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ZEEMAN EFFECT: NEW OUTLOOK ON OLD PERTURBATION THEORY

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A b s t r a c t

The problem of hydrogen atom placed in constant external magnetic field is studied. We investigate the properties of ordinary perturbation theory (in powers of the field) in the framework of a new approach proposed earlier. It is shown that the "wave function corrections" with in this approach are simpler than within ordinary one and contain a finite number of harmonics with polinomial coefficients. Some coefficients of these polinomials are found explicitly.

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The weak field Zeeman effect in simple atoms was one of the first problems studied in quantum mechanics [1]. Nevetheless the problem remains open now and full understanding is still lacking. It worth noting that the Zeeman effect plays a fundamental role in many aspects of astrophysics, solid state and plasma physics [2,3]. Due to the above reasons the interest to the description of this effect has not died up to now (see e.g. [2-8]).

In this Letter I want to look at Zeeman effect in hydrogen from the new point of view following the so called "nonlinearization method" [9,10] (see too [11]). I restrict myself to investigation of the structure of ordinary divergent perturbation theory (PT) (in powers of the field) (see [5,6]). The ground state will be considered in detailed while the excited states will be discussed only in brief. I try to demonstrate the advantages of our method in comparison with the standard one.

For the spinless hydrogen Zeeman Hamiltonian the Schrödinger equation has the form (for the ground state)

$$\Delta \Psi + \left(E + \frac{2\alpha}{r} - \frac{B^2}{8}(x^2+y^2)\right)\Psi = 0 \qquad (1)$$

where B is the strength of the magnetic field and $\vec{B}$ = = (0,0,B). In this paper we will be interested only in PT in powers of B

$$E(B) = \sum_{n=0}^{\infty} E_n \left(\frac{B^2}{8}\right)^n \qquad (2)$$

Here $E_0 = -\alpha^2$. We will apply the so called nonlinearization method. Let us remind its basic features. The potential vector field $\vec{y}$ is introduced instead of wave function ψ

$$\vec{y} = -\vec{\nabla}\psi/\psi \qquad (3)$$

Then, the equation

$$\operatorname{div}\vec{y} - \vec{y}^{\,2} = E + \frac{2\alpha}{r} - \frac{B^2}{8}(x^2+y^2) \qquad (4)$$

holds, being equivalent the initial equation (1). As usual, let us expand

$$\vec{y} = \sum_{n=0}^{\infty} \vec{y}_n \left(\frac{B^2}{8}\right)^n \qquad (5)$$

and substitute eqs. (2), (5) into eq. (4). If we want the coefficient of $(B^2/8)^n$ to vanish, then we must require the following equation to hold

$$\Delta\varphi_n - 2\vec{y}_0\vec{\nabla}\varphi_n = E_n - Q_n\,, \quad \vec{\nabla}\varphi_n = \vec{y}_n \qquad (6)$$

where

$$\vec{y}_0 = \alpha\frac{\vec{r}}{r}\,, \qquad Q_1 = (x^2+y^2)\,, \quad n=1$$

$$Q_n = -\sum_{i=1}^{n-1} \vec{y}_i\,\vec{y}_{n-i}$$

and [9–10]

$$E_n = \int Q_n \psi_0^2\, d^3x \Big/ \int \psi_0^2\, d^3x \qquad (7)$$

where $\psi_0 = \exp\{-\alpha r\}$ is the Coulomb wave function. In order to solve eq. (6), we may look for φ_n in the form of a series

$$\varphi_n = \sum_{m=0}^{\infty} R_{n,m}(r)\, P_{2m}(\cos\theta) \qquad (8)$$

where $P_{2m}(\cos\theta)$ stand for the Legendre polinomial. In this way one obtaines the following equation

$$R''_{n,m} + \left(\frac{2}{r} - 2\alpha\right) R'_{n,m} - \frac{2m(2m+1)}{r^2} R_{n,m} = (E_n - Q_n)\Big|_{P_{2m}} \qquad (9)$$

where the r.h.s. represents, by definition, the coefficient of P_{2m} in the expansion of $(E_n - Q_n)$. The boundary conditions for eq. (9) are the following: (i) vanishing of $R_{n,m}(r)$ at the origin $(R_{n,m}(0) = 0)$, and (ii) the absence of exponential growth at infinity. It is readily seen that $R_{n,m} \equiv 0$, if the r.h.s. of eq. (9) is identical zero. Let us look for the solution of eq. (9) in the form

$$R_{n,m}(r) = \sum_{k=0}^{\infty} a_{n,m,k} \cdot r^k \qquad (10)$$

Substituting (10) into eq. (9) one obtaines recurrence relations which are not written out here because of their cumbersome structure. A simple analysis shows that $R_{n,m}$ are polinomials:

$$a_{n,m,k} = 0 \quad at \quad \begin{array}{l} k = 0, 1 \\ k > 2n+1 \\ k < m \end{array} \qquad (11)$$

and

$$E_n = 6 a_{n,0,2} = \frac{18}{\alpha} a_{n,0,3} \tag{11'}$$

$$2\alpha \cdot a_{n,1,2} = 3 a_{n,1,3}$$

Thus, in the n-th order of PT the polinomial coefficient in front of the highest Legendre polinomial P_{2n} has two terms, the preceeding polinomial (in front of P_{2n-2}) has four terms, etc. Summarizing the general structure of these polinomials is the following

