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Exact solution of the Dirac-Coulomb equation and its application to bound-state problems. I. External fields

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An exact treatment of relativistic effects in bound-state problems in hydrogenlike atoms is given. In this paper we discuss the Zeeman effect and the Stark effect for relativistically bound electrons in a Coulomb field. For the Zeeman effect, the exact solution obtained by Darwin is used, and results of Crubellier and Feneuille for the Breit-Margenau correction are obtained in a simple way. For the Stark effect, the solution of Wong and Yeh is used. The exact expression can be readily compared with that of the Pauli approximation, and all correction terms can be identified. In the following paper we discuss interaction of the bound electron with radiation in an exact relativistic way. In the evaluation of the radial r^k matrix elements with $n'\neq n$, we present a closed-form expression as a sum over three parameters, derived from the method of the generating function of Laguerre polynomials.

I. INTRODUCTION

It is interesting to note that although nonrelativistic treatment of bound-state problems in hydrogenlike atoms has been developed in great detail, there exists very little treatment of the relativistic case in an exact way. One of the reasons is that the exact solution of the Dirac-Coulomb equation given by Darwin[1] and Gordon[2] is very complicated. So far, an exact treatment of the bound electron in an external field can only be found in the Zeeman effect, leading to the Breit[3]-Margenau[4] correction. The correction term has been evaluated by Crubellier and Feneuille,[5] with the simple result

$$\int_0^\infty f_{nlj}^2 r^2 dr = \tfrac{1}{2}(1-\epsilon) , \tag{1.1}$$

where

$$\epsilon = E/E_0 , \tag{1.2}$$

and f is the radial wave function for the "small component" as given in Eq. (14.37) of Bethe and Salpeter.[6] In most other cases, the Pauli approximation is used, where the small component of the wave function is neglected, and the radial wave function is replaced by the nonrelativistic Schrödinger solution.

This situation is now remedied since we have found a simplified solution[7] to the Dirac-Coulomb equation. This solution is very similar to the solution of the Schrödinger equation and leads directly to the Pauli approximation if one (1) neglects the small component and (2) replaces $(l^2-\alpha^2Z^2)^{1/2}$ by l. Therefore instead of using the Pauli approximation, we can now give an exact treatment of relativistic effects by using the exact solution of the Dirac-Coulomb equation. We find that our solution can be applied to the Stark effect, which will be treated in this paper, and interaction of bound electrons with radiation, which will be treated in the following paper.

In this paper we discuss the bound electron in external fields, i.e., the Zeeman effect, where the external field is magnetic, and the Stark effect, where the external field is electric. In the following paper, we discuss interaction of the bound electron with radiation, obtaining transition probabilities and sum rules in an exact, relativistic way.

In Sec. II we discuss the radial r^k matrix elements which will be used repeatedly in subsequent sections. For the case $n'\neq n$, we obtain a closed-form expression for the radial integral using the method of the generating function for the Laguerre polynomials. In Sec. III we discuss the Zeeman effect and obtain Eq. (1.1) in a simple way. In Sec. IV we discuss the Stark effect, using the solution of Wong and Yeh[7] for the Dirac-Coulomb equation.

II. HYDROGENIC RADIAL r^k MATRIX ELEMENTS

In this section we shall consider the integral

$$\int_0^\infty R_{n\lambda} r^k R_{n'\lambda'} r^2 dr , \tag{2.1}$$

where $R_{n\lambda}$ (or $R_{n'\lambda'}$) is a radial wave function containing one term of a confluent hypergeometric function. n and λ need not be integers. In fact, they are irrational in all the cases under consideration. However, the radial quantum number

$$n_r=n-\lambda-1 \tag{2.2}$$

is always a non-negative integer.

The integral (2.1) can be divided into two parts: (1) $n=n'$ (2) $n\neq n'$. For $n=n'$, the integral has been evaluated by Pasternack and Sternheimer,[8] Armstrong,[9] and many others. This integral is connected with the group O(2,1) or SU(1,1), and is, in fact, reducible to the Clebsch-Gordan coefficients of SU(1,1) obtained by Ui.[10] For $n\neq n'$, the integral can be evaluated by using a recurrence relation obtained by Gordon,[11] or by repeated differentiation of a formula obtained by Menzel.[12] A closed-form expression has been obtained by Badawi, Bessis, Bessis, and Hadinger.[13] We shall also give a closed-form expression for the integral directly as a sum over three parameters.

