidimensional case in Refs. 33 and 35. Furthermore, it was shown that when a standard perturbation theory can be realized this approach becomes a purely algebraic procedure which reduces to the solution of recurrence relations.[38]

At present this approach is being developed rapidly. Essentially all the familiar problems of quantum mechanics are being reexamined both from the standpoint of studying ordinary perturbation theory and for an analytic study of the region of arbitrary perturbations: the anharmonic oscillator (see, for example, Refs. 30–33), the Stark effect (Refs. 17 and 39, for example), the Zeeman effect,[18,40] the screened Coulomb potential (Ref. 41, for example), the hydrogen atom in crossed fields,[42] etc. We might add that a perturbation theory which does not require knowledge of the entire eigenvalue spectrum of the unperturbed problem has been given various names in the literature: a "perturbation theory in quadratures,"[22–26] "Dalgarno's F-function method,"[27] the "logarithmic perturbation theory,"[36] and the "nonlinearization method."[32,33,35,36,38] We will use the last of these names here.

Despite the rather long history and intense development of the problem, there has been no coherent exposition of the method. The one review on the topic[27] dealt with the F-function method and referred to perturbation theory alone. It contains essentially no examples. We are attempting to fill this void here.

2. PERTURBATION THEORY

We preface the construction of a perturbation theory with some general comments.

The wave function of an arbitrary bound state in a smooth potential can obviously be written in the form

$$\psi(x) = f(x) \exp[-\phi(x)], \tag{2.1}$$

where the functions $f(x)$ and $\phi(x)$ have no singularities at real $x \in \mathbb{R}^k$. Representation (2.1) is of course ambiguous. We will discuss the resolution of this ambiguity below, but that procedure is unimportant at this point. We now assume that the potential of the problem consists of two parts, an unperturbed part V_0 and a perturbation V_1:

$$V = V_0 + \lambda V_1, \tag{2.2}$$

where λ is a formal parameter. We wish to solve the initial problem by a perturbation theory in the parameter λ. There are several ways to construct a perturbation theory, by using various expansions of the wave function in series[5] in λ:

a) $\phi(x) \equiv 0, \quad f(x) = \sum_n \lambda^n f_n(x).$

This is none other than the standard Rayleigh-Schrödinger perturbation theory (see Ch. 6 in Ref. 11). Another possibility is

b) $\phi(x) = \phi_0(x), \quad f(x) = \sum_n \lambda^n f_n(x).$

This procedure is called Dalgarno's F-function method.[27] In particular, this method has been used successfully by Banks, Bender, and Wu to study one- and two-dimensional anharmonic oscillators.[2,3,43,44] A third possibility is

c) $\phi(x) = \sum_n \lambda^n \phi_n(x), \quad f(x)$

$$= \begin{cases} 1 \text{ in the case of the ground state,} \\ f_0(x) \text{ in the case of excited states with known positions} \\ \text{of the node surfaces,} \\ \sum_n \lambda^n f_n(x) \text{ in the general case of excited states.} \end{cases}$$

The contents of the present review are basically to construct, study, and use this form of perturbation theory, which is the most general form for representation (2.1).

We begin with the case of a ground state whose wave function does not vanish at the end points.

a) Ground state

Looking at the method from a slightly different angle, we can say that it essentially consists of (a) a transformation procedure, which we call a *nonlinearization*,[36,37] which is used to transform a k-dimensional Schrödinger equation, a linear second-order equation,

$$\Delta\psi + (E - V)\psi = 0, \tag{2.3}$$

into an equation which is nonlinear but which is of first order and has a right side and (b) the construction of a perturbation theory specifically for this equation. The transformation which implements this procedure in the case of the ground state is[6]

$$\mathbf{y} = -\frac{\nabla\psi}{\psi} = -\nabla(\ln\psi), \tag{2.4}$$

where Δ and ∇ are the ordinary k-dimensional Laplacian and gradient operators, respectively. Using (2.3) and (2.4), we find the equation

$$\operatorname{div}\mathbf{y} - \mathbf{y}^2 = E - V, \tag{2.5}$$

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

$$\mathbf{y} = \nabla\phi(x), \tag{2.6}$$

where $\phi(x)$ is a scalar function. In other words, the cross derivative must vanish:

$$\partial_i y_j - \partial_j y_i = 0. \tag{2.6'}$$

Equation (2.5) with conditions (2.6) or (2.6') is the basic equation which is used to construct our method. In the one-dimensional case, this equation becomes the Riccati equation (see, for example, Kamke[49]). We will discuss the boundary condititions on (2.5) below.

[5]The index 0 specifies the unperturbed problem.

[6]This transformation has been used previously in a variety of physical situations: by Wentzel, Kramers, and Brillouin in deriving a semiclassical approximation; by Rytov in the theory of oscillations (see the discussion in Ref. 45); and by Bijl,[46] Bogolyubov and Zubarev,[47] and Penrose and Onsager[48] in problems in statistical physics.

We now proceed to construct a perturbation theory after having made the following. The potential $V(x)$ of interest obviously can always be written as a sum (2.2) or in the general case as

$$V(x)=\sum_n \lambda^n V_n(x), \tag{2.2'}$$

where λ is a formal parameter introduced for convenience. The equation

$$\Delta\psi_0+(E_0-V_0)\psi_0=0 \tag{2.7}$$

has an explicit solution. Alternatively, the problem could be formulated as follows: we take any sufficiently smooth function $\psi_0(x)\in L_2(\mathbb{R}^k)$ and find the potential

$$V_0-E_0=\frac{\Delta\psi_0}{\psi_0} \tag{2.7'}$$

which corresponds to it. The perturbation potential $V_1(x)$ is then the difference $(V-V_0)$. It should be noted that

$$\mathbf{y}_0=-\frac{\nabla\psi_0}{\psi_0}. \tag{2.8}$$

This point will prove very useful below. We turn now to the construction of a perturbation theory for the ground state.

As mentioned above, for sufficiently smooth potentials the wave function of the ground state vanishes nowhere. This means that the vector function $\mathbf{y}$ contains no pole singularities at real values of[7] x. We now expand E and $\mathbf{y}$ in Taylor series in the parameter λ:

$$\mathbf{y}=\mathbf{y}_0+\lambda\mathbf{y}_1+\lambda^2\mathbf{y}_2+\ldots=\sum_{n=0}^{\infty}\lambda^n\mathbf{y}_n, \tag{2.9}$$

$$E=E_0+\lambda E_1+\lambda^2E_2+\ldots=\sum_{n=0}^{\infty}\lambda^nE_n; \tag{2.10}$$

where E_0 and $\mathbf{y}_0$ are given by (2.7') and (2.8), respectively. Subsituting (2.9) and (2.10) into (2.5), and collecting terms with like powers λ^n, we find the following equation for determining E_n and $\mathbf{y}_n$:

$$\operatorname{div}(\psi_0^2\mathbf{y}_n)=(E_n-Q_n)\psi_0^2, \tag{2.11}$$

or, equivalently,

$$\operatorname{div}\mathbf{y}_n-2\mathbf{y}_0\mathbf{y}_n=E_n-Q_n; \tag{2.11'}$$

The vector field $\mathbf{y}_n$ must also satisfy potential condition (2.6) or (2.6'). Here

$$Q_1=V_1,\quad Q_n=-\sum_{i=1}^{n-1}\mathbf{y}_i\mathbf{y}_{n-i},\quad n\geqslant 2. \tag{2.12}$$

We wish to emphasize a curious fact: To find the nth correction we must solve the same equation, (2.11), but with different right sides. Consequently, Q_n for $n>1$ may be thought of as an effective perturbation potential. Equation (2.11) along with the condition under which the field $\mathbf{y}_n$ is a potential field is the equation of ordinary (but multidimensional) electrostatics, in which ψ_0^2 and $\mathbf{y}_n$ serve as the dielectric permittivity and the field, respectively, while $(E_n-Q_n)\psi_0^2$ is the charge density.

We turn now to the boundary conditions. Since we are interested in the bound-state problem, we can write the boundary condition in our initial equation (2.5) as the condition that there must be no current of particles at infinity:

$$|\mathbf{y}\psi^2|\to 0 \quad \text{as} \quad |x|\to\infty. \tag{2.13}$$

For Eq. (2.11) we can write the boundary condition in the following form, working from condition (2.13):

$$|\mathbf{y}_n\psi_0^2|\to 0 \quad \text{as} \quad |x|\to\infty. \tag{2.14}$$

Since the wave functions of bound states usually decay exponentially at infinity, (2.14) means that the vector field $\mathbf{y}_n$ must not increase more rapidly than a power function at large distances. This boundary condition can be understood from the physical standpoint: If the perturbation potential is zero, all the corrections E_n and $\mathbf{y}_n$ are identically zero; i.e., the solution of the homogeneous equation (2.11) or (2.11') must be identically zero.

Condition (2.14) can be quickly converted into information about the corrections E_n. For this purpose we integrate (2.11) over the entire space and transform the integral on the right side into a surface integral, using Gauss's theorem. Using condition (2.14), we then find[33,35-37]

$$E_n=\int_{\mathbb{R}^k}Q_n\psi_0^2\,dx\left(\int_{\mathbb{R}^k}\psi_0^2\,dx\right)^{-1}. \tag{2.15}$$

Expression (2.15) gives us an arbitrary correction to the energy level of the ground state of the unperturbed problem. The expression for the first correction, E_1, is the same as the standard expression of the Rayleigh-Schrödinger perturbation theory.[11] The second correction,

$$E_2=-\int\mathbf{y}_1^2\psi_0^2\,dx\left(\int\psi_0^2\,dx\right)^{-1},$$

is always negative, as it should be.

In order to evaluate the various corrections E_n for $n\geqslant 2$, however, we need to solve the electrostatic problem (2.11); equivalently, we must solve an elliptical equation of the general form

$$\frac{1}{\psi_0^2}\operatorname{div}(\psi_0^2\operatorname{grad}\phi_n)=E_n-Q_n \tag{2.16}$$

with boundary condition (2.14), where $\mathbf{y}_n=\operatorname{grad}\phi_n$, and E_n is given by (2.15). The operator

$$\frac{1}{\psi_0^2}\frac{\partial}{\partial x_i}\left(\psi_0^2\frac{\partial}{\partial x_i}\right)$$

on the right side of (2.16) is the Laplacian in a curved space with a conformally plane metric; ψ_0 serves as the determinant of the metric tensor. The problem of constructing a perturbation theory is thus equivalent to one of finding the Green's function of a Laplacian in a conformally plane space with a special type of metric.

The problem of calculating the corrections is thus not an eigenvalue problem (E_n and Q_n are assumed to be known from the preceding iterations), so the problem of finding the corrections E_n and, correspondingly, $\mathbf{y}_n$ is much simpler

[7] Here and below we will streamline the notation and write simply x, which is to be understood as a point in the space $\mathbb{R}^k$ with the coordinates $(x_1,x_2,\ldots,x_k)$.

from the standpoint of numerical calculations than that of solving the original Schrödinger equation. Furthermore, the equivalence of this problem to the electrostatic problem means that we could in principle use analog computers.

We now seek more concrete expressions for the corrections $\mathbf{y}_n$. A solution of Eq. (2.11) with the auxiliary condition that the field must be a potential field, (2.6), is

$$\psi_0^2 \mathbf{y}_n(x) = \int_{R^k} \mathbf{G}_k(x, x')(E_n - Q_n)\psi_0^2 \, dx', \tag{2.17}$$

where $\mathbf{G}_k(x,x')$ is the Green's function of Eq. (2.11) with auxiliary condition (2.6), and the index k specifies the dimensionality of the space. In the general case in which ψ_0^2 is an arbitrary function such that $\psi_0 \in L_2(\mathbb{R}^k)$, the Green's function is not known and apparently cannot be constructed explicitly. In several particular cases, however, it can be. First, for spherical ψ_0^2 and V_1 the Green's function is

$$\mathbf{G}_k(x, x') = \frac{1}{\sigma_k} \frac{\mathbf{x}-\mathbf{x}'}{|x-x'|^k}, \tag{2.18}$$

where $\sigma_k = 2\pi^{k/2}/\Gamma(k/2)$ is the area of a k-dimensional sphere of unit radius. After we integrate over the angular variables, we can then write the solution (2.17) as

$$r^{k-1}\psi_0^2 y_n(r) = \int_0^r (E_n - Q_n)\psi_0^2 r'^{(k-1)} \, dr', \quad \mathbf{y}_n = y_n(r)\frac{\mathbf{r}}{r}. \tag{2.19}$$

We wish to emphasize that this expression also gives the general solution in the one-dimensional case. Second, the problem can be solved explicitly even when the dielectric permittivity is Gaussian:

$$\psi_0^2 = a\exp(-\alpha \mathbf{x}^2).$$

The general solution of Eq. (2.11) is

$$\mathbf{y}_n = \frac{1}{2\pi^{k/2}} \int_{R^k} dx' (E_n - Q_n(x')) \int_0^\infty \frac{dt}{\sqrt{t}} (t+\alpha)^{(k-2)/2} \times \exp[-(\sqrt{t}\,\mathbf{x} - \sqrt{t+\alpha}\,\mathbf{x}')^2](\sqrt{t}\,\mathbf{x} - \sqrt{t+\alpha}\,\mathbf{x}'), \tag{2.20}$$

and is derived in the Appendix. Although we know no other explicit Green's functions, a perturbation theory can be constructed explicitly for the perturbed two-particle Coulomb problem by virtue of the phenomenon of "algebraization" (Section 3), despite the lack of an explicit expression for the Green's function. If a spherically asymmetric potential contains a finite number of harmonics, the procedure for constructing a perturbation theory also simplifies considerably. The zeroth order approximation is taken to be spherically symmetric, and the corrections are sought as finite expansions in the harmonics. The coefficient functions of the harmonics are found from the solutions of one-dimensional equations. This approach has been used to study the problem of a two-dimensional asymmetric anharmonic oscillator.[35] Numerical methods are generally necessary for solving Eq. (2.11).

b) Excited states

We turn now to excited states. There are several reasons why they must be treated separately. First, nonintegrable singularities arise in integrals (2.15) in the case of excited states since the zeros of the excited wave functions transform into pole singularities of the vector function $\mathbf{y}$, and the integrals (2.15) depend on the quantities Q_n, which are quadratic forms of $\mathbf{y}_i$. It has been shown[34] for the one-dimensional case that by moving the integration contour into the complex plane in order to avoid these singularities one can obtain correct results. This method is technically complicated; furthermore, its generalization to the multidimensional case is not clear. We will describe a simpler method[33,35] in which the dimensionality of the space does not play an important role. Second, there has been essentially no analytic study of the question of excited states in the multidimensional case. In particular, we do not have a solution of the state classification problem.[8)] This circumstance seriously aggravates the situation.

It thus seems plausible that the wave function of an excited state can be characterized by some set S_0 on which it vanishes. The wave function can thus be written in the form (2.1):

$$\psi(x) = f(x)\exp[-\phi(x)],$$

where $f(x)$ and $\phi(x)$ contain no singularities at finite $x \in \mathbb{R}^k$; $f(x)$ increases no more rapidly than a power function as $|x| \to \infty$; and $f(x) = 0$ and $\nabla f(x) \neq 0$ for[9)] $x \in S$. In other words, we explicitly single out a function $f(x)$ which embodies information on the node surfaces, where the original wave function vanishes. This procedure is ambiguous. To eliminate the ambiguity, we impose a *minimality condition*, requiring that $f(x)$ contain a minimum of information which does not pertain to the node surfaces. We will explain the essence of this requirement using a one-dimensional example. We know that the wave function of the l th excited state is characterized by l zeros. We thus require that $f(x)$ be a polynomial of degree l with real roots. We now introduce the vector $\mathbf{g} = \nabla\phi(x)$, so that the vector function $\mathbf{y}$ in (2.4) becomes

$$\mathbf{y} = -\frac{\nabla\psi}{\psi} = \mathbf{g} - \frac{\nabla f}{f}. \tag{2.21}$$

We have thus explicitly singled out that part of the vector field $\mathbf{y}$ which contains the singularities associated with the vanishing of the wave function. Substituting (2.21) into (2.5), and multiplying the result by $f(x)$, we find the equation[33,35]

$$f\nabla\mathbf{g} - f\mathbf{g}^2 - \Delta f + 2\mathbf{g}\nabla f = (E-V)f. \tag{2.22}$$

This equation is the foundation of the entire approach. If $\mathbf{g} = 0$, this equation becomes the ordinary Schrödinger equation, while if $f(x) = 1$ it becomes Eq. (2.5).