$$R_{n,m}(r) = \sum_{k=\max\{2,2m\}}^{2n+1} a_{n,m,k} \cdot r^k \tag{10'}$$

Most probably the property (10') is a consequence of a hidden dynamical symmetry in the problem considered. The above recurrence relations allow for a calculation of PT coefficients order-by-order. These calculations are rather simple. As an example I write out the first corrections explicitly

$$R_{1,0} = \frac{r^2}{3\alpha^2} + \frac{r^3}{9\alpha} \, , \quad - R_{1,1} = \frac{r^2}{6\alpha^2} + \frac{r^3}{9\alpha}$$

$$-R_{2,0} = \frac{53}{36\alpha^6} r^2 + \frac{53}{108\alpha^5} r^3 + \frac{11}{90\alpha^4} r^4 + \frac{2}{135\alpha^3} r^5 \tag{12}$$

$$R_{2,1} = \frac{193}{36\alpha^6} r^2 + \frac{193}{540\alpha^5} r^3 + \frac{79}{630\alpha^4} r^4 + \frac{17}{945\alpha^3} r^5$$

$$-R_{2,2} = \frac{11}{1260\alpha^4} r^4 + \frac{1}{315\alpha^3} r^5$$

and

$$E_1 = \frac{2}{\alpha^2}, \quad E_2 = -\frac{53}{6\alpha^6}, \quad E_3 = \frac{5581}{36\alpha^{10}} \tag{13}$$

Expressions (13) coincide with ordinary ones [4,6].

From the above recurrence relations it is easy to find a few polinomials $R_{n,n-k}$ ($k = 0,1,\ldots$) explicitly. For instance, the polinomial $R_{n,n}$ is

$$-R_{n,n}(r) = \frac{((2n)!)^2 (2n-3)!}{(4n)!(n-2)!(n-1)!} \frac{8\, r^{2n+1}}{6^n \alpha^{2n-1}} + \frac{((2n)!)^2}{(4n)!}\left[1 + 2^{1-2n} \frac{(2n-1)!}{(n-1)!\, n!}\right] \left(\frac{2}{3}\right)^n \frac{r^{2n}}{\alpha^{2n}} \tag{14}$$

It is worth noting that the above recurrence relations may be easily used for numerical calculations by means of computer.

A few words about the relation of our approach and the standard Rayleigh-Schrödinger one. Since $\varphi = \ln \psi$ (ψ - wave function) this relation is obvious. One may confront our expressions (10') (as well as (12), (14)) with usual ones [4]. Our formulas are simpler namely, our polinomials are of a lower power and contain a smaller number of terms. Besides that, the recurrence relations may be written to determine the corrections to the wave function. They are convenient for computer calculations. Futher discussion will be given elsewhere.

Let us briefly discuss excited states as well. Obviously a wave function may be represented in the form [10]

$$\psi(x) = f(x)\exp\{-\varphi(x)\} \tag{15}$$

where $\varphi(x)$ does not contain singularities at the finite points of $\mathbb{R}^3$ and $f(x)$ does not grow exponentially at infinity (indeed, $f(x)$ describes node surfaces). Expanding the functions $f(x)$ and $\varphi(x)$ in powers of $(B^2/8)$ and substituting these expansions into (1) *), one obtains the equations for f_n and φ_n of the type of eq. (6). The solutions of these equations contain a finite number harmonics with polinomial (in r) coefficients. For example, for the state (2,0,0)

$$f_n = \sum_{m=0}^{n} f_{n,m}(r) P_{2m}(\cos\theta), \quad \varphi_n = \sum_{m=0}^{n} R_{n,m} P_{2m}(\cos\theta) \tag{16}$$

It is easily to show that

$$f_{n,m} = A_{n,m} + B_{n,m} r \qquad R_{n,m} = \sum_{k=1}^{2n+1} a_{n,m,k} r^k \tag{17}$$

$$f_{n,0} = A_{n,0}$$

In particular, the first correction is of the form **)

$$-f_1 = \frac{2}{3\alpha^4} + \frac{r}{\alpha^3} P_2(\cos\theta)$$

$$R_{1,0} = -\frac{2}{3\alpha^3} r + \frac{1}{2\alpha^2} r^2 + \frac{1}{9\alpha} r^3, \quad E_1 = \frac{7}{\alpha^2} \tag{18}$$

$$-R_{1,1} = \frac{r}{\alpha^3} + \frac{r^2}{3\alpha^2} + \frac{r^3}{9\alpha}$$

*) For simplisity the only case of $L_z = 0$ ($m = 0$) is considered only.

**) For this state $\psi_0 = (1-\alpha r)\exp\{-\alpha r\}$, $E_0 = -\alpha^2$, $V_0 = -4\alpha/r$.

Expressions (18) are simpler than the usual ones [4]. It is obvious that the calculation of the next corrections is not on difficult task. It is well-defined theoretically.

So, in the framework of approach considered the construction of PT in the powers of the field reduces to a solution of recurrent relations. This is much simpler than the calculation of the intermediate-state sum or the solution of differential equations of the second order with a right hand side in the usual approach.

In a paper which is under preparation now, I shall consider a convergent perturbation theory for the Zeeman effect in sence of my preceeding papers [9-10].

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