The radial solution we have obtained for the Dirac-Coulomb equation can be expressed as

$$N(\tilde{\omega})\phi_{n\lambda}=N(\tilde{\omega})\frac{[\Gamma(n+\lambda+1)\Gamma(n-\lambda+1)]^{1/2}}{\Gamma(2\lambda+2)} \times\rho^{\lambda}e^{-\rho/2}{}_1F_1(-n+\lambda+1,2\lambda+2,\rho)\ , \tag{2.3}$$

where $N(\tilde{\omega})$ is a normalization constant. We would like to take this opportunity to point out that m and $E\kappa/\gamma$ in Eq. (3.45) of Ref. 7 should be interchanged. Therefore $N(\tilde{\omega})$ should read

$$N(\tilde{\omega})=(4\mu^3/n)^{1/2}[(n-\lambda+\tfrac{1}{2}\tilde{\omega}-\tfrac{1}{2})!(n-\lambda+\tfrac{1}{2}\tilde{\omega}-\tfrac{3}{2})!]^{-1/2} \times[(n-\lambda+\tfrac{1}{2}\tilde{\omega}-\tfrac{1}{2})(n-\lambda+\tfrac{1}{2}\tilde{\omega}+\tfrac{1}{2})(E\kappa/\gamma-\tilde{\omega}m)+(E\kappa/\gamma+\tilde{\omega}m)]^{-1/2}\ , \tag{2.4}$$

$$|\gamma|=\lambda-\tfrac{1}{2}\tilde{\omega}+\tfrac{1}{2}\ , \tag{2.5}$$

$$\rho=2\mu r\ , \tag{2.6}$$

$$\mu=(m^2-E^2)^{1/2}\ , \tag{2.7}$$

$$\kappa=\tilde{\omega}(j+\tfrac{1}{2})=\tilde{\omega}l-\tfrac{1}{2}+\tfrac{1}{2}\tilde{\omega}\ . \tag{2.8}$$

In terms of the normalized Schrödinger solution $R_{n\lambda}$, we have

$$\phi_{n\lambda}=[(n-\lambda)!]^{1/2}[(n-\lambda-1)!]^{1/2}(2n)^{1/2}(2\mu)^{-3/2}R_{n\lambda}\ . \tag{2.9}$$

For the radial solution obtained by Darwin, each component contains the sum of two confluent hypergeometric functions. However, each term in the sum can be expressed in the form of (2.3) with appropriate definitions for n and λ. Thus, for example, we can write

$$f=\tilde{N}(1-\epsilon)^{1/2}[n'f_1+(N-\kappa)f_2]\ , \tag{2.10}$$

$$g=\tilde{N}(1+\epsilon)^{1/2}[-n'f_1+(N-\kappa)f_2]\ , \tag{2.11}$$

where f_1 and f_2 are of the form (2.3).

Then for $n'=n$, we have

$$\int_0^\infty r^k R_{n\lambda}R_{n\lambda'}r^2dr=(2\mu)^{-k}A(-k-2,0,\lambda n\,|\,\lambda' n)\tfrac{1}{2}\Gamma(\lambda+\lambda'+k+3)[\Gamma(2\lambda+2)\Gamma(2\lambda'+2)n^2]^{-1/2}\ , \tag{2.12}$$

$$A(k,q,\lambda n\,|\,\lambda' n')=[\Gamma(2\lambda+2)\Gamma(2\lambda'+2)\Gamma(\lambda'+n'+1)\Gamma(n'-\lambda')\Gamma(n-\lambda)/\Gamma(n+\lambda+1)]^{1/2} \times\delta(n',q+n)\sum_t(-1)^{q+t+\lambda-\lambda'}[\Gamma(n-\lambda-t)\Gamma(\lambda+\lambda'+q+t+2)]^{-1} \times\begin{bmatrix}\lambda-\lambda'-k-1\\ q+\lambda-\lambda'+t\end{bmatrix}\begin{bmatrix}k-q\\ t\end{bmatrix}. \tag{2.13}$$

For $n\neq n'$, we wish to point out that the integral can be evaluated by the method of the generating function for the Laguerre polynomials.[14] Thus we obtain

$$\int_0^\infty r^k R_{n\lambda} R_{n'\lambda'} r^2 dr = 2^{\lambda+\lambda'+k+3}(2\mu)^{-k-3/2}(2\mu')^{3/2}(\mu/\mu')^{\lambda'}\tfrac{1}{2}(nn')^{-1/2}[\Gamma(n-\lambda)\Gamma(n'-\lambda')]^{1/2}$$
$$\times[\Gamma(n+\lambda+1)\Gamma(n'+\lambda'+1)]^{-1/2}\Gamma(\lambda+\lambda'+k+3)$$
$$\times\sum_{\sigma,\rho,\tau}(1+\mu'/\mu)^{-n'+n-2\lambda+\rho-\sigma-2\tau-k-3}(\mu'/\mu-1)^{n'-n-\lambda'+\lambda-\rho+\sigma+2\tau}(-1)^{\rho+n-\lambda-1}$$
$$\times\begin{bmatrix}-\lambda+\lambda'+k+1\\ \sigma\end{bmatrix}\begin{bmatrix}\lambda-\lambda'+k+1\\ \rho\end{bmatrix}\begin{bmatrix}-\lambda-\lambda'-k-3\\ \tau\end{bmatrix}$$
$$\times\begin{bmatrix}-\lambda-\lambda'-k-\tau-3\\ n'-n-\lambda'+\lambda-\rho+\sigma+\tau\end{bmatrix}\begin{bmatrix}-k-2\lambda-n'+n+\rho-\sigma-2\tau-3\\ n-\lambda-1-\sigma-\tau\end{bmatrix}. \quad (2.14)$$