We now begin to construct the perturbation theory. We assume that the potential is of the form in (2.2') and that ψ_0 is the wave function of Eq. (2.7) written in the form in (2.1). The

[8)] Korsch[102] reviews the present state of this problem.

[9)] At self-intersections of the node surfaces, where branching occurs, the condition $\nabla f(x) = 0$ must hold.

set s_0 on which $\psi_0(x)$ vanishes is determined by the condition $f_0(x) = 0$. We now expand in series in λ not only E and $\mathbf{g}$ [see (2.8) and (2.10)] but also the function $f(x)$, which characterizes the set of zeros and their deformation[10]:

$$f = f_0 + \lambda f_1 + \lambda^2 f_2 + \ldots = \sum_{n=0}^{\infty} \lambda^n f_n. \tag{2.23}$$

We collect the terms of first order in λ; after some simple mathematical transformations we find

$$\operatorname{div}(\psi_0^2 \mathbf{g}_1 + e^{-2\phi_0}(f_1 \nabla f_0 - f_0 \nabla f_1)) = (E_1 - V_1)\psi_0^2, \tag{2.24}$$

where the index 0 specifies the zeroth order approximation. Integrating (2.24) over the entire space, and using condition (2.14) (with $\mathbf{y}$ replaced by $\mathbf{g}$), we find an expression for E_1 which is the same as (2.15) in the case $n = 1$. If we set $\mathbf{g}_1 = 0$, we find that Eq. (2.24) becomes the Dalgarno-Lewis equation (see the review by Hirschfelder *et al.*[27]) The general solution of Eq. (2.24) can be written

$$\psi_0^2 \mathbf{g}_1 + e^{-2\phi_0}(f_1 \nabla f_0 - f_0 \nabla f_1) = \int_{R^k} dx'\, \mathbf{G}_{ex}(x, x')(E_1 - V_1)\psi_0^2, \tag{2.25}$$

where $\mathbf{G}_{ex}(x,x')$ is the Green's function of Eq. (2.24). The expression $\psi_0^2\, G_{ex}(x,x')$ must satisfy the potential condition (2.6) or (2.6′) in terms of the variable x. Another condition imposed on the Green's function is that the right side of (2.25) must be a vector directed along Δf_0 for $x \in S_0$. The deformation of the set S_0 is thus characterized in first order in λ by the condition

$$f_1(x) = \frac{\nabla f_0 \cdot \int \mathbf{G}_{ex}(x, x')(E_1 - V_1)\psi_0^2\, dx'}{(\nabla f_0)^2 \exp[-2\phi_0(x)]}, \quad x \in S_0. \tag{2.26}$$

Equations for determining the higher-order corrections are found in an analogous way. These other equations are structurally similar to (2.24), differing from it only by their right sides:

$$\operatorname{div}[\psi_0^2 \mathbf{g}_n + e^{-2\phi_0}(f_n \nabla f_0 - f_0 \nabla f_n)] = (E_n - \tilde{Q}_n)\psi_0^2, \tag{2.27}$$

or, equivalently,

$$\nabla \mathbf{g}_n - 2\mathbf{g}_0 \mathbf{g}_n - \frac{\Delta f_n - 2\mathbf{g}_0 \nabla f_n - 2\mathbf{g}_n \nabla f_0}{f_0} + f_n \frac{\Delta f_0 - 2\mathbf{g}_0 \nabla f_0}{f_0^2} = E_n - \tilde{Q}_n, \tag{2.28}$$

where

$$Q_n \equiv -\sum_{i=1}^{n-1} \mathbf{g}_i \mathbf{g}_{n-i} - \frac{1}{f_0}\left[\sum_{k=1}^{n-1} f_k \left(\sum_{i=0}^{n-k} \mathbf{g}_i \mathbf{g}_{n-k-i} - \nabla \mathbf{g}_{n-k} + E_{n-k} - V_{n-k}\right) - 2\sum_{k=1}^{n-1} \mathbf{g}_k \nabla f_{n-k}\right], \quad n \geqslant 2. \tag{2.28′}$$

The correction to the energy is found on the basis of the same arguments as in the case of the ground state. It is similar in form to (2.15):

$$E_n = \int dx\, \tilde{Q}_n \psi_0^2 \left(\int dx\, \psi_0^2\right)^{-1}, \tag{2.29}$$

where $\tilde{Q}_n$ for $n \geqslant 2$ is given by (2.28′), and $\tilde{Q}_1 = V_1$. Recalling that the field $\mathbf{g}$ is a potential field, we see that, as in the case of the ground state, the problem of finding the corrections reduces to one of solving the electrostatic problem with a variable dielectric permittivity. In this case the role of the electric field vector is played by the quantity $[\mathbf{g}_n - \nabla(f_n/f_0)]$.

We can write the solution of Eq. (2.27) in the same form as the solution of Eq. (2.24):

$$\psi_0^2 \mathbf{g}_n + (f_n \nabla f_0 - f_0 \nabla f_n)\, e^{-2\phi_0} = \int_{R^k} dx'\, \mathbf{G}_{ex}(x, x')(E_n - \tilde{Q}_n)\psi_0^2, \tag{2.30}$$

with the same Green's function $\mathbf{G}_{ex}(x,x')$ as in (2.25). Information on the higher-order corrections f_n, characterizing the deformation of the set of zeros, is found from

$$f_n(x) = \frac{\nabla f_0 \cdot \int \mathbf{G}_{ex}(x, x')(E_n - \tilde{Q}_n)\psi_0^2\, dx'}{(\nabla f_0)^2 \exp(-2\phi_0)}, \quad x \in S_0. \tag{2.31}$$

It might thus appear that we have everything we need in order to construct a perturbation theory for the excited states. However, this is not quite the case, as we will now show.

The problem is that we need to know the properties of the node surfaces. If we can guess their positions on the basis of considerations of one sort or another, there is no difficulty in constructing a perturbation theory, because the problem actually reduces to that in the case of a ground state, since

$$f_n = 0, \quad n \geqslant 1,$$

and thus[11]

$$\tilde{Q}_1 = Q_1 = V_1, \quad \tilde{Q}_n = Q_n = -\sum_{i=1}^{n-1} \mathbf{g}_i \mathbf{g}_{n-i}. \tag{2.32}$$

A situation of this type arises, for example, in a study of levels with a zero radial quantum number in a spherically symmetric problem, in the case of zero parabolic quantum numbers in the Stark effect, and for certain states in the Zeeman effect (more on this below).

In the general case, on the other hand, the situation is quite indefinite, since in order to find the deformations of the manifold of zeros $f_n(x)$ we need to appeal to additional con-

[10] In the one-dimensional case, S is a discrete set of points, and f is the polynomial

$$f(x) = \prod_i^m (x - \alpha_i),$$

where m is the number of zeros. In principle we can thus directly expand the positions of the zeros α_i in series in λ; i.e., we can write $\alpha_i = \sum \lambda^k \alpha_{ik}$, as suggested in Refs. 31 and 34. This method, however, cannot be generalized to the multidimensional case (as discussed below). Furthermore, it is not efficient, since the accuracy is exceeded in the coefficient of the exponential function: The corrections $f_n \lambda^n$ contain contributions from higher orders. In other words, in order to construct a perturbation theory it is superfluous to know how the fragments of the node surfaces deform; it is sufficient to know how the overall picture changes.

[11] The correction E_2 is always negative, as in the case of the ground state.

siderations in order to continue $f_n(x)$ from the region $x \in S_0$ [see (2.31)], in which they are defined, to the entire space $\mathbb{R}^k$. In the one-dimensional case, this additional information is given by the oscillation theorem (§21 in Ref. 11).

In the multidimensional case we do not have additional information of this type, since we do not have at this point a multidimensional analog of the oscillation theorem. All that is known about the node surfaces is that the node surfaces of level n partition the space into no more than n parts[16] (see the discussion in Ref. 102). This difficulty reflects the absence of a classification of states in the multidimensional case. Before we construct a perturbation theory we must therefore solve the classification problem. The classification problem can be solved technically, through the solution of a secular equation, in certain particular cases (in which the unperturbed problem is exactly solvable). In principle, this difficulty can be circumvented by using a variational principle and keeping track of the orthogonality of the trial wave functions.

c) One-dimensional case

We now take a more detailed look at the one-dimensional case, since here the perturbation theory can be constructed completely. For the ground state, Eq. (2.5) converts in the one-dimensional case into the well-known Riccati equation, and condition (2.6) or (2.6′) holds identically. It is easy to show that a solution of Eq. (2.11) is given by (2.18), which can be put in the form[22]

$$y_n = \psi_0^{-2} \int_{-\infty}^{x} (E_n - Q_n)\, \psi_0^2(x')\, dx', \tag{2.33}$$

where Q_n is defined in (2.18). The energy corrections E_n are again given by (2.15).

In the case of excited states, a solution of Eq. (2.27) of the form in (2.30) transforms to a solution of the form[33,35]

$$g_n(x) = \left(\frac{f_n}{f_0}\right) + \psi_0^{-2} \int_{-\infty}^{x} (E_n - \tilde{Q}_n)\, \psi_0^2\, dx', \tag{2.34}$$

while the deformation of the manifold of zeros f_n is given by (2.31). Since the set S is the set of several points on a straight line in the one-dimensional case, the quantities determining the deformations of their postitions are

$$f_n(x_i^0) = \int_{-\infty}^{x_i^0} (E_n - \tilde{Q}_n)\, \psi_0^2\, dx' \,[f_0'(x_i^0)\, e^{-2\Phi_0(x_i^0)}]^{-1},$$
$$\times x_i^0 \in S_0, \quad i = 1, \ldots, l, \tag{2.35}$$

where l is the index of the level under consideration, and $\tilde{Q}_n$ is given by (2.28). To find the deformations of the manifold of zeros $f_n(x)$ we appeal to the oscillation theorem (see Ref. 11, for example), which can be summarized as follows: The coefficient $f(x)$ of the exponential function is a polynomial of degree equal to the index of the level of interest, so that the corrections $f_n(x)$ must be polynomials of degree no higher than the level index. The problem of finding the corrections $f_n(x)$ thus reduces to one of determining the coefficients of a polynomial of degree $(l-1)$, $P_n^{(l-1)}(x)$, specified at the points $x_i^0 (P_n^{(l-1)}(x_i^0) = f_n(x_i^0))$. This problem can be solved by solving a system of l linear equations with l unknowns, which are the coefficients of the polynomial, a_j $(P_n^{(l-1)}(x) = \Sigma_{j=0}^{l-1} a_j x^j)$. This is a standard problem of linear algebra. Its solution is given in Ref. 50 (Section 3), among other places. We wish to emphasize that when we are dealing with the first excited level the corrections $f_n(x)$ are constants, and the equations are the same as those given in Ref. 31. It is also worth mentioning that the corrections $g_n(x)$ have no singularities on the real axis.

Equations (2.33)–(2.35) are modified in the obvious way in the case of a multidimensional spherically symmetric problem. For the ground state, these equations are given in Refs. 23–26 and 30. We wish to call attention to an important circumstance: It is a particularly simple matter to construct a perturbation theory for excited states with a zero radial quantum number, since the node surfaces are not deformed, and the problem essentially reduces to the ground-state case.

In our approach, we find the nth correction to the wave function and the $(n+1)$th correction to the energy after n interactions. Polikanov[28,34] and Au[51] have shown that in the one-dimensional case the convergence of the iterations in this method can be accelerated significantly by some slight modifications: The nth iteration can yield the $(2^n - 1)$th correction to the wave function and that to the energy. As before, all the corrections are expressed as explicit quadratures. To demonstrate the approach we consider for simplicity the ground state, following Ref. 51. We assume that we have found the first correction, y_1. What potential corresponds to the function $(y_0 + \lambda y_1)$? Substituting $(y_0 + \lambda y_1)$ into the Riccati equation (2.5), we find that this potential is $V_0 + \lambda V_1 - \lambda^2 y_1^2$. We now go through the first-order perturbation-theory calculation, with a zeroth order approximation $y_0^{(1)} = y_0 + \lambda y_1$ and a perturbation potential $-\lambda^2 y_1^2$. As before, we adopt $y_0^{(1)} + \lambda^2 y_1^{(1)} \equiv y_0^{(2)}$ as a zeroth order approximation. The perturbation potential is then of the order of λ^4; specifically, it is $-\lambda^4 y_2^{(1)2}$. The corrections in the preceding step were accordingly of the order of λ^3. After the nth iteration, the perturbation potential is evidently of the order of λ^{2n}, so that the nth iteration is of the order of λ^{2n-1}. The generalization of this procedure to excited states is quite obvious.[34] We should emphasize that the algebraization is lost in the course of this procedure (Section 3 below).

d) Relationship with standard perturbation theory

How is this perturbation theory related to the standard Rayleigh-Schrödinger perturbation theory? The relationship is easy to trace by comparing the expansion of the wave function in the standard approach,

$$\psi = \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \ldots = \sum \lambda^n \psi_n, \tag{2.36}$$

with that in the approach of the present paper:

$$\psi = (f_0 + \lambda f_1 + \lambda^2 f_2 + \ldots) \exp(-\phi_0 - \lambda\phi_1 - \lambda^2\phi_2 - \ldots)$$
$$= \left(\sum \lambda^m f_m\right) e^{-\sum \lambda^m \phi_m}. \tag{2.37}$$

We recall the expressions for ψ_m and E_m in the standard approach (see, for example, §38 in Ref. 11), and we compare them with the corresponding expressions in our approach

[the exponential function in (2.37) must be expanded in a series for this purpose].[12] We then find two families of sum rules (for brevity, we reproduce here only a single member of each family)[13]:

$$\psi_1^{(n)} = \sum_m{}' \frac{\langle m|V_1|n\rangle}{E_0^{(n)} - E_0^{(m)}} \psi_0^{(m)} = \left(-\phi_1 + \frac{f_1}{f_0}\right) \psi_0^{(n)}, \tag{2.38}$$

$$E_2^{(n)} = \sum_m{}' \frac{|\langle m|V_1|n\rangle|^2}{E_0^{(n)} - E_0^{(m)}}$$

$$= \int \tilde{Q}_2 \{\psi_0^{(n)}\}^2 \, dx \left(\int \{\psi_0^{(n)}\}^2 \, dx\right)^{-1}, \tag{2.39}$$

where the subscript specifies the order of the correction, and the superscript the index of the particular level. The fact that sum rules of this type arise has been pointed out in many places.[23,28,30–37] These sum rules were constructed explicitly for the ground state in the one-dimensional case in Refs. 31 and 37. In particular, Aharonov and Au[31] proved (2.39) directly, while expansion (2.38) was essentially proved in the pioneering paper by Zel'dovich.[23] Studies of these sum rules yield information on the spectrum of the unperturbed problem.

