Algebraization of the perturbation theory in quantum chromodynamics

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It is shown that if an unperturbed problem is a multidimensional harmonic oscillator or a hydrogen-like system and the perturbation is a polynomial, then the formulation of perturbation theory must be a purely algebraic problem. A hydrogen-like system in an electric field $\mathscr{E}$ parallel to the magnetic field $\mathscr{H}$ is analyzed. The correction to the ground-state energy of order $\mathscr{E}^2$ and $\mathscr{H}^2$ is calculated. Some structures of the arbitrary "correction to the wave function" are determined in the explicit form.

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1. The Rayleigh-Schrödinger perturbation theory (PT) is one of the more widely used methods of solving problems associated with the spectrum of bound states. A serious deficiency of this method, however, is that it requires knowledge of the total spectrum of the unperturbed problem and it deals with problems such as the calculation of the matrix elements and summation of the multiple series, which are often technically difficult to overcome. We shall show in this paper that in the case of frequently occurring problems such as the polynomial perturbation of the harmonic oscillator or of the Coulomb system, the formulation of PT is a *purely algebraic problem* which reduces to the solution of recursion formulas that allow a simple formalization on a computer.

2. A method of dealing with the spectrum in quantum mechanics, which is based on the "nonlinearization procedure" (see also Refs. 2 and 3), was formulated in Ref. 1. Its main advantage is that the total spectrum of the unperturbed problem does not have to be known. We shall briefly review the salient features of this method. We shall use the logarithmic derivative $\mathbf{y} \equiv - \nabla \phi = - \nabla \ln \psi$ of the wave function ψ instead of the wave function itself. The Schrödinger equation in this case has the form[1,2]

$$\operatorname{div} \mathbf{y} - \mathbf{y}^2 = E - V. \tag{1}$$

Suppose that $V = V_0 + \lambda V_1$. We shall develop a PT for (1) according to the parameter λ

$$\mathbf{y} = \Sigma \lambda^n \mathbf{y}_n, \qquad E = \Sigma \lambda^n E_n. \tag{2}$$

We can determine the correction from the following equation[1,2] in this case:

$$\Delta \phi_n - 2 \mathbf{y}_0 \nabla \phi_n = E_n - Q_n, \qquad n \geqslant 1, \tag{3}$$

where $y_0 = - \nabla \ln \psi_0$ and E_n and Q_n are determined from the preceding iterations

$$Q_1 = V_1, \quad Q_n = - \sum_{i=1}^{n-1} y_i \, y_{n-i}, \quad E_n = \int Q_n \, \psi_0^2 \, dx / \int \psi_0^2 \, dx. \quad (4)$$

Notice that Q_n can have the meaning of a perturbation potential. The formula for E_n in Eq. (4) must be modified slightly for the excited states.[3] However, since this formula will not be used here, we shall not discuss it.

3. Our goal in this paper is to formulate a PT for the unperturbed potential that corresponds to the harmonic oscillator

$$V_0 = \sum_{i=1}^{n} a_i x_i^2, \quad a_i > 0 \quad (5)$$

and to the hydrogen-like system

$$V_0 = - \frac{2a}{r}, \quad a > 0, \quad (6)$$

but the perturbation is a polynomial

$$V_1 = \sum_{i_1 i_2 \cdots i_n}^{i_{1\,max} \cdots i_{n\,max}} a_{i_1 i_2 \cdots i_n} x_1^{i_1} x_2^{i_2} \cdots x_n^{i_n} \quad (7)$$

or [for the potential (6)]

$$V_1 = \sum_{l,m}^{l_{max}} R_{lm}(r) \, Y_l^m (\mu, \phi), \quad R_{lm} = \sum_{k=1}^{k_{max}} a_k r^k \quad (8)$$

where $r = (x_1^2 + x_2^2 + x_3^2)^{\frac{1}{2}}$, $\mu = \cos \Theta$, and Y_l^m are the spherical harmonics. We shall now formulate the main propositions of our study.

Proposition 1. The corrections to ϕ_n are polynomials in the PT for the ground state of the potential (5) when the perturbation is a polynomial. If, moreover, the maximum power of the x_k variable is equal to I_k, then the maximum power x_k in the correction to ϕ_n must be in the range of $nI_k - 2n + 2$ to nI_k.

Proposition 2. The correction to ϕ_n has a finite number of harmonics with polynomial coefficients in the PT for the ground state of the potential (6) when the perturbation contains a finite number of harmonics with polynomial coefficients of r.

Both of these propositions, which seem to be rather obvious, can be easily proved inductively. If we assume that ϕ_l are polynomials for $l < n$, then ϕ_n [see Eq. (4)] must also be polynomials. The problem, therefore, reduces to proving whether a polynomial solution of Eq. (3), whose right-hand side is a polynomial, exists. Rather than proving this, we shall mention only that the correction to ϕ_1 in the case of the potential (5), where $y_0 = (a_1 x_1, a_2 x_2, \cdots, a_n x_n)$, contains the same conminations of the $(i_1 i_2 \cdots i_n)$ powers as the V_1 potential, as well as combinations similar to them $(i_1 - 2k_1, i_2 - 2k_2, \cdots, i_n - 2k_n)$, where $k_1, k_2, \cdots k_n$ are positive integers.[1] We can show that such assumptions (with some modifications) are valid for the excited states.