We have formulated a nonstandard perturbation theory. In constructing it we have nowhere made use of knowledge of the entire eigenvalue spectrum of the unperturbed problem. We have had to call upon our knowledge of only that level to which the correction is being sought. The situation can be explained particularly simply in the one-dimensional case. Let us asume that we know $\psi_0^{(n)}$, the unperturbed wave function of the n-th state, with an energy $E = E_0^{(n)}$, which is the solution of a linear second-order differential equation (which is what the Schrödinger equation is). Furthermore, if we know one solution, then we can construct a second, linearly independent solution by means of quadratures. Consequently, since we know two linearly independent solutions, we can construct a Green's function for a fixed energy $E = E_0^{(n)}$. On the other hand, the Green's function which appears in all the perturbation-theory equations is that for the energy $E = E_0^{(n)}$, since the equation for the mth correction is

$$\Delta\psi_m^{(n)} + (E_0^{(n)} - V_0)\psi_m^{(n)} = F(E_i^{(n)}, \psi_i^{(n)}), \quad i < m. \tag{2.40}$$

For this reason, all the equations can be written in quadratures, as was actually shown by Zel'dovich.[23] Unfortunately, no corresponding procedure has been developed for constructing the Green's function in the multidimensional case.

3. ALGEBRAIZATION OF THE PROCEDURE FOR CONSTRUCTING A PERTURBATION THEORY

In the preceding section we described the general structure of the perturbation theory. We now begin our discussion of some more specific problems. The subject of this section is a situation in which a standard Rayleigh-Schrödinger perturbation theory can be constructed, i.e., a situation in which the unperturbed problem is exactly solvable. We will show that in this case the construction of our perturbation theory is a purely algebraic problem, which reduces to one of solving some rather simple recurrence relations. In this case it is possible to analyze the structure of an arbitrary correction of the perturbation theory series for arbitrary perturbations of a polynomial type; we will find certain substructures of this correction explicitly. In the course of doing so we find an algebraic method for calculating various matrix elements based on the use of sum rules of the type in (2.38).

a) The harmonic oscillator as the unpertubed problem

1) General discussion

The zeroth order approximation potential, corresponding to a harmonic oscillator, is

$$V_0 = \sum_{i=1}^{d} a_i x_i^2, \quad a_i > 0, \tag{3.1}$$

while the perturbation potential is a polynomial potential:

$$V_1 = \sum_{\{i_1 i_2 \ldots i_d\}}^{i_1 \max \ldots i_d \max} a_{i_1 i_2 \ldots i_d} x_1^{i_1} x_2^{i_2} \ldots x_d^{i_d}. \tag{3.2}$$

The requirement that the perturbation be a polynomial form does not restrict the generality of our discussion, since the potential could otherwise be expanded in a Taylor series, and (3.2) could be treated as an infinite sum. For simplicity we assume that the harmonic oscillator is spherically symmetric, i.e., $a_i = 1$. We will show below that this condition is unimportant. We will also assume that the problem of the classification of the excited states has been solved.

Before we go into detail, let us see why an algebraization arises. We write, say, the first correction of the ordinary Rayleigh-Schrödinger perturbation theory:

$$\psi_1^{(n)} = \sum_k{}' \frac{V_{nk}}{E_0^{(n)} - E_0^{(k)}} \psi_0^{(k)}.$$

The unperturbed wave function $\psi_0^{(k)}$ is a Hermite polynomial (or a combination of Hermite polynomials) multiplied by a Gaussian function. On the other hand, we know (see Ref. 11, for example) that if a perturbation is of polynomial form there is a bounded number of nonvanishing transition matrix elements[14] V_{nk}. This assertion in turn means that a series in intermediate states contains a finite number of terms and that the expression for the correction is a superposition of Hermite polynomials with certain weights, multiplied by the same Gaussian function. The coefficient of the exponential function is thus a finite polynomial. Analogous arguments can be made for an arbitrary correction $\psi_i^{(n)}$; this is the explanation for the algebraization phenomenon. This phenomenon was first pointed out and used by Bender and Wu,[2,3] who worked in the formalism of Dalgarno's F-functions. They wrote recurrence relations which they used to calculate 75 coefficients in the expansion of the ground-state energy of a one-dimensional anharmonic oscillator, and they found the asymptotic behavior of these coefficients. Along

[12] Once we have found the first m correction in the expansion (2.37), we can reproduce not only the first m corrections in the expansion (2.36) but also some of the contributions from higher orders.

[13] For simplicity we consider only the case in which the problem has no continuous spectrum and no degeneracy. Incorporating these factors does not alter the right side of the resulting sum rules.

[14] This is a trivial consequence of the properties of the Gaussian integrals which arise in this problem.

with Banks,[43,44] they pursued an analogous procedure for the ground state of a two-dimensional, asymmetric anharmonic oscillator. The algebraization formalism under discussion in the present paper was used for the ground state in the one-dimensional case in Refs. 30 and 52 and in the two-dimensional case in Ref. 33. An algebraization of the perturbation theory for the ground state was advanced in Ref. 38 for an arbitrary polynomial perturbation in the multidimensional case. This approach is presently being developed intensely in the direction of the use of both Dalgarno's F-function method (and its modifications) and the method of the present paper (see Refs. 39–42 and 53–55, for example).

Let us examine Eq. (2.28). The first remarkable feature that we find is a cancellation in the combination

$$\frac{f_n}{f_0^2}(\Delta f_0 - 2\mathbf{g}_0\nabla f_0) = -2k\frac{f_n}{f_0}, \quad \mathbf{g}_0 = \mathbf{x}, \tag{3.3}$$

since in this case f_0 is a multidimensional Hermite polynomial or a linear combination of such polynomials,[56] and k is the "principal quantum number." For example, if $f_0 = H_{k_1}\times(x_1)\ldots H_{k_d}$, where $H_i(y)$ is an ordinary Hermite polynomial, then we have

$$k = k_1 + k_2 + \ldots + k_d. \tag{3.3'}$$

Equation (2.28) with (3.3) then becomes

$$\nabla g_n - 2g_0 g_n + \frac{2g_n\nabla f_0 - (\Delta f_n - 2g_0\nabla f_n + 2kf_n)}{f_0} = E_n - \tilde{Q}_n. \tag{3.4}$$

Now making use of the potential nature of the field,

$$\mathbf{g}_n = \nabla\phi_n, \tag{3.5}$$

we finally find ($\mathbf{g}_0 = \mathbf{x}$)

$$\Delta\phi_n - 2\mathbf{x}\nabla\phi_n + \frac{2\nabla\phi_n\nabla f_0 - (\Delta f_n - 2\mathbf{x}\nabla f_n + 2kf_n)}{f_0} = E_n - \tilde{Q}_n. \tag{3.6}$$

If f_0 is a Hermite polynomial with a principal quantum number k, the expression in parentheses vanishes.

We can now formulate the basic assertion of this subsection.

Theorem 1. The construction of a perturbation theory for a harmonic oscillator in the case of a polynomial perturbation potential is an algebraic problem. This means that ϕ_n and f_n are multidimensional polynomials, whose coefficients can be found from the recurrence relations which follow from (3.6). In particular, if the highest power of the variable x_i in the perturbation potential is I_i, then the highest power of this variable in an arbitrary correction ϕ_n lies between $(nI_i - 2n + 2)$ and nI_i, depending on the particular perturbation potential (3.2).

Proof. The proof in the case of the ground state is actually given in Ref. 38. We consider the more general case here, assuming that the classification problem has been solved, i.e., that f_0 is some multidimensional polynomial which is a superposition of multidimensional Hermite polynomials with a given principal quantum number. The proof is by induction.

We consider the equation for the first correction:

$$\Delta\phi_1 - 2\mathbf{x}\nabla\phi_1 + \frac{2\nabla\phi_1\nabla f_0 - (\Delta f_1 - 2\mathbf{x}\nabla f_1 + 2kf_1)}{f_0} = E_1 - V_1. \tag{3.7}$$

Obviously, ϕ_1 is some multidimensional polynomial which contains the same combinations of powers $\{i_1 i_2 \ldots i_d\}$ as the potential V_1 (since the operator $\mathbf{x}\nabla$ is a uniform operator) and also similar combinations of powers.[15] One condition for finding the correction f_1 is the requirement that the fraction in (3.7) cancel out, since the correction ϕ_1 must not have singularities at finite values of x (see the discussion in Subsection 2b). We can thus write

$$\frac{2\nabla\phi_1\nabla f_0 - (\nabla f_1 - 2\mathbf{x}\nabla f_1 + 2kf_1)}{f_0} \equiv R_1, \tag{3.8}$$

where R_1 is some polynomial which we are to find. Equivalently, we could write

$$\Delta f_1 - 2\mathbf{x}\nabla f_1 + 2kf_1 = 2\nabla\phi_1\nabla f_0 - R_1 f_0. \tag{3.9}$$

We recall that f_0 is a superposition of multidimensional Hermite polynomials with a principal quantum number k and that f_0 satisfies the homogeneous equation (3.9). We expand the right side of (3.9) in a series in multidimensional Hermite polynomials,[16] and we require that this expansion contain no terms with principal quantum numbers larger than or equal to k. From this condition we can immediately determine the coefficients of the polynomial R_1. It is then a straightforward matter to find a solution of (3.9) as a series in Hermite polynomials. It should be noted that R_1 contains the same combinations of powers as ϕ_1, with the natural restriction that not all the p_i can vanish simultaneously.

In the first step we thus find recurrence relations for the coefficients of R_1. In the second step we find recurrence relations for the coefficients of ϕ_1 which follow from the equation

$$\Delta\phi_1 - 2\mathbf{x}\nabla\phi_1 + R_1 = E_1 - V_1. \tag{3.10}$$

We introduce the function R_n as a generalization of R_1. Since $n > 1$, the function R_n will have a contribution from the right side of (3.4), i.e., from $\tilde{Q}_n$, which includes terms with f_0 in the denominator:

$$R_n = [2\nabla\phi_n\cdot\nabla f_0 - (\Delta f_n - 2\mathbf{x}\nabla f_n + 2kf_n) - \sum_{i=1}^{n-1}\{f_i[-\Delta\phi_{n-i} + 2\mathbf{x}\nabla\phi_{n-i} + (E_{n-i} - V_{n-i}) + \sum_{j=1}^{n-i}\nabla\phi_j\nabla\phi_{n-i-j}] - 2\nabla f_i\nabla\phi_{n-i}\}]f_0^{-1}. \tag{3.11}$$

Alternatively, noting that the expression in (square) brackets is R_{n-i}, we can write

$$R_n = [2\nabla\phi_n\cdot\nabla f_0 - (\Delta f_n - 2\mathbf{x}\nabla f_n + 2kf_n) - \sum_{i=1}^{n-1}(f_i R_{n-i} - 2\nabla f_i\nabla\phi_{n-i})]f_0^{-1}. \tag{3.12}$$

[15] "Similar combinations of powers" are combinations which contain powers $(i_1 - 2p_1, i_2 - 2p_2, \ldots, i_d - 2p_d)$, where $p_1, p_2, \ldots, p_d$ are positive integers, and the condition $(i_l - 2p_l) \geqslant 0$ holds for arbitrary l.

[16] The right side will of course have a finite number of terms, and the leading term will be characterized by the quantum number

$$M = k + i_{1\max} + i_{2\max} + \ldots + i_{d\max} - 2.$$

The equation for f_n thus takes a form analogous to that of (3.9):

$$\Delta f_n - 2x\nabla f_n + 2kf_n = \sum_{i=0}^{n-1} (2\nabla f_i \nabla \phi_{n-i} - f_i R_{n-i}). \quad (3.13)$$

We now assume that $\phi_i f_i$, and R_i for $i < n$ are polynomials and that f_i contains Hermite polynomials with principal quantum numbers less than or equal to k, by analogy with the assumptions used for f_1. We find first R_n and then f_n. We then find recurrence relations for ϕ_n from the equation.

$$\Delta\phi_n - 2x\nabla\phi_n + R_n = E_n - Q_n, \quad (3.14)$$

where $Q_n = -\Sigma_{i=1}^{n-1} g_i g_{n-i}$, since Eq. (3.14) has a polynomial solution, because its right side is a polynomial by construction, as we have been required to prove.

The discussion above cannot of course be regarded as rigorous proof; it would be more accurate to say that these arguments are very similar to those of the actual proof.

Finally, we note that an analysis of the higher powers of the correction ϕ_n does not require knowledge of R_i and f_i, since they do not contribute to these higher powers. These coefficients are thus independent of the particular level, depending on only the higher powers in the perturbation potential V_1. These coefficients can be found explicitly, as will be done below.

2) One-dimensional anharmonic oscillator

We now take up our first specific example: the familiar problem of a one-dimensional anharmonic oscillator,

$$V = x^2 + gx^4. \quad (3.15)$$

We will construct a perturbation theory in the coupling constant g. In this case the unperturbed wave function of the k th level is

$$\psi_0 = H_k(x) \exp\left(-\frac{x^2}{2}\right), \quad (3.16)$$

where $H_k(x)$ is the k th Hermite polynomial; i.e., $f_0 = H_k(x)$. Equation (3.4) then becomes

$$\phi_n'' - 2x\phi_n' + \frac{2\phi_n' f_0' - (f_n'' - 2xf_n' + 2kf_n)}{f_0} = E_n - \tilde{Q}_n. \quad (3.17)$$

Alternatively, recalling definition (3.12),

$$R_n = \frac{2\phi_n' f_0' - (f_n'' - 2xf_n' + 2kf_n) - \sum_{i=1}^{n-1} (f_i R_{n-i} - 2f_i'\phi_{n-i}')}{f_0}, \quad (3.18)$$

we can write this equation in the more convenient form

$$\phi_n'' - 2x\phi_n' + R_n = E_n - Q_n, \quad (3.19)$$

where $Q_1 = V_1$ and $Q_n = -\Sigma_{i=1}^{n-1} \phi_i' \phi_{n-i}'$. We begin with the first-order calculation. Clearly, $g_1 = \phi_1'$ is a third-degree polynomial which contains only odd powers (by virtue of the symmetry of the problem), while the function R_1 is a polynomial of the form $\alpha x^2 + \beta$. Substituting R_1 into the right side of (3.18), and expanding in a series in Hermite polynomials, we obtain an expansion containing the polynomials H_{k+2}, H_k, H_{k-2}, H_{k-4}. We set the coefficients of H_{k+2} and H_k equal to zero; in this manner we can determine the polynomial R_1. We now substitute R_1 into (3.19), and then we can immediately find ϕ_1. We have now determined the right side of the equation for the correction f_1 [see (3.9)]. We seek f_1 as a superposition of H_{k-2} and H_{k-4}. Since H_k is the solution of the equation for the correction, it can appear with an arbitrary coefficient in f_1. We set this coefficient equal to zero, since it fixes the normalization of the wave function, which is of no importance here. The final expression for the first correction is

$$\phi_1 = \frac{x^4}{8} + \frac{x^2}{4}\left(k + \frac{3}{2}\right), \quad E_1 = \frac{3}{2}\left(k^2 + k + \frac{1}{2}\right),$$
$$f_1 = k\frac{k!}{(k-2)!} H_{k-2} + \frac{1}{4}\frac{k!}{(k-4)!} H_{k-4}. \quad (3.20)$$

The second correction can be found just as easily and simply:

$$-\phi_2 = \frac{x^6}{48} + \frac{x^4}{64}(6k+11) + \frac{x^2}{32}(9k^2 + 25k + 21),$$
$$f_2 = \left(-\frac{85}{32}k^2 - \frac{3}{32}k - \frac{9}{8}\right)\frac{k!}{(k-2)!} H_{k-2}$$
$$+ \left(\frac{k^2}{2} - \frac{23}{16}k + \frac{17}{32}\right)\frac{k!}{(k-4)!} H_{k-4}$$
$$+ \left(\frac{k}{8} - \frac{7}{24}\right)\frac{k!}{(k-6)!} H_{k-6} + \frac{1}{32}\frac{k!}{(k-8)!} H_{k-8},$$
$$-E_2 = \frac{34k^3 + 51k^2 + 59k + 21}{16}. \quad (3.21)$$

The expression for E_1 and E_2 are the same as the standard expressions (see Ref. 57, for example). The coefficients f_1 and f_2 contain polynomials of degrees lower than that in H_k. Lowering ϕ_1 and ϕ_2 from the exponential function, i.e., expanding the exponential function in a series, we can reconstruct all possible transition matrix elements V_{mk}. We note that E_1 gives us a diagonal matrix element. We have thus algebraically found relations between different matrix elements (see the discussion in Subsection 2*d*).

It is easy to show on the basis of (3.17)–(3.19) that an arbitrary correction has the functional form

$$\phi_n = \sum_{i=0}^{n} a_i^{(n)} x^{2i+2},$$
$$R_n = \sum_{i=0}^{n} \alpha_i^{(n)} x^{2i}, \quad f_n = \sum_{i=1}^{2n} A_i^{(n)} H_{k-2i}(x), \quad (3.22)$$

and in practice there is no particular difficulty in finding the leading coefficients in (3.22), by explicitly solving the recurrence relations, going from top to bottom (from the highest coefficient to the lowest). For ϕ_n we find

$$\left.\begin{aligned} a_n^{(n)} &= (-1)^{n-1}\frac{(2n-2)!}{2^{2n}(n+1)!\,(n-1)!}, \\ a_{n-1}^{(n)} &= \frac{(-1)^{n+1}}{n}\left[\frac{1}{4} + \left(k+\frac{1}{2}\right)\frac{(2n-1)!}{2^{2n}n!\,(n-1)!}\right], \\ a_{n-2}^{(n)} &= (-1)^{n+1}\left\{\frac{1}{2}\left(k+\frac{1}{2}\right)\right. \\ &\quad + \frac{(2n-2)!}{3\cdot 2^{2n+3}n!\,(n-1)!}\left[12(4n+1)\left(k+\frac{1}{2}\right)^2\right. \\ &\quad \left.\left. + 40n^3 - 20n + 9\right]\right\}, \end{aligned}\right\} \quad (3.23)$$

and for f_n we find

$$A_{2n}^{(n)}=\frac{1}{2^{2n}n!}\frac{k!}{(k-4n)!},$$
$$A_{2n-1}^{(n)}=\frac{k-\frac{7}{3}(n-1)}{2^{2n-1}(n-1)!}\frac{k!}{(k-4n+2)!}. \tag{3.24}$$

The succeeding coefficients can be found in an analogous way, but the calculations become rapidly more tedious for each successive coefficient. This problem can be solved easily on a computer with the help of symbolic programming languages which can be used to carry out analytic calculations. We note that the leading coefficient in (3.23) does not depend on the particular index, and it should not. This coefficient was first calculated for the ground state in Ref. 30.

Let us briefly analyze the properties of the coefficients $a_{n-i}^{(n)}$ and $A_{2n-i}^{(n)}$ [see (3.22)]. The coefficient $A_{2n-i}^{(n)}$ has a factor of $k!/(k-4n+2i)!$. The rest of the expression is a polynomial of degree i in k. In the case of the first excited state, $k=1$, the coefficients are $A_i^{(n)}\equiv 0$, while for $k=2$ the correction f_n is a constant determined exclusively by the index n. The coefficient $a_{n-i}^{(n)}$ is a polynomial of degree i and k; in particular, the coefficient of the lowest degree of x in the correction ϕ_n is a polynomial of degree n in k. At large values of n, we find $a_{n-i}^{(n)}\sim n^i$. Accordingly, while these coefficients vary with the power at small values of i, their growth becomes factorial at $i\sim n$. In principle, an analysis of the recurrence relations can yield expressions describing the asymptotic behavior of the coefficients $a_{n-i}^{(n)}$ and $A_{2n-i}^{(n)}$ and thus of E_n.

A similar procedure could be used to construct a perturbation theory for a system of d coupled harmonic oscillators perturbed by a polynomial potential. Although the calculations become more laborious, the first few corrections can still be found explicitly, and the functional structure of an arbitrary correction can be analyzed. This program was carried out in Ref. 63 for the case in which the perturbation potential is a multidimensional polynomial of fourth degree. One of the results which we wish to emphasize is the appearance of nontrivial phenomena in the transition to an infinite number of oscillators.

b) Coulomb system perturbed by an arbitrary static multipole interaction

1) General discussion

In the preceding subsection we considered a harmonic oscillator perturbed by a polynomial interaction. We demonstrated the algebraization of the procedure for constructing the perturbation theory. In the present subsection we do the same for a Coulomb system described by the potential

$$V_0=-\frac{2\alpha N}{r} \tag{3.25}$$

(the parameters α and N are introduced for convenience) perturbed by an arbitrary static multipole potential containing a finite number of harmonics,

$$V_1=\sum V_{lm}(r)\,Y_l^m(\theta,\ \varphi), \tag{3.26}$$

under the restriction

$$V_{lm}(r)=\sum^{k_{max}} a_k r^k. \tag{3.27}$$

The algebraization of the construction of a perturbation theory for the Coulomb problem was mentioned in Refs. 38 and 58 and has been used by various investigators; see, for example, Ref. 41 (the problem of the screened Coulomb interaction), Ref. 39 (the Stark effect), Ref. 40 (the Zeeman effect), and Refs. 38 and 42 (the hydrogen atom in crossed fields). Excited states have been considered as well as the ground state. It has been demonstrated in all these studies that the use of this method makes it a simple matter to find essentially any desired number of coefficients of the perturbation-theory series.

We begin our discussion of this problem by noting that, as in the case of a harmonic oscillator, a cancellation occurs in the expression

$$\frac{f_n}{f_0^2}(\Delta f_0-2\mathbf{g}_0\nabla f_0)=-\frac{2\alpha(N-1)}{r}\frac{f_n}{f_0}, \tag{3.28}$$

where N is some combination of quantum numbers; the particular combination is determined a little later. If ψ_0 is a Coulomb wave function in spherical coordinates (we are not concerned with the normalization here), given by

$$\psi_0=r^l\tilde{R}_{n_r,\,l}(2\alpha r)\,Y_l^m(0,\ \varphi)\,e^{-\alpha r},\quad E_0=-\alpha^2, \tag{3.29}$$

then

$$f_0^{(N)}=r^l\tilde{R}_{n_r,\,l}(2\alpha r)\,Y_l^m(\theta,\ \varphi),\qquad \mathbf{g}_0=\alpha\frac{\mathbf{r}}{r}, \tag{3.29'}$$

where $\tilde{R}_{n_r,l}(2\alpha r)$ is the Laguerre polynomial, and

$$Y_l^m=P_l^m(\theta)\begin{cases}\cos m\varphi, & m\geqslant 0,\\ \sin|m|\varphi, & m<0\end{cases}$$

are spherical harmonics in the normalization of Bateman and Erdélyi.[56] In this case the parameter N is given by

$$N=n_r+l+1 \tag{3.30}$$

and has the meaning of a principal quantum number [see also (3.25)]; the radial quantum number n_r gives us the number of zeros of the Laguerre polynomial. If we use parabolic coordinates we can write

$$N=n_1+n_2+1, \tag{3.31}$$

where n_1 and n_2 are parabolic quantum numbers. Using (3.28), we can rewrite (2.28) as

$$\nabla\mathbf{g}_n-2\mathbf{g}_0\mathbf{g}_n+\frac{2\mathbf{g}_n\nabla f_0-\left(\Delta f_n-2\mathbf{g}_0\nabla f_n+\frac{2\alpha(N-1)}{r}f_n\right)}{f_0}$$
$$=E_n-\tilde{Q}_n. \tag{3.32}$$

We note that $f_0^{(N)}$ from (3.29') satisfies the equation

$$\Delta f_0^{(N)}-2\mathbf{g}_0\nabla f_0^{(N)}+\frac{2\alpha(N-1)}{r}f_0^{(N)}=0. \tag{3.33}$$

We introduce functions R_n analogous to those in (3.12),

$$R_n = \frac{2g_n\nabla f_0 - \left[\Delta f_n - 2g_0\nabla f_n + \frac{2\alpha(N-1)}{r} f_n\right] - \sum_{i=1}^{n-1}(f_i R_{n-i} - 2\nabla f_i g_{n-1})}{f_0}, \tag{3.34}$$

and we state a theorem analogous to Theorem 1.

Theorem 2. The construction of a perturbation theory for a Coulomb problem with the interaction (3.26)–(.327) is a purely algebraic problem. The corrections ϕ_n and f_n contain a finite number of harmonics with coefficients which are polynomials in r and which are determined from the recurrence relations which follow from Eqs. (3.32) and (3.34).

Proof. We will go through all the details of this proof, which is very similar to the proof of Theorem 1. We simply review the most important aspects.

The correction f_n is found from an equation analogous to (3.13) which follows from (3.34):

$$\Delta f_n - 2g_0\nabla f_n + \frac{2\alpha(N-1)}{r} f_n = \sum_{i=0}^{n-1}(2\nabla f_i g_{n-i} - f_i R_{n-i}). \tag{3.35}$$

The right side of this equation can be expanded in a series in functions of the type $f_0^{(N)}$ [see (3.29′)] with various values of n_r and l. The function R_n is found by requiring that this expansion contain no terms with $N_i > N$, where $N_i = n_r^i + l^i + 1$. Once the function R_n has been found, it is substituted into the equation

$$\Delta\phi_n - 2g_0\nabla\phi_n + R_n = E_n - Q_n. \tag{3.36}$$

We seek a solution of this equation as a series in spherical harmonics,

$$\phi_n = \sum_{l,m} \phi_{lm}^{(n)} Y_l^m(\theta, \varphi). \tag{3.37}$$

It is easy to see that this expansion contains a finite number of harmonics with coefficient functions $\phi_m^{(n)}(r)$ which are polynomials in r. The coefficients in $\phi_m^{(n)}$ are found from the obvious recurrence relations QED.

We thus see that the phenomenon of algebraization also arises in the perturbed Coulomb problem. Since we know that algebraization occurs for the perturbed harmonic oscillator, however, this fact should perhaps not be surprising: The Coulomb problem is equivalent to a four-dimensional harmonic oscillator (see Ref. 59, for example).

We will now demonstrate how algebraization works for Coulomb problems, considering the Zeeman effect as an example.

2) The hydrogen atom in a static magnetic field (the Zeeman effect)

The study of the deformation of the spectrum of the hydrogen atom upon the application of a static magnetic field is one of the oldest problems in quantum mechanics. Since the problem is substantially three-dimensional, however, its solution is still far from complete: Even the problem of classifying the states has not been solved. Only the low-lying states of the spectrum have been analyzed regularly (see the review by Garstang[60] and the bibliography there). This problem has recently attracted considerable interest because of possible astrophysical applications, and a steady stream of papers is being published (see, for example, Refs. 18, 40, 60, and 63 and the bibliographies there).

We will look in detail at the situation in the case of a weak field for a certain class of states, including the ground state, and we will calculate the coefficients of the perturbation-theory series up to terms $\sim\mathscr{H}^6$ inclusively. For simplicity we assume that the atom is spinless.

The problem of the classification of states has not yet been solved for a hydrogen atom in a static magnetic field. Consequently, we do not know even the first correction to the energy for the quadratic Zeeman effect in the general case. There are, however, several classes of states which are not degenerate (and which therefore do not mix). In particular, these states include the extreme and near-extreme components of Coulomb multiplets for a zero radial quantum number:

$$n_r = 0, \quad m = \pm l, \quad \pm(l-1), \tag{3.38}$$

where m is the magnetic quantum number (see Ref. 62, for example). Let us examine this class of states.

The energy expansion is

$$E = -\alpha^2 + \mathscr{H}m + E_1\mathscr{H}^2 + E_2\mathscr{H}^4 + \ldots + E_n\mathscr{H}^{2n} + \ldots, \tag{3.39}$$

where $\mathscr{H}$ is the magnetic field (in dimensionless units), which is directed along the z axis. The perturbation potential (3.26) is $V_1 = \mathscr{H}^2(x^2+y^2)/4$, and $\alpha = 1/N$. We wish to find E_1, E_2, and E_3.

The coefficient of the exponential function for this class of states, (3.38), is

$$f = f_0 = r^l Y_l^m(\theta, \varphi), \quad |m| = l, \; l-1, \tag{3.40}$$

and does not change when perturbation are imposed, i.e., we have $f_n = 0$ for $n > 0$. In the exponential function, an arbitrary correction contains a finite number of harmonics[17]:

$$\phi_n = \sum_{i=0}^{n} R_{n,2i}(r)\, Y_{2i}^0. \tag{3.41}$$

Using (3.40), we can rewrite Eq. (3.32) for the corrections ϕ_n as

$$\Delta\phi_n - 2\alpha\frac{\partial\phi_n}{\partial r} + 2\frac{\nabla\phi_n\nabla f_0}{f_0} = E_n - Q_n, \tag{3.42}$$

where Q_n is given by (2.13). By virtue of theorem 2 the coefficient functions are polynomials, and their functional form

$$R_{n,2i} = \sum_{k=\max(2,\,2i)}^{2n+1} a_{n,2i,k} r^k \tag{3.43}$$

can be found easily by analyzing the recurrence relations which follow from (3.42). It should be noted that the polynomial preceding the highest-order harmonic, Y_{2n}^0, contains only two terms; that of the next highest, Y_{2n-2}^0, contains

[17]This assertion applies to any level of interest, since only the coefficients of the exponential functions are mixed.

only four; etc. As in the case of a perturbed harmonic oscillator, we can find the coefficient functions for the higher harmonics. Explicit expressions for these functions are given in Refs. 40 and 18.

The calculations of the first few corrections in the perturbation-theory series are quite simple and are easily formalized for numerical solution. We have used the REDUCE-2 analytic calculation program. Here is the series found for the energy[18]:

$$
\begin{aligned}
E = & -\frac{1}{N^2} + \mathcal{H}m + \mathcal{H}^2 \frac{N^2(N+1)(N-k)}{4} \\
& - \mathcal{H}^4 \frac{N^6(N+1)}{16}\left[\frac{46}{45}N^3 + \frac{137}{60}N^2 + \frac{17}{15}N\right. \\
& \left. - \frac{1}{45} - \left(\frac{185}{180}N^2 + \frac{359}{108}N + \frac{61}{54}\right)k + \left(\frac{3}{4}N + \frac{7}{6}\right)k^2\right] \\
& + \mathcal{H}^6 \frac{N^{10}(N+1)}{64}\left[\frac{407}{135}N^5 + \frac{16\,373}{1\,080}N^4\right. \\
& \qquad + \frac{3\,071}{108}N^3 + \frac{3\,182}{135}N^2 \\
& + \frac{22}{3}N - \left(\frac{513\,433}{68\,040}N^4 + \frac{8626\,423}{249\,480}N^3 + \frac{278\,5715}{49896}N^2\right. \\
& \qquad \left. + \frac{25\,985\,163}{748\,440}N + \frac{183\,107}{249\,48}\right)k \\
& + \left(\frac{1055}{168}N^3 + \frac{2\,759}{108}N^2 + \frac{24\,851}{756}N + \frac{673}{54}\right)k^2 \\
& \left. - \left(\frac{7}{4}N^2 + \frac{221}{36}N + \frac{11}{2}\right)k^3\right] + \ldots,
\end{aligned}
\tag{3.44}
$$

where N is the principal quantum number ($N = l + 1$), and

$$
k = \begin{cases} 0 & \text{for} \quad m = \pm l, \\ 1 & \text{for} \quad m = \pm (l-1). \end{cases}
$$

A few words are in order regarding the general structure of the correction E_n. It can be shown that an arbitrary term of series (2.10) has the functional form

$$
E_n = (-1)^{n+1} N^{4n-2} (N+1) P_{2n-1}(N), \tag{3.45}
$$

where $P_{2n-1}(N)$ is a polynomial of degree $2n-1$. The coefficient of the highest power of this polynomial, N^{2n-1}, does not depend on m, the angular momentum projection, i.e., does not depend on the number k, and is positive. At the nonphysical points $N = 0, -1$ the contribution to the energy from the quadratic Zeeman effect is zero. We wish to emphasize that E_n *vanishes at* $N = 0$ *not only for the states under consideration here but also for any other states. All the corrections* ϕ_n *also vanish at this point.* The nature of this phenomenon is not clear, but it should be recalled that a similar situation arises in a study of the anharmonic oscillator $V(r) = r^2 + gr^4$ in a d-dimensional space, in which case all the corrections to the energy vanish at a nonphysical dimensionality of the space, $d = -2$ (Ref. 30). In this situation it turns out to be possible to find an exact solution of the Schrödinger equation for the ground state with $d = -2$, and an attempt has been made to construct a perturbation theory in the dimensionality of the space, i.e., in the quantity $\epsilon = d + 2$. Unfortunately, it has not been found to solve the Schrödinger equation with $N = 0$ or $N = -1$ in this case.