The determination of the corrections to ϕ_n and E_n,[2] therefore, reduces to the

solution of recursion formulas, i.e., it is an algebraic problem. Moreover, we can easily write the explicit solution of these recursion formulas for the coefficients of the leading powers of these polynomials. They can also be solved rather easily on a computer.

4. We shall briefly discuss the obtained results. Proposition 1 seems to be quite reasonable if we recall that the perturbations (7) have a rather limited number of nontrivial matrix elements of the transitions (see, for example, Ref. 4). The sums of the intermediate states in this case are finite and the corrections to the wave function are expressed as a polynomial multiplied by the exponent. This was first systematically investigated by Bender and Wu[5] for a one-dimensional anharmonic oscillator and in collaboration with Banks[6] for a two-dimensional anharmonic oscillator. They have obtained recursion formulas, investigated the properties of polynomials, and determined 75 terms in the PT series for the ground-state energy. The polynomial ϕ_n was also used in the one-dimensional case in other investigations, for example, in Ref. 7 and in the two-dimensional case in Ref. 3.

Proposition 2 is considerably more important. However, the polynomial nature of PT in this case can be almost immediately evident if we assume that the Coulomb system is equivalent to the four-dimensional harmonic oscillator.[8] The polynomial PT has been noted in Ref. 2 in connection with the multipole static perturbation and in Refs. 9 and 10 in the Stark effect and in the Zeeman effect in hydrogen.

5. To demonstrate the possibilities of the method described by us, we shall examine the classical hydrogen-like system (hydrogen-like atom, exciton) in an electric field ξ parallel to the magnetic field $\mathcal{H}$. This problem, which has been analyzed qualitatively[11] but not quantitatively to any extent, has important applications in astrophysics, in semiconductor physics, and in spectroscopy.

We limit ourselves here to the study of the ground state, calculate the term $\sim \xi^2 \mathcal{H}^2$, which is important in weak fields, and describe the general structure of the corrections to ϕ_{kn}. Thus, the $\xi \| \mathcal{H}$ ground-state potential has the form

$$V_1 = \xi z + \mathcal{H}^2 (x^2 + y^2) = -\xi r P_1(\mu) + \mathcal{H}^2 r^2 P_2(\mu) . \tag{9}$$

We shall build the PT for the ξ and $\mathcal{H}$ fields,

$$E = \sum_{k,n} E_{kn} \xi^k \mathcal{H}^{2n}, \qquad \phi = \sum_{k,n} \phi_{kn} \xi^k \mathcal{H}^{2n} \tag{10}$$

where $\phi_0 = ar$, $E_0 = -a^2$; here Eqs. (4) have a slightly modified form. Analysis of Eq. (3) shows that the arbitrary correction of ϕ_{kn} has the structure

$$\phi_{kn} = \sum_{l=0}^{n+[k/2]} R_{k,n,2n+k-2l} P_{2n+k-2l}(\mu) ;$$

$$R_{k,n,2n+k-2l} = \sum_{\substack{m=2n+k-2l \\ m \neq 0}}^{2n+k+1} a_m r^m \tag{11}$$

We emphasize that the polynomial of the leading harmonic P_{2n+k} is a binomial and that the preceding harmonic P_{2n+k-2} is a quadrinomial, etc. An analogous structure was previously observed in the study of the Zeeman effect $(\xi = 0)$.[10] Some coefficients of these polynomials can be easily determined in the explicit form. For example, the polynomial of the leading harmonic is

$$-R_{k,n,2n+k} = \frac{(2n+k)!^2(2n+2k)!\,2^{-2k}}{(4n+2k)!\,(n+k)!\,k!\,n!\,(2n+2k-1)!}\frac{r^{2n+k+1}}{3^n\,a^{2n+2k-1}}$$

$$+\frac{(2n+k)!^2(n+k-1)!}{2(2k+4n)!\,k!\,n!}\left\{1+\frac{(2n+2k)!\,(n+k)2^{-2n-2k+1}}{(n+k)!^2(2n+k)}\right\}$$

$$\times\left(\frac{4}{3}\right)^n\frac{r^{2n+k}}{a^{2n+2k}}. \qquad (12)$$

For $k=0(\xi\equiv0)$ Eq. (12) becomes an equation which was previously obtained in Ref. 10. The E_{kn} corrections are connected with ϕ_{kn}. We write the first terms of the E expansion in the explicit form

$$E = -a^2 - \frac{9}{8a^4}\xi^2 + \frac{2}{a^2}\mathcal{H}^2 - \frac{53}{6a^6}\mathcal{H}^4 - \frac{3555}{512a^{10}}\xi^4 + \frac{317}{48a^8}\xi^2\mathcal{H}^2 + \cdots. \qquad (13)$$

Notice that the coefficients of the fourth-order terms have almost the same values. In principle, the subsequent corrections can be determined without much difficulty. However, because of the asymptotic nature of the series (13), it is not clear whether they should be determined. The excited states can be analyzed in the same manner as in Ref. 10 for $\xi\equiv0$. The results of this analysis will be discussed in another paper.

We showed that the formulation of PT is an algebraic problem in two important special cases. Evidently, this also applies to other cases in which the zeroth approximation is an exactly solvable problem.

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[1] Of course, $i_l - 2k_l \geqslant 0$ in these combinations.
[2] The correction to E_n is expressed in terms of the ϕ_n coefficients of the terms $\sim x_i^2$.

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