[18]The calculations were carried out on an ES-1060 computer.

We turn now to expression (3.44). In the case $N = 1$ (the ground state) this expression is the same as the results of the standard calculations, which are given in Ref. 61, among other places. With $N = 2$ and $l = 1$, however, there is a slight numerical discrepancy with the result calculated in Ref. 64. The coefficient of the $\mathcal{H}^2$ term for arbitrary N agrees with that which has been found elsewhere (see Ref. 60, for example).

Let us discuss expression (3.44) and the type of information which can be extracted from it. We know that perturbation-theory series (3.44) is divergent; its coefficients increase factorially, and it has a zero convergence radius.[61,62] For highly excited states, the coefficients of the perturbation-theory series also depend in a power-law fashion on the principal quantum number; they grow. As a result, the range of applicability of the perturbation theory contracts rapidly with increasing N. The range of applicability can be estimated quite simply for $N \gg 1$:

$$
(\mathcal{H}^2)_{\text{PT}} \lesssim \frac{4}{N^6}. \tag{3.46}
$$

This estimate means that for states with $N \gtrsim 30$–40 even standard laboratory fields of 2–4 T are "strong," the perturbation theory is inapplicable, and the situation becomes indefinite.

c) Conclusion

To conclude this section we discuss the algebraization of the procedure for constructing a perturbation theory for other exactly solvable problems. We begin by noting that essentially all such known problems have the property that a polynomial which gives the positions of the node surfaces can be factored out explicitly. This polynomial is usually given by some hypergeometric function. The factorization process is carried out in some special coordinates. For example, for the Morse potential $V(x) = A(e^{-2\alpha x} - 2e^{-\alpha x})$ the new coordinates are $\xi = e^{-\alpha x}$ (Ref. 11). The factor which remains in the wave function after the polynomial has been factored out, however, is not always an exponential function of the type in (2.1). This is the situation for the potential $V(x) = -V_0/\text{ch}^2 \alpha x$. In other exactly solvable problems, however, this factor is an exponential function in terms of certain coordinates. It can thus be concluded that if an exactly solvable problem allows a representation of the wave function in the form in (2.1), and if the potential of the perturbation is a polynomial in the coordinates in which representation (2.1) is possible, then the procedure for constructing a perturbation theory is purely algebraic. This is the case for the following potentials[63]:

$$
V(x) = A(e^{-2\alpha x} - 2e^{-\alpha x}), \quad \xi = e^{-\alpha x}, \tag{3.47}
$$

$$
V(r) = \frac{A}{r^2} - \frac{B}{r}, \quad \xi = r, \tag{3.48}
$$

$$
V(r) = \frac{A}{r^2} + Br^2, \quad \xi = r^2. \tag{3.49}
$$

In (3.47)–(3.49) we have also listed the coordinates in which the perturbation should be of polynomial form.[19] We see

[19]Burenin[101] has recently demonstrated explicitly that the procedure for constructing a perturbation theory for (3.48) is algebraic.

that, with certain modifications, a polynomial form of the perturbations will lead to an algebraization in other exactly solvable problems also. In particular, when the wave function cannot be written in the form in (2.1), an algebraization can be carried out in an implementation of Dalgarno's F-function method.

This concludes our examination of problems in which the zeroth order approximation is an exactly solvable problem.

4. ARBITRARY PERTURBATIONS: PERTURBATION THEORY AND THE VARIATIONAL METHOD

In the preceding section we demonstrate the applicability of our approach in situations in which the standard method, based on the Rayleigh-Schrödinger perturbation theory, can be used, and we demonstrated the advantages of our own approach in comparison with the standard method. Much more common and attractive, however, are applications in which the standard method cannot be used since the zeroth order approximation is not an exactly solvable problem. We have not yet made any use of a powerful property of our approach: It does not require knowledge of the entire eigenvalue spectrum of the unperturbed problem. In the present section we will make use of this property. It allows us to construct a procedure which converges for an arbitrary perturbation parameter, choosing the zeroth order approximation potential almost arbitrarily. On the other hand, it allows us to evaluate the accuracy of variational calculations! Furthermore, we have at our disposal a criterion for judging the "reasonableness" of a particular choice of zeroth order approximation (trial wave functions) in variational calculations based on Dyson's argument.[1]

In this section we describe a regular method for studying the strong-coupling region in quantum mechanics. As examples we consider several standard problems in quantum mechanics which serve as test cases for any method.

a) The variational method from the standpoint of perturbation theory

Since we hve an iterative procedure for finding the eigenvalues of a Schrödinger operator without knowing the entire eigenvalue spectrum of the unperturbed problem, we have a great deal of latitude in the choice of a potential for the unperturbed problem. We can exploit this flexibility to write the potential under study, V, as a sum $V_0 + V_1$ in essentially any way we wish, so that we can construct a converging perturbation theory which establishes the relationship between the perturbation theory and the variational principle.

We preface the discussion of this question with an obvious comment: Any sufficiently smooth function $\psi_0 \in L_2(\mathbb{R}^k)$ is an eignfunction of some state in a potential V_0 given by

$$V_0 - E_0 = \frac{\Delta\psi_0}{\psi_0}, \tag{4.1}$$

where E_0 is the energy of this state. We now assume that we wish to find the position of some level in the potential V by means of a variational principle and to construct for this level a class of trial wave functions[20] $\psi_0(\lambda)$. To determine how these trial functions correspond to the poentials $V_0(\lambda)$, we use (4.1). Let us examine a variational calculation from the standpoint of perturbation theory. The variational energy is

$$E_{\text{var}} = \min_{\{\lambda\}} \int \psi_0 \hat{H} \psi_0 = \min_{\{\lambda\}} \left[E_0 + \int \psi_0 (\hat{H} - \hat{H}_0) \psi_0 \right]$$
$$= \min_{\{\lambda\}} (E_0 + E_1); \tag{4.2}$$

here $\hat{H}(\hat{H}_0) = p^2 + V(V_0)$, $\hat{H}_0\psi_0 = E_0\psi_0$ and $E_1 = \int \times\psi_0(V - V_0)\psi_0$ is the first correction to the energy level in the case in which the perturbation potential V_1 is $V - V_0$. We thus find that a variational calculation gives us the first two terms of the perturbation-theory series [see (2.10)], in which the perturbation potential is equal to the deviation of the initial potential from that corresponding to the trial function $\psi_0(\lambda)$ [see (4.1)]. Evaluating the succeeding terms in perturbation theory series (2.10), E_2, E_3, . . ., we find that we can evaluate the accuracy of the variational calculations, and we can refine them by an iterative method.[21] Furthrmore, by comparing the potentials V and V_0 we can see just how reasonably the class of trial functions has been constructed (this point will be explained below).

b) Dyson's argument. How can a converging perturbation theory be constructed?

We turn now to the equation of the convergence of the procedure described above, i.e., to the question of just when series (2.9), (2.10), and (2.23) converge. We will first determine why perturbation theory series usually diverge.[22] As an example we consider the anharmonic oscillator $V = x^2 + gx^4$ ($V_0 = x^2$, $V_1 = x^4$). If $g > 0$ (Fig. 1a), there are an infinite number of bound states in the potential, while at $g < 0$ (for arbitrarily small g; Fig. 1(b) tunneling occurs; i.e., the level energy $E(g)$ changes from real to complex. This assertion means that the function $E(g)$ has a singularity at $g = 0$, and since the perturbation theory series is an expansion at the origin, i.e., right at the singularity, the perturbation theory series has a zero convergence radius. This is the explanation for the divergence of the perturbation theory. This phenomenon was first analyzed rigorously by Vaĭnshteĭn[65] using the example of an anharmonic oscillator and by Langer[66]; they showed that a cut begins for the ground-state energy at the point $g = 0$, and they calculated the discontinuity at this cut in the limit $g \to -0$.

We now understand that one reason for the divergence of a perturbation theory series is that the perturbation potential is more singular at infinity than an unperturbed potential. In this case, there is a fundamental change in the structure of the eigenvalue spectrum upon a variation of the perturbation parameter g: A level may become quasistation-

[20] Here λ is a set of parameters with respect to which a minimization is performed. For the discussion below, however, it is unimportant whether this minimization is performed.

[21] If, of course, the perturbation theory series converges.

[22] The arguments below are usually called "Dyson's instability argument."[1] He has proved in a similar way that a perturbation theory series in α diverges in quantum electrodynamics.

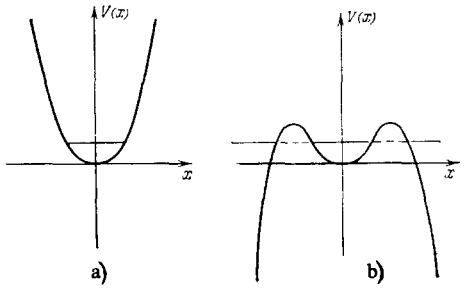

FIG. 1. The anharmonic oscillator potential $V(x) = x^2 + gx^4$. a—$g > 0$; b—$g < 0$. The horizontal line in each part of the figure is a representative position of one level.

ary, as in the example just described, and it may go into the continuum. The general recipe for obtaining a convergent perturbation-theory series then runs as follows[32,33,37]:

A zeroth order approximation wave function is constructed in such a manner that the potential V_0 to which this wave function corresponds [see (4.1)] reproduces as many of the characteristic properties of the potential of interest, V, as possible. Of particular importance is that all the singularities and the asymptotic behavior of the original potential be reproduced.

In terms of wave functions, this means that ψ_0 must embody as many properties of the true wave function ψ as possible: the behavior at infinity, the behavior at the origin, the behavior near singularities of the potential, information about the zeros, etc. It is not difficult to see that this recipe (in terms of wave functions) is actually the same as that which is ordinarily followed in constructing a class of trial functions in the nonlinear Ritz variational method (see Chapter 9 in Ref. 15 and the excellent monograph by Epstein[67]).

We turn now the the convergence question, and we state the following theorem regarding the ground-state case[33]:

Theorem 3. If the first correction, $\mathbf{y}_1$, is a bounded vector function, i.e., if (1) the condition $|\mathbf{y}_1| < a_1$ holds; if furthermore (2) the condition $|\psi_0^{-2}| \int |\mathbf{G}(x,x')\psi_0^2| dx \leqslant A$, holds; and if (3) we have $a_1 A < 1/8$, then series (2.9) and (2.10) converge.

Proof. The proof is by mathematical induction. It follows immediately from conditions (1) and (2) that all the corrections are bounded vector functions,

$$|\mathbf{y}_1| \leqslant 2A \sum_{i=1}^{n-1} a_i a_{n-i} \equiv a_n, \quad n \geqslant 2, \tag{4.3}$$

with

$$|E_n| \leqslant \sum_{i=1}^{n-1} a_i a_{n-i}, \tag{4.4}$$

where the number a_n is a bound on the modulus of the vector function $\mathbf{y}_n$. To find the convergence region of series (2.9) and (2.10) we evaluate the sum

$$S = \sum_{i=1}^{\infty} a_i. \tag{4.5}$$

Using (4.3), we can easily show that

$$2AS^2 + a_1 = S. \tag{4.6}$$

The solution of (4.6) which we want is

$$S = \frac{1 - \sqrt{1 - 8Aa_1}}{4A}. \tag{4.7}$$

We have thus constructed majorizing sequences for $\mathbf{y}_n$ and E_n, which converge if

$$8Aa_1 \leqslant 1, \tag{4.8}$$

proving the theorem.

This theorem is a rather feeble assertion and can be strengthened considerably. It is nearly obvious that in the case in which $|\mathbf{y}_0|$ is an increasing function in the limit $|x| \to \infty$, the satisfaction of condition (1) is sufficient for the convergence of series (2.9) and (2.10). It should be noted that an analogous theorem can be proved for excited states, in which case we would replace condition (1) of the theorem by the condition that the vector function $\mathbf{g}_1$ must be bounded. We note that in Section 3, where we considered problems for which it was known at the outset that the perturbation theory series diverge in all cases, condition (1) did not hold.

In summary, we wish to emphasize that the question of the convergence of perturbation theory series is a rather subtle and delicate one. Unfortunately, we know of no constructive results in this field with anything approaching rigor.

c) Examples

We now consider some examples in which the use of Dyson's argument, along with an appropriate choice of zeroth order approximation wave functions, yields highly accurate results quite simply and rapidly.

1) One-dimensional anharmonic oscillator

Let us consider the anharmonic oscillator described by the potential

$$V(x) = m^2x^2 + gx^{2n}, \tag{4.9}$$

with $n = 2$. At sufficiently small values of g we can use ordinary perturbation theory in powers of g, so we will begin by looking at the region of extremely strong coupling, $g \to \infty$; i.e., we examine the spectrum problem in the potential

$$V = x^{2n}. \tag{4.9'}$$

That potential (4.9') describes the region of extremely strong coupling can be seen easily from the rescaling relation (see Ref. 4, for example) for the spectrum:

$$E^{(k)}(m^2, g) = g^{1/(n+1)} E^{(k)}\left(\frac{m^2}{g^{2/(n+1)}}, 1\right), \tag{4.10}$$

where k is the level index.

One of the simplest ground-state functions which satisfy the requirments listed in Subsection 4b is, for example,[32]

$$\psi_0^{(0)} = \exp\left(-\frac{ax^2}{2} - \frac{\sqrt{g}}{n+1}|x|^{n+1}\right), \tag{4.11}$$

where the subscript specifies the order of the approximation. This function is the wave function of the ground state in the polynomial potential

$$V_0^{(0)} = -(\sqrt{g}\, n \mid x\mid^{n-1} - 2a\sqrt{g} \mid x \mid^{n+1}) + a^2x^2 + gx^{2n}, \tag{4.12}$$

where the parameter a will be specified below.

We digress somewhat to emphasize an important point: The exact wave function for the ground state for the polynomial potential (4.12) is given by (4.11). Furthermore, it is clear that any exponential function of a polynomial with a negative leading coefficient is the exact wave function of the ground state for some polynomial potential with definite relations between coefficients. The generalization to the case of excited states is quite straight-forward: The wave function must be taken in the form of a polynomial multiplied by an exponential function of a polynomial; the potential will then contain poles, which can frequently be removed through an appropriate choice of the coefficients of the polynomials in the argument of the exponential function and in the coefficient of the exponential function. It might appear at first glance that some new exactly solvable problems could be sought in this way, but it has not proved possible to find *more than one* state for a given potential except in the well-known exactly solvable cases! Apparently this is an indication that the other wave functions of the spectrum do not factorize into an exponential multiplied by another function. All this activity in searching for exact solutions for polynomial potentials apparently began with Refs. 32 and 68. It continues at a high level even now (see, for example, Refs. 69 and 70 and the bibliographies there). In particular, eigenfunctions hve been found for polynomial potentials in the form of definite integrals.

1.1) The potential $V(x)=x^{2n}$ We assume that the parameter g is equal to 1 in (4.11) and (4.12). There is an important fact to be noted here: With $g = 1$, potential (4.12) reproduces the behavior of the potential of interest at infinity, so that it is reasonable from the standpoint of Dyson's argument. A perturbation potential which is the difference between the potential under study and potential (4.12) is given by

$$V_1^{(0)}(x) = (n \mid x \mid^{n-1} - 2a \mid x \mid^{n+1}) - a^2x^2. \tag{4.13}$$

We now substitute (4.11) and (4.12) into (2.15) and (2.33) and evaluate the corrections y_k and E_k. Table I shows the corrections E_k ($k = 1,2$) found in this manner for the case $a = 1$ (Refs. 32 and 37). The convergence of the method is seen to be quite good, especially for the x^2 potential. Incorporating E_3 leads to an accuracy better than 1%, even in the worst case of the x^4 potential.

We now minimize the expression $(E_0 + E_1)$ with respect to the parameter a (Subsection 4a). As a result we find the variational value of the ground-state energy with trial function (4.11). Calculating E_2 for $a = a_{\min}$, we can immediately evaluate the accuracy of the variational calculation, which turns out to be at the level of 1%. After determining the correction E_3, we see that the absolute accuracy of the calculation is $\sim 10^{-4}$ in terms of the energy (Table I).

We now calculate the energy of the first excited level. We take the trial function for the zeroth order approximation in the form

$$\psi_0^{(1)} = x\psi_0^{(0)}, \tag{4.11'}$$

since it must vanish once. It is clear from the symmetry of the problem ($x \to -x$) that this vanishing occurs at $x = 0$. The perturbation potential is

$$V_1^{(1)} = ((n+2) \mid x \mid^{n-1} - 2a \mid x \mid^{n+1}) - a^2x^2. \tag{4.13'}$$

In this case we will not perform a minimization with respect to a; we give the results calculated for $a = 1$ (Table I). As in the case of the ground state, the results are worst for the x^4 potential. The reason is that the perturbation potential is "higher" than in the x^6 case. A minimization with respect to the parameter a greatly improves the accuracy of the calculations and eliminates the "prominence" of the x^4 potential.

1.2) Anharmonic oscillator. The anharmonic oscillator is one of the oldest problems in quantum mechanics. The one-dimensional anharmonic oscillator has been studied

TABLE I. Calculated energies of the ground and first excited states in an x^{2n} ($n = 2,3$) potential.

Potential			Ground state				First excited state	
Approximation			$V(x) = x^4$		$V(x) = x^6$		$V(x) = x^4$	$V(x) = x^6$
0	E_0	$E_0 = a_{\min}$	1	0,47	1	0.85	3	3
1	E_1		0,13359	0,598448	0,158409	0,302627	0.94939	1,35903
	E_0+E_1		1,13359	1,068448	1,158409	1,152627	3.94939	4,35903
2	$-E_2$		0.04841	0,007720	0,010936	0,007319	0,10458	0,01927
	$E_0+E_1+E_2$		1,08518	1,060728	1,147473	1.145308	3,84482	4.33976
3	$-E_3$		0,01542	0,000304	0,002033	0.000406	—	—
	$E_0+E_1+E_2+E_3$		1,06976	1.060424	1,145440	1,144902	—	—
E_{exact}			1,060362		1.14480246		3,7996732	4.338599

Here $a_{\min}$ is that value of the parameter a [see (4.11)] at which the minimum of $(E_0 + E_1)$ is reached. The values of E_{exact} were found by M. S. Marinov and V. E. Shestopal through a numerical solution of the Schrödinger equation.

TABLE II. Ground-state energy for an anharmonic oscillator.

g'	a_{min}	E_1'	$-\Delta E_2'$	E_2'	E' (Ref. 81)
0.1	0.77	0,561738	0,002569	0,559169	0.559146
	1.2380	0,55914111	0,00000278	0,55914634	
1	0,86	0.809320	0,005607	0,803113	0,803771
	2.4416	0,8038481	0,0000764	0,8037717	
10	1.41	1,51622	0,001150	1,50472	1,50497
	8.23	1,505310	0,000332	1,504978	
100	2.82	3,15516	0,02438	3,13078	3,13138
	35,146	3,132241	0,000841	3,131399	
1000	5,98	6,74521	0,05230	6,69291	6,69422
	160,3500	6,696134	0,001877	6,694257	

The normalization of E and g is the same as in Ref. 81.($E' = E/2, g' = g/2$). The upper row corresponds to approximation (4.11), and the lower row to the analog of the leading log approximation, (4.40).

most comprehensively and in most detail by Bender and Wu.[2,3] The list of papers on this problem is extremely long. There has been particular interest in this problem in the past decade, for many reasons: First, for all its apparent simplicity the anharmonic oscillator is not a trivial problem, and it is frequently used to test new spectrum calculation methods. In particular, the anharmonic oscillator has very recently been discussed in connection with various methods for summing perturbation theory series[71-73]; modifications of semiclassical,[74,75] variational,[76] and moment[77] methods; various perturbation-theory and iteration methods[30,33,78-81]; etc. A second reason for the hightened interest in this problem is that the anharmonic oscillator is a one-dimensional field theory[2] which embodies many problems inherent in realistic four-dimensional field-theory models. It thus seems important to attempt to study these problems on the example of a rather simple model. Third, the anharmonic oscillator has important applications in atomic and molecular physics and also in solid state physics.

Semiclassical methods were used in Refs. 2, 3, 65, 66, and 82 for a detailed study of the structure of the perturbation theory series in the coupling constant. Simon[4] and Crutchfield[82] studied the analytic structure of the Riemannian energy surface as a function of the coupling constant g and found it to be rather complicated. We will show below how to construct one version of a converging perturbation theory for an anharmonic oscillator by the approach of this paper. We will follow Ref. 33 in this discussion. Various versions of converging perturbation theories have been proposed previously in several places[23] (Refs. 30, 33, 35, 37, 78, and 104).

As a trial wave function of the zeroth order approximation for the ground state we take the function (4.11) with $n = 2$. The perturbation potential is then

$$V_1^{(0)} = m^2x^2 + 2\sqrt{g}\,|\,x\,|\,(1-ax^2) - a^2x^2. \tag{4.14}$$

We now develop a perturbation theory, substituting (4.11) and (4.14) into (2.15) and (2.33). For the energy we then find the series

$$E = E_0 + E_1 + \ldots = a + \frac{\int_0^\infty [(m^2-a^2)x^2 + 2\sqrt{g}\,x(1-ax^2)]\exp\left(-ax^2 - \frac{2\sqrt{g}}{3}x^3\right)dx}{\int_0^\infty \exp\left(-ax^2 - \frac{2\sqrt{g}}{3}x^3\right)dx}. \tag{4.15}$$

It is easy to see that series (4.15) incorporates many properties of the actual energy function, and although the expansion for $g = 0$ contains not only integer powers of g there is also a cut in the g plane which runs from 0 to $-\infty$. The discontinuity at this cut becomes exponentially small as $g \to -0$.

We now minimize with respect to the parameter a, evaluate E_2 and compare the results with the results of the numerical integration of the Schrödinger equation. In can be seen (Table II) that the accuracy of this method is such that even the simplest trial function, (4.11), can reproduce several decimal places at both small and large values of the coupling constant g. Expression (4.15) can be used to study the analytic structure of the energy as a function of the coupling constant. The incorporation of the higher-order corrections does not alter the structure of the singularities.

2) The hydrogen atom in static fields. The case of electric field (the Stark effect)

The behavior of the hydrogen atom in a static electric field is the first multidimensional problem which we will discuss. In weak fields, $\mathscr{E} \lesssim 0.1$ a.u., the level shift is described well by a perturbation theory in powers of the field $\mathscr{E}$, and this theory has recently been analyzed in some detail.[83-85,39] However, since the perturbation theory series are divergent and of constant sign,[85] attempts to go beyond the range of applicability of the perturbation theory by appealing to various methods for summing the series have been unsuccessful.

Consequently, calculations on the Stark effect outside the range of applicability of perturbation theory are carried out primarily by various numerical methods,[86-89] which, however, yield inconsistent results on both the level shift and

[23]The converging iterative procedure proposed by Dolgov and Popov[30] is a particular case of the approach of the present paper: the case in which the unperturbed potential is $V_0 = V - V'\sqrt{V}/2$, and the perturbation potential is accordingly $V_1 = V'\sqrt{V}/2$ (Ref. 37).

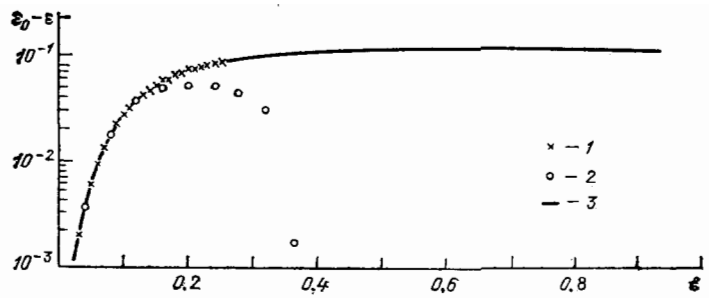

FIG. 2. Shift of the ground state energy ($\varepsilon_0 = -1/2$) as a function of the electric field. 1—Calculations from Ref. 87; 2—Ref. 89; 3—Ref. 17.

the level width at fields $\mathscr{E} \gtrsim 0.15$ a.u. An analytic calculation for the ground state was carried out in Ref. 17 by a nonlinearization method, which was the same as the perturbation theory within the latter's range of applicability and agreed with the results of Ref. 87 outside this range. To illustrate this procedure, we will follow Ref. 17. The various approaches to the Stark effect are reviewed in detail by Damburg and Kolosov[90] and also in a recent paper by Korsch and Mohlenkamp.[103]

The Schrödinger equation for a hydrogen atom in a static electric field is

$$\left(\frac{1}{2}\Delta+\varepsilon+\frac{1}{r}-\mathscr{E}z\right)\psi=0, \tag{4.16}$$

where ε is the level energy, and $\mathscr{E}$ is the electric field, in atomic units. Transforming to the parabolic coordinates $\xi = r+z$, $\eta = r-z$, and introducing $\psi = F(\xi)G(\eta) \times (\xi\eta)^{-1/2}$, for the ground state,[24] we find the following system of equations (see Ref. 11, for example):

$$\xi F'' + \left(\frac{1}{4\xi}+\frac{1}{2}\varepsilon\xi-\frac{1}{4}\mathscr{E}\xi^2+\alpha\right)F=0, \tag{4.17}$$

$$\eta G'' + \left(\frac{1}{4\eta}+\frac{1}{2}\varepsilon\xi+\frac{1}{4}\mathscr{E}\xi^2+\beta\right)G=0, \tag{4.17'}$$

where the separation constants α and β are related by the condition

$$\alpha+\beta=1. \tag{4.18}$$

The quantities G and β are the analytic continuations of F and α, respectively, along the parameter $\mathscr{E}$:

$$G(\mathscr{E}) = F(-\mathscr{E}), \quad \beta(\mathscr{E}) = \alpha(-\mathscr{E}). \tag{4.19}$$

An important point is a transformation from Eq. (4.17) to a Riccati equation through the substitution $f = F'/F$ [cf. (2.4) and (2.5)]:

$$f'+f^2+\frac{1}{4\xi^2}+\frac{\varepsilon}{2}-\frac{\mathscr{E}\xi}{4}+\frac{\alpha}{\xi}=0. \tag{4.20}$$

We will construct a perturbation theory for this equation. As a zeroth order approximation we choose a function which correctly describes solution (4.20) in the limits $\xi\to\infty$ and $\xi\to 0$:

$$f_0=\frac{1}{2\xi}-\frac{1}{2}\sqrt{1+\mathscr{E}\xi}. \tag{4.21}$$

We construct a perturbation-theory series in the deviation from f_0:

$$f(\xi)-f_0(\xi)=\sum_{n=1}^{\infty}f_n(\xi), \quad \alpha=\sum_{n=1}^{\infty}\alpha_n, \quad \varepsilon=\sum_{n=1}^{\infty}\varepsilon_n. \tag{4.22}$$

The quantities $f_n(\xi)$, α_n, and ε_n are determined in each successive order by means of a system of recurrence relations [cf. (2.11)],

$$f_n'+2f_nf_0=\varkappa_n-\frac{\alpha_n}{\xi}-\varphi_n(\xi), \tag{4.23}$$

where $\varkappa_n = -(2\varepsilon_n+\delta_{n1})/4$ and $\varphi_1 = -\frac{\sqrt{1+\mathscr{E}\xi}}{2\xi} - \frac{\mathscr{E}}{4\sqrt{1+\mathscr{E}\xi}}$. Here φ_1 serves as a perturbation potential; at $n>1$, we have $\varphi_n = \Sigma_{i=1}^{n-1} f_i(\xi) f_{n-i}(\xi)$.

A solution of Eq. (4.23) which decays as $\xi\to\infty$ is

$$f_n=-\frac{1}{\xi}e^{K(\xi)}\int_{\xi}^{\infty}dt\,te^{-K(t)}\left(\varkappa_n-\varphi_n-\frac{\alpha_n}{t}\right), \tag{4.24}$$

where $K(t)=\left(\frac{2}{3\mathscr{E}}\right)(1+\mathscr{E}t)^{3/2}$. From the condition $\xi f(\xi) \to 0$ as $\xi\to 0$ we find

$$\alpha_n = \langle t(\varkappa_n-\varphi_n)\rangle, \tag{4.25}$$

where

$$\langle\varphi\rangle=\int_0^{\infty}dte^{-K(t)}\varphi(t)\left(\int_0^{\infty}dte^{-K(t)}\right)^{-1}.$$

Using conditions (4.18) and (4.19), we can expand the energy eigenvalue:

$$\varkappa_n=\frac{\langle t\varphi_n\rangle+\overline{\langle t\varphi_n\rangle}+\delta_{n1}}{\langle t\rangle+\overline{\langle t\rangle}}, \tag{4.26}$$

where δ_{n1} is the Kronecker delta, and the superior bar means the analytic continuation from $\mathscr{E}$ to $-\mathscr{E}$.

The quantities $\varkappa_n$ in (4.3) are complex and determine both the shift and width of the hydrogen ground level. A reexpansion of $\Sigma\varkappa_n$ is powers of $\mathscr{E}$ reproduces the series of the ordinary perturbation theory. The imaginary part of $\varkappa_1$ is exponentially small in the limit $\mathscr{E}\to 0$ and differs from the semiclassical expression[91] only in the coefficient of the exponential function. In strong fields we find from (4.26)

$$\varkappa_n = c_n e^{-i\pi/3}\mathscr{E}^{2/3}[1+O(\mathscr{E}^{-1/3})], \tag{4.27}$$

where $c_1 = -(1/2)(3/2)^{2/3}/\Gamma(4/3)$ and $c_2 \approx 0.2c_1$. If the series Σc_n converges, then the result in (4.27) contradicts Ref.

[24]This transformation is required to reduce the problem to a "nearly" one-dimensional problem, for which a perturbation theory can be realized in quadratures (Subsection 2c).

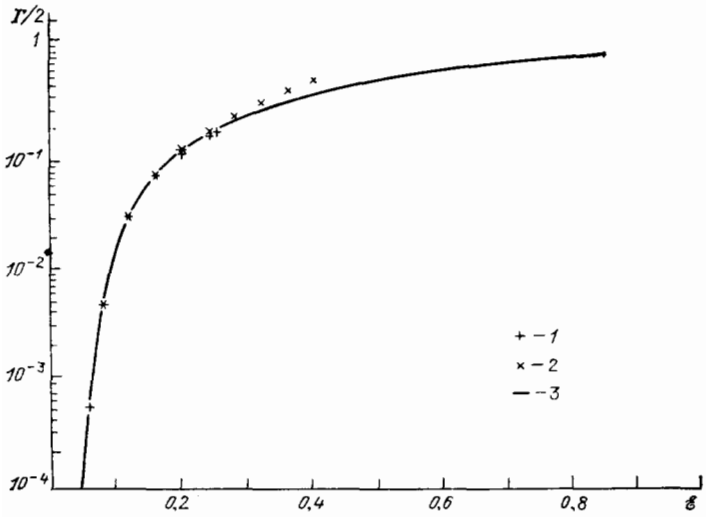

FIG. 3. Width of the ground state as a function of the electric field. 1—Calculations from Ref. 87; 2—Ref. 89; 3—Ref. 17.

85, where $\varkappa \sim \mathscr{E}^{2/3}\ln\mathscr{E}$ was found. It can be shown that our procedure converges in weak fields, and it appears likely that it also converges in strong fields.

We have calculated the energy shift and width of the ground level of hydrogen from the first two orders of this perturbation theory; the results are shown in Figs. 2 and 3. Figure 4 shows the ratio of the second-order contribution to the first-order contribution for the real and imaginary parts of the energy. We see that the second-order contribution is small in comparison with the first-order contribution everywhere, demonstrating the numerical accuracy of the method. These ratios increase in strong fields $\mathscr{E}$, but expression (4.27) shows that they do not exceed 0.2 in the limit $\mathscr{E}\to\infty$.

3) The hydrogen atom in an arbitrary static magnetic field (the Zeeman effect)

We discussed the case of weak magnetic fields in Subsection 3b2 and showed that the range of applicability of the ordinary perturbation theory describing the behavior of hydrogen in a weak field depends strongly on the degree of excitation of the atom. In the present section we will demonstrate that our approach can be used to study this overall problem in a field of arbitrary strength. We will actually restrict the discussion to a "correct" variational calculation with a trial wave function which is reasonable in the spirit of Dyson's argument. We will discuss only the states in (3.38).

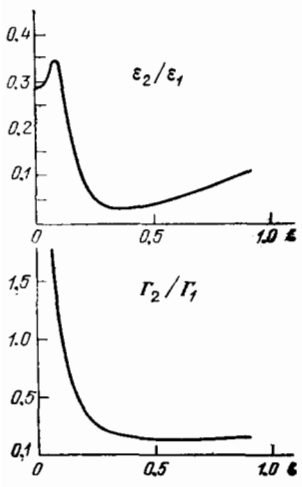

FIG. 4. Ratio of the second-order contribution to the first-order contribution to the level shift and the level width as functions of the electric field.

A zeroth order approximation wave function which is reasonable for arbitrary fields should thus correspond to a potential which has a Coulomb behavior near the origin and which reproduces the potential of a two-dimensional harmonic oscillator at long range. The simplest wave function which satisfies the requirements and which describes states (3.38) is[18]

$$\psi_0 = r^{|}Y_{|}^{m}(\theta,\ \varphi)\exp\left[-\frac{\alpha r}{N}-\frac{\mathscr{H}}{4}(x^2+y^2)\right], \tag{4.28}$$

The corresponding potential is

$$V_0 = -\frac{2\alpha}{r}+\frac{\mathscr{H}^2}{4}(x^2+y^2)+\frac{\alpha\mathscr{H}}{N}\,\frac{x^2+y^2}{r}, \tag{4.29}$$

and the energy is

$$E_0 = -\frac{\alpha^2}{N^2}+\mathscr{H}\,(|m|+m+1), \tag{4.30}$$

where the parameter α will be set equal to unity. We immediately see that his choice of a wave function is a good one: The deviation of V_0 from the actual potential is small not only in the asymptotic regions but also at intermediate values of r, and the magnitude of the deviation falls off with increasing index of the state. Furthermore, the energy E_0 in (4.30) reduces to the energy for a Coulomb spectrum in weak fields, while in strong fields it converts into the Landau formula describing the spectrum of an electron moving in a static magnetic field.[11]

We now develop a perturbation theory in the deviation of potential (4.29) from the original potential. The perturbation potential is

$$V_1 = V - V_0 = -\alpha\mathscr{H}r\sin^2\theta\cdot N^{-1}. \tag{4.31}$$

From the standpoint of Dyson's argument this is a converg-

TABLE III. Energies (in atomic units) of the 1s and $2p_{+1}$ levels as functions of the magnetic field.

$\mathscr{H}$, a.u.	1s					$2p_{+1}$		
	Brandi [94]	Kaschiev [93]	Galindo [64]	Expression (4.32) with $\alpha=1$	(4.28) with minims.	Praddaude [95]	Galindo [64]	(4.32) with $\alpha=1$
0				−1	−1			−0,25
0.1	−1	−0,999957	−0,99505	−0,9916	−0,9932	−0,10169	−0,10039	−0,08971
1	−1	−0,66228	−0,66331	−0,6056	−0,6201	2,08682	2,37576	2,1402
5		2,2396	2,21382	2,392	2,387	13.28*	14.3397	13,453
20	15,68	15,59		15.95	15,79			57,586
100	92,74	92.5223	92,4045	93,65	92,20	294,7*	299.33	296,20

Asterisk denotes results obtained by Larsen.[96]

ing perturbation theory; the convergence accelerates with increasing principal quantum number. The first correction to the energy, E_1, can be reduced to the following form[18]:

$$E_1 = -\mathscr{H}(k+1)(N-k) \times \frac{\int_0^\infty d\eta \frac{\eta^N e^{-\eta}}{\left(1+\frac{\mathscr{H}N^2}{2}\eta\right)^{N+1}}\left(\frac{\mathscr{H}N^2k}{2}\eta^2+k\eta-N\right)}{\int_0^\infty d\eta \frac{\eta^N e^{-\eta}}{\left(1+\frac{\mathscr{H}N^2}{2}\eta\right)^{N}}\left(\frac{\mathscr{H}N^2k}{2}\eta^2+k\eta-(N-k)\right)}. \quad (4.32)$$

We recall that N is the main quantum number, and

$$k=\begin{cases} 0, & |m|=l, \\ 1, & |m|=l-1. \end{cases}$$

The expression for (E_0+E_1) embodies many characteristic properties of the actual energy of the level: In weak fields $\mathscr{H}$ it gives a correct description of the linear Zeeman effect, although the coefficient of $\mathscr{H}^2$ differs from the actual coefficient by a factor of two. In the limit $\mathscr{H}\to\infty$, in which the Coulomb part of the potential is unimportant, it gives a correct description of the spectrum of an electron in a static magnetic field, adding to it some corrections logarithmic in the field. In the case $\mathscr{H}^2=0$, there is a singularity which leads to a divergence of the perturbation theory series in the field. As in the case of an anharmonic oscillator, there is a cut in the complex $\mathscr{H}^2$ plane, running from $\mathscr{H}^2=0$ to $-\infty$. Avron[62] has calculated the discontinuity at this cut in the limit $\mathscr{H}^2\to -0$ and has found it to be exponenetially small. Expression (4.32) also contains a cut $[0,-\infty)$; the discontinuity is exponentially small in the limit $\mathscr{H}^2\to -0$, although the coefficient of the exponential function does not agree with that derived by Avron.

In addition to its advantages, the expression for (E_0+E_1) has some disadvantages. Odd powers of $\mathscr{H}$ arise in the expansion of this expression in powers of $\mathscr{H}$, but an *a priori* inspection of the situation indicates that they should not. It can be shown, however, that incorporating the following corrections (E_2,E_3, etc.) successively eliminates these odd powers. In the limit $\mathscr{H}\to\infty$ an asymptotic term $\sim\ln^2\mathscr{H}$ following the leading terms does not appear, and the expansion begins with the term $\sim\ln\mathscr{H}$. This defect is also eliminated by the higher-order corrections. Nevertheless, expressions (4.30) and (4.32) give a highly accurate description of the situation at any value of $\mathscr{H}$. Table III shows results calculated from these expressions for states with $N=1$ and 2 and with nonnegative angular momentum projections. In strong fields the field dependence of the energy becomes nearly linear, but none of the states considered goes into the continuum; i.e., their energies remain below the energy of a free electron in a magnetic field. Table III compares the results with the calculations by other investigators; there is a fair agreement. We will discuss the accuracy of our calculations below; at this point they may be regarded as variational calculations with trial wave function (4.28).

How are the Coulomb states (weak fields) related to the states to a two-dimensional harmonic oscillator (strong fields, the Landau regime)? Expressions (4.30) and (4.32) immediately tell us which states correspond to which. There is a complete agreement with the correspondence scheme given in the review by Garstang[60] for the first few excited states. Our analysis yields some more general results. An obvious result is that all the low-lying components of multiplets with

TABLE IV. Crossings of various levels found from expression (4.32)

	$3d_{-2}$	$3d_{-1}$	$4f_{-3}$	$4f_{-2}$	$5g_{-4}$	$5g_{-3}$
$2p_{+1}$	0,062	0,090	0,087	0,119	0,105	0,137
$3d_{+1}$			0.015	0,021	0,023	0,030
$3d_{+2}$			0.011	0,013	0,016	0,019
$4f_{+2}$					0,0042	0,005
$4f_{+3}$					0,0035	0,0040

$m = -l, -l+1$ go into the zeroth Landau band, while the upper components go into various Landau bands. Accordingly, all possible level crossings occur. In particular, all the levels with $m = -l, -l+1$ at $l \geqslant 2$ ($N \geqslant 3$) cross the $3p_{+1}$ level; at $l \geqslant 3$ ($N \geqslant 4$) they cross the $3d_{+2}$ and $3d_{+1}$ levels; at $l \geqslant 4$ ($N \geqslant 5$) they cross the $4f_{+3}$ and $4f_{+2}$ levels; etc. There is a true crossing of levels, since the levels have different symmetries by virtue of the conservation of magnetic quantum number. Table IV shows the positions of the first few crossings. The crossing of the $2p_{+1}$ and $3d_{-2}$ levels occurs in fields on the order of 10^8 G.

Since the projection of the angular momentum is an exact integral of the problem, the upper and lower components of the multiplets are related by the obvious condition

$$\Delta E_l^m \equiv E_l^m - E_l^{-m} = 2\mathscr{H}m, \tag{4.33}$$

which holds for all fields. Condition (4.33) yields another exact relation:

$$\hat{\Delta} E_l^m = \Delta E_l^m - \Delta E_l^{m-1} = \delta^+ E_l + \delta^- E_l = 2\mathscr{H}, \tag{4.34}$$

where $\delta + E_l = E_l^m - E_l^{m-1}$ is the distance between the upper components, and $\delta - E_l = E_l^{-m+1}$ is the distance between the lower components, for states (3.38). The right side of (4.34) does not depend on the principal quantum number N. The quantities $\delta^{\pm} E_l$ may prove useful for identifying spectral lines. It is easy to see from (4.30) and (4.32) how these quantities depend on the field: While they are essentially equal in weak fields, $\delta^+ E_l = \delta^- E_l$, since the splitting is proportional to the field, a deviation from this equality sets in with increasing $\mathscr{H}$: $\delta^+ E_l > \delta^- E_l$. At $\mathscr{H} \gg 1$ we find $\delta^+ E_l = 2\mathscr{H} - O(\ln \mathscr{H})$. This effect has been observed experimentally,[92] particularly clearly for states with $N = 2$. The situation is shown schematically in Fig. 5.

The situation at large values of the principal quantum number is quite interesting. A study of expressions (4.30) and (4.32) yields the following expression for the extreme components at $\mathscr{H} \gg 1$:

$$E_N = \mathscr{H}(|m| + m + 1) - \frac{2^{5/4}}{e} N^{-7/4} \mathscr{H}^{-3/4} + \ldots, \tag{4.35}$$

where $e = 2.718\ldots$. At large values of N the Landau regime thus sets in quite rapidly. Since the correction to the Landua formula is negative, the levels never go into the continuum. The levels approach the continuum boundary in a power-law fashion, more rapidly, the stronger the field. We wish to emphasize that taking the limit of strong fields does not commute with taking the limit of high excitations.

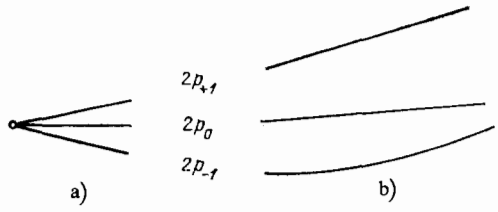

FIG. 5. Distance between the upper and lower components of the multiplet in weak fields (a) and strong fields (b).

How accurate are these results? We have used the first two terms of the perturbation series everywhere above; this approach is equivalent to carrying out a variational calculation (as discussed above). Since Dyson's argument gives us faith in the convergence of the perturbation series, the calculation of E_2 not only gives us a term in this series but also allows us to evaluate the accuracy of the variational calculation with trial function (4.28). There is an important circumstance to be noted here: Since the node surfaces do not become deformed, the second correction to the energy is always negative [see (2.32)], so that our results on the state energies $(E_0 + E_1)$ are upper limts. To calculate E_2 we need to know the correction ϕ_1 [see (2.29)]; i.e., we need to solve the electrostatic equation (2.24). To do this we use the following iterative procedure: We find the asymptotic expressions for the function ϕ_1,

$$\begin{aligned} &\phi_1 \xrightarrow[r\to 0]{} \frac{E_1 r^2}{2(2N+1)}, \\ &\phi_1 \xrightarrow[r\to\infty]{} Nr(1-|\mu|), \end{aligned} \tag{4.36}$$

and we construct the interpolation function

$$\phi_1 = \frac{E_1 r^2}{2(2N+1)} \left[1 + \frac{E_1 r}{2(2N+1)N(1-|\mu|)}\right]^{-1}. \tag{4.37}$$

Adopting (4.37) as a zeroth approximation, we substituted it into (2.24). After one iteration we see that it is small in comparison with (4.37). Substituting (4.37) into expression (2.29) for E_2, we find an estimate of E_2. Carrying out this procedure for $\mathscr{H} = 1$, we find that the relative accuracy of our calculations is of the order of 10^{-N}.

A detailed variational calculation can be carried out by using (4.28) as a trial function and leaving α as an adjustable parameter. Table III shows the results of a minimization for the ground-state energy. We note that α should be understood as a parameter which is a measure of the screening of the charge of the proton. The screening increases with increasing field.

5. QUANTUM-MECHANICAL ANALOG OF THE LEADING LOG APPROXIMATION

In this section we would like to propose a new method of continuing the results which hold in the weak-coupling region into the region of strong coupling and large perturbations. This method is radically different from the Pade, Pade-Borel, and other methods which are ordinarily used in these situations; it is essentially a close analog of the leading log approximation of quantum field theory. Accordingly, before we construct and discuss this approximation, we will briefly review the leading log approximation itself.

The leading log approximation is one of the methods most commonly used for studying renormalizable models in quantum field theory. It can be summarized as follows: The contribution of any n-loop perturbation-theory diagram is represented by a polynomial in the logarithm of the momentum plus power-law terms. The leading log approximation is the sum of the highest powers of the polynomials. The range of applicability of the leading log approximation is estimated by requiring that the term in the polynomial with the next-

TABLE V. Calculated values of the first four levels for an x^4 potential with the analog of the leading log approximation used as the zeroth order approximation [see (4.40)]

Approximation		Level: Zeroth	First	Second	Third
0	$a_{\min}$	1,003960	1,431950	1,800056	2,1223
	$f_0(x)$	1	x	$2{,}997103\cdot x^2-1$	$x(1{,}166267\cdot x^2-1)$
	E_0	0	0	0	0
1	$f_1(x)$	0	0	0,007604	$0{,}004420\,x$
	E_1	1,0606687	3,8002786	7,4567270	11,6463337
2	$-E_2$	0,0003010	0,0006056	0,0010410	0,0016802
	E_1+E_2	1,0603677	3,7996729	7,4556860	11,6446535
E_{exact}		1,06036211	3,79967315	7,45569862	11,6447475

to-highest power be small in comparison with the term with the highest power. In all the calculations carried out to date the sums over the leading powers of the logarithm have a finite convergence radius,[25] although we know quite well the perturbation theory series in the same theories diverge, having a zero convergence radius. The leading log approximation thus singles out a converging subseries from a diverging series with factorially increasing coefficients. It can be suggested that the divergence of a perturbation theory series is manifested in a divergence of the sums over the lower powers of the logarithm. Here, however, we have the question of whether it is legitimate to change the order of the summation and just how valid the approximation itself is. At present we do not have ironclad answers to these questions.

This has been the situation regarding the leading log approximation in quantum field theory. In quantum mechanics we do not have a direct physical analog of the leading log approximation of quantum field theory, but it is possible to construct an approximation which is mathematically similar to it. Since quantum mechanics is much simpler than quantum field theory, this approximation can be studied in detail.

The approximation is based on the phenomenon of the algebraization of the procedure for constructing a perturbation theory in the weak-coupling region (Theorems 1 and 2 in Section 3). We have already seen that the corrections $\phi_n(x)$ are polynomials, and there is no particular difficulty in finding the coefficients of the higher-order powers for essentially arbitrary perturbations. The perturbation theory series which incorporate only the highest powers turn out to converge. The idea of the approach is to use these sums as zeroth order approximations for a perturbation theory. All this will be explained on a simple example.

We consider a one-dimensional anharmonic oscillator, (4.9), with $n = 2$. It was shown in Subsection 3a2 that the correction $\phi_n(x)$ is a polynomial of degree $2n + 2$ [see (3.22)], which we write in the form

$$\phi_n(x) = x^{2n+2} \sum_{i=0}^{n} (a_{n-i}^{(n)} x^{2i}), \tag{4.38}$$

[25] As do the sums over some of the powers of the logarithm following the leading powers.

where the coefficients $a_n^{(n)}, a_{n-1}^{(n)}$, and $a_{n-2}^{(n)}$ are known [see (3.23)]. It is easy to find a sum of the perturbation theory series over the higher powers of the polynomials:

$$\hat{\phi}(x) = \sum_{n=0}^{\infty} g^n a_n^{(n)} x^{2n+2} = \frac{1}{3g}[(m^2 + gx^2)^{3/2} - m^3]. \tag{4.39}$$

This series converges if $|gx^2| < m^2$, and the approximation of the higher powers of the polynomials is meaningful if $x \gtrsim 1$. Consequently, if we understand (4.39) as the analytic continuation along x of the sum of a series of a perturbation theory in the higher powers into the region $|gx^2| \geqslant m^2$, then $\hat{\phi}(x)$ should be a correct approximation of $\phi(x)$ in this region. This is what we actually find. Furthermore, $\hat{\phi}(x)$ reproduces the correct asymptotic behavior in the limit $x \to 0$.

As a zeroth order approximation wave function for the k th level we thus use

$$\psi_0^{(k)} = P_k(x) \exp[-\hat{\phi}(x)], \tag{4.40}$$

where $P_k(x)$ is a polynomial of degree k, which has k real roots. The potential corresponding to function (4.40) is

$$V_0^{(k)} = m^2x^2 + gx^4 - g_0(x) - \frac{gx^2}{g_0(x)} + \frac{P_k''(x) - 2xg_0(x)P_k'(x)}{P_k(x)}, \tag{4.41}$$

where $g_0(x) = (m^2 + gx^2)^{1/2}$. Potential (4.41) obviously gives a correct reproduction of the asymptotic behavior of the original potential as $|x| \to \infty$. The perturbation potential is

$$V_1^{(k)} = (1 - m^2)x^2 + g_0(x) + \frac{gx^2}{g_0(x)} - \frac{P_k''(x) - 2xg_0(x)P_k'(x)}{P_k(x)}. \tag{4.42}$$

At first glance, the perturbation potential $V_1^{(k)}$ looks terrible: It contains simple poles. However, precisely the same poles, with the same residues, are incorporated in $V_0^{(k)}$. They accordingly cancel out. Nowhere in the construction of the perturbation theory do divergent integrals arise. The potential $V_0^{(k)}(x)$ reproduces the behavior of the original potential $V(x)$ in the limit $|x| \to \infty$. Consequently, the perturbation theory series converges from the standpoint of Dyson's argument.

We will refer to this procedure of using construction (4.39) and developing a perturbation theory in the potential

TABLE VI. Energy of the second level of an anharmonic oscillator, with the analog of the leading log approximation used as a zeroth order approximation [see (4.40)]. The normalization is as in Table II; x_0 and $\Delta_1 x_0$ are the position and deformation of the zero of the wave function.

g	$a_{\min}$	x_0	$-\Delta_1 x_0$	E_1	$-E_2$	E_1+E_2	from Ref. 81
0,1	1,4817	0,6306	0,0010	3,1386452	0,0000269	3,1386183	3,13862
1	3,6945	0,4902	0,0013	5,179652	0,000452	5,179200	5,17929
10	14,009	0,3469	0,0014	10,34831	0,00175	10,34656	10,3471
100	62,200	0,2383	0,0009	21,90991	0,00371	21,90619	21,9069
1000	286,555	0,1626	0,0006	47,02409	0,00745	47,01663	47,0173

of the zeroth order approximation, (4.41), everywhere as the "analog" of the leading log approximation.

We have calculated the energies of the first four levels of the oscillator (4.9); Table V shows the results calculated for the potential $V(x)=x^4$ [an oscillator in the region of extremely strong coupling; see (4.10) and the discussion in Subsection 4c1]. We see that E_1 (from the variational calculation) gives us an absolute accuracy of $\sim 10^{-3}$–10^{-4}, while the incorporation of E_2 (the correction to the variational calculation) leads to an absolute accuracy of $\sim 10^{-5}$–10^{-6}. An estimate of the accuracy in the spirit of Theorem 3 shows that incorporating E_3 improves the absolute accuracy to $\sim 10^{-7}$–10^{-8}. We wish to point out that the absolute accuracy of the calculation depends only weakly on the level index. Tables II and VI show results calculated for the zeroth and second levels for various values of the parameter g by the first two approximations. The results agree with the results calculated in Ref. 81. The absolute accuracy of the calculations is essentially independent of g, oscillating around 10^{-6}–10^{-7}. Table II can be used to compare the results calculated for the ground state in this approximation with the results calculated in the approximation based on the use of wave function (4.11). The analog of the leading log approximation is obviously preferable.

We conclude this section with a few words about the analog of the leading approximation in the case of a multidimensional, spherically asymmetric problem. Here we immediately run into some difficulties, which we will demonstrate using the example of the Zeeman effect. It has been shown earlier that the correction ϕ_n is of the form in (3.41). We use (3.43) and write (3.41) in the form

$$\phi_n = \sum_{j=2}^{2n+1} r^j \sum_{i=0}^{n} a_{n,i,j} \sin^{2i}\theta. \tag{4.43}$$

To construct the analog of the leading log approximation we must calculate the double sum

$$\hat{\phi} = \sum_{n=0}^{\infty} r^{2n+1} \mathscr{H}^{2n} \sum_{i=0}^{\infty} a_{n,i,2n+1} \sin^{2i}\theta, \tag{4.44}$$

and we immediately encounter a problem. On the one hand, it is a straightforward matter to find the first few ordinary sums, e.g.,

$$\hat{\phi}_0 = \sum_{n=0}^{\infty} r^{2n+1} \mathscr{H}^{2n} a_{n,n,2n+1} \sin^{2n}\theta = \frac{2r}{N}\sqrt{1+\frac{\mathscr{H}^2 r^2}{12N^2}\sin^2\theta},$$
$$\hat{\phi}_1 = \sum_{n=0}^{\infty} r^{2n+1} \mathscr{H}^{2n} a_{n,n-1,2n+1} \sin^{2n-2}\theta = -\frac{\mathscr{H}^4 r^8 \sin^2\theta}{90\hat{\phi}_0^3}, \tag{4.45}$$

but it can be shown rigorously that $\hat{\phi}_{n-1}$ cannot be written in finite form.[26] The function $\hat{\phi}_0$ has the correct behavior at $r\to 0$—the same behavior as that of a Coulomb function. In this limit we can ignore the contributions from $\hat{\phi}_1, \hat{\phi}_2$, etc. In the limit $r\to\infty$ we find $\hat{\phi}_0 \to \mathscr{H}(x^2+y^2)/2\sqrt{3}$, corresponding to a two-dimensional oscillator, but its strength is smaller by a factor of $1/\sqrt{3}$ than that in the original potential. It can be shown that the sums $\hat{\phi}_1$ and $\hat{\phi}_2$ are of the same order of magnitude as $\hat{\phi}_0$ in the limit $r\to\infty$.

The only constructive way out of this situation is to modify $\hat{\phi}_0$ to reconcile it with the oscillator, writing

$$\hat{\phi}_0^{(1)} = \frac{2r}{N}\sqrt{1+\frac{\mathscr{H}^2 r^2}{4N^2}\sin^2\theta} \tag{4.46}$$

or

$$\hat{\phi}_0^{(2)} = \frac{2r}{N}\sqrt{1+\frac{\mathscr{H}^2 r^2}{4N^2}\sin^4\theta}. \tag{4.47}$$

Either version is acceptable. If we carry out a variational calculation with N as an adjustable parameter, the accuracy will be much higher than in a calculation with the function (4.28) (see Table VII).

We can thus draw the following conclusion: When an analog of the leading log approximation can be constructed, the calculations will be quite accurate. If it is a difficult matter to construct an analog of the leading log approximation completely, this approach will suggest an appropriate trial function.

6. CONCLUSION

We have described an unconventional approach to the problem of the eigenvalue spectrum in quantum mechanics, an approach which might be considered a strong-coupling theory. It has many advantages: Its implementation is simple and transparent, it does not require knowledge of the entire eigenvalue spectrum of the unperturbed problem, it reveals the accuracy of variational calculations, and in some cases it leads to an algebraization of the procedure for constructing the perturbation theory. The idea of comparing potentials—the original potential with that corresponding to the zeroth order approximation trial function—instead of comparing wave functions proves extremely useful. We thus acquire a means for judging the reasonableness of the zeroth

[26] The procedure is as follows: Working from the recurrence relations, we write an equation for ϕ_{n-1}, which turns out to be a Riccati equation which does not fall in the class of equations whose solutions can be expressed in finite form.

TABLE VII. Energy of the $1s$ state for $\mathscr{H} = 1$ according to calculations from (4.28) and (4.46) without and with minimization with respect to α.

Eq. (4.28)		(4.46)		Acc. Ref. 93
$\alpha = 1$	$\alpha = \alpha_{\min} = 0{,}879$	$\alpha = 1$	$\alpha = \alpha_{\min} = 1{,}1359$	
$-0{,}6056$	$-0{,}6201$	$-0{,}6352$	$-0{,}6543$	$-0{,}6623$

order approximation. The many examples above have demonstrated the power of this approach, for all its simplicity, and in essentially no case have we found negative results. Two-center problems have also come under study recently: the hydrogen molecular ion and the hydrogen molecule in a static magnetic field.[105] The simplest trial functions, which are obvious generalizations of (4.28), have led to a unified description of the entire range of fields which occur in nature, up to 10^{12}–10^{13} G. The results are in excellent agreement with earlier calculations (for the H_2^+ ion), carried out by far more complicated and refined methods, while for the H_2 molecule the results are the first available at fields above 10^9 G.

I believe that this approach has an important feature. It could be applied to the more complicated many-body problems, and an attempt might be made to take a look at field theory from the stand-point of quantum mechanics. In particular, it would be interesting to analyze the three-body problem in terms of perturbation theory by this approach. Relativistic generalizations have now been proposed to both the case of the Klein-Gordon equation and the case of the Dirac equation.[97,98] It would clearly be interesting to look at scattering problems by this formalism. We should also emphasize the attempts made in Refs. 106 and 107 to develop a similar approach to problems in field theory, where the original action S is broken up into a nontrivial sum $S_0 + S_1$, and a perturbation theory in S_1 is developed. An important condition on the partitioning here is that it be reasonable from the standpoint of Dyson's argument.

There are, of course, many difficulties. In practice, for the Laplacian in a curved, conformally planar space which even comes close to being one of the nontrivial Green's functions we do not know a single Green's function which we need for a nontrivial realization of this procedure in the multidimensional case. For complicated problems, the procedures for constructing the zeroth order approximation wave functions are far from simple, especially in multiple dimensions. There are also some purely mathematical problems. In particular, it is totally unclear how to construct zeroth order approximations for the excited states in multidimensional problems and how to go beyond the limits of variational calculations, since the state classification problem has not been solved. In this connection it would be interesting to study at least a very simple problem in which a level quasicrossing occurs, e.g., the two-dimensional anharmonic oscillator.

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APPENDIX
Electrostatics with a Gaussian dielectric permittivity

To solve the electrostatic problem with a Gaussian dielectric permittivity

$$\varepsilon \equiv \psi_0^2 = a \exp(-\alpha \mathbf{x}^2), \tag{A.1}$$

we use Eq. (2.12), in which we immediately incorporate the potential condition (2.6). Recalling that $\mathbf{y}_0 = 2\alpha\mathbf{x}$, we find that the original equation transforms to

$$\Delta\phi_n - 2\alpha\mathbf{x}\nabla\phi_n = q_n(x), \tag{A.2}$$

where $q_n(x)$ is some function which is related in an obvious way to the charge density, and $\phi_n(x)$ is a polynomial ($\mathbf{y}_n = \nabla\phi_n$; for convenience, we will omit the index n below). There are various ways to solve this equation, but the simplest and most elegant is as follows: We adopt the similarity transformation $x \to xt$, and we note that the operator

$$\mathbf{x}\nabla_x\phi(xt) = t\frac{\partial}{\partial t}\phi(xt) \tag{A.3}$$

is homogeneous. Equation (A.2) then becomes

$$\frac{1}{t^2}\Delta_x\phi(x, t) - 2\alpha t\frac{\partial\phi(x, t)}{\partial t} = q(x, t); \tag{A.4}$$

we seek a solution of this equation which has the form of a function of the product xt. To find this solution, we use Fourier transforms in the variable x. As a result we find the equation

$$-\frac{p^2}{t^2}\tilde{\phi} - 2\alpha t\frac{\partial\tilde{\phi}}{\partial t} = \tilde{q}, \tag{A.5}$$

where p is the variable which is the conjugate of x, and $\tilde{\phi}$ and $\tilde{q}$ are the Fourier transforms of the function being sought and of the right side of Eq. (A.4), respectively. After some simple and not very lengthy calculations, we find that the solution of Eq. (A.2) is

$$\phi(x) = \int dx' q(x') \int_0^\infty dt \frac{(t+\alpha)^{(k-2)/2}}{4\pi^{k/2}t} \times \exp[-(\sqrt{t}\mathbf{x} - \sqrt{t+\alpha}\mathbf{x}')^2]. \tag{A.6}$$

The electric field corresponding to this potential is

$$\mathbf{y} = \int dx' q(x') \int_0^\infty dt \frac{(t+\alpha)^{(k-2)/2}}{2\pi^{k/2}t^{1/2}} \exp[-(\sqrt{t}\mathbf{x} - \sqrt{t+\alpha}\mathbf{x}')^2] \times (\sqrt{t}\mathbf{x} - \sqrt{t+\alpha}\mathbf{x}'), \tag{A.7}$$

and gives us the expression which we are seeking, (2.20).

The equations derived here are interesting from several

points of view. First, they give us a solution of a nontrivial electrostatic problem. Second, from the standpoint of gravitation, this is a conformally planar world which is closed, since the integral of the metric tensor converges. Third, the equations with the dielectric permittivity (A.1) may be useful for constructing a perturbation theory for quasistationary states in which α plays the role of a parameter for the regularization of the resulting integrals (see the paper by Zel'dovich[99] and the monograph by Baz' *et al.*,[24] §6 in Ch. 7). Finally these equations are of course important for implementing the approach described in the present review.

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