Equation (2.14) can be compared with the result of Badawi *et al.*,[13] where the radial integral is computed for the Schrödinger case.

III. ZEEMAN EFFECT OF THE RELATIVISTICALLY BOUND ELECTRON

In the Zeeman effect where the magnetic field is weak compared to the separation of neighboring fine-structure levels, the unperturbed states can be taken from the exact solution of the Dirac-Coulomb equation. The magnetic field can be considered as a perturbation. The perturbing term is $-e\vec{\alpha}\cdot\vec{A}$. This case has been considered by Breit[3] and Margenau.[4] For the relativistically bound electron, Margenau obtained a correction to the Landé g factor $\kappa/(\kappa+\frac{1}{2})$. The relativistic Landé g factor is

$$g_R = \frac{2m_0c}{\hbar}\tilde{\omega}\frac{(2j+1)}{2j(j+1)}\int_0^\infty fgr^3dr \quad (3.1)$$

$$= \frac{\kappa}{\kappa+\frac{1}{2}}\left[1-\frac{4\kappa}{2\kappa-1}\int_0^\infty f^2r^2dr\right], \quad (3.2)$$

where f and g are given explicitly by Bethe and Salpeter,[6] in their Eq. (14.37).

Crubellier and Feneuille[5] evaluated the radial integral in (3.1) and obtained a simple result for the radial integral in (3.2), i.e.,

$$\int_0^\infty f_{nlj}^2 r^2 dr = \tfrac{1}{2}(1-\epsilon), \quad (3.3)$$

where

$$\epsilon = E/E_0 . \quad (3.4)$$

We now give a simple proof of Eq. (3.3). First, we write f and g according to (2.10) and (2.11). Then, using (2.12) and (2.13), we can easily show that

$$\int_0^\infty f_1 f_2 r^2 dr = 0 . \quad (3.5)$$

Therefore

$$\int_0^\infty f^2r^2dr = \tilde{N}^2(1-\epsilon)\times\left[n'^2\int_0^\infty f_1^2r^2dr + (N-\kappa)^2\int_0^\infty f_2^2r^2dr\right] = \tilde{N}^2(1-\epsilon)h , \quad (3.6)$$

but f and g are normalized. Thus

$$\int_0^\infty g^2r^2dr + \int_0^\infty f^2r^2dr = 1 , \quad (3.7)$$

or

$$\tilde{N}^2(1+\epsilon)h + \tilde{N}^2(1-\epsilon)h = 1$$

with

$$\tilde{N}^2h = \tfrac{1}{2} . \quad (3.8)$$

Setting (3.8) into (3.6), we get

$$\int_0^\infty f^2r^2dr = \tfrac{1}{2}(1-\epsilon) , \quad (3.9)$$

Q.E.D.

IV. STARK EFFECT OF THE RELATIVISTICALLY BOUND ELECTRON

In this section we consider the Stark effect of the relativistically bound electron, where the electric field is weak compared to the separation of neighboring fine-structure levels. Then the unperturbed states can be taken from the exact solution of the Dirac-Coulomb equation, and the external electric field can be considered as a small perturbation. As far as we know, no exact treatment in the relativistic case has been given. Bethe and Salpeter[11] discussed this case in the Pauli approximation.

We find that this case can be treated exactly in a relativistic way using the simplified solution of

Wong and Yeh for the Dirac-Coulomb equation. This treatment is much simpler with the Wong-Yeh solution than with the Darwin solution, even though in principle both solutions can be used. Moreover, the Wong-Yeh solution leads immediately to the Pauli approximation as we shall show later.

The perturbing term caused by the external electric field $\vec{F}$ in the z direction can be written as eFz. Thus in the Stark effect we wish to calculate the matrix element

$$\langle u_-^* \mid eFz \mid u_+ \rangle , \tag{4.1}$$

where u_+ is a 4×1 column matrix with $\tilde{\omega}=+1$, and u_-^* is a 1×4 row matrix with $\tilde{\omega}=-1$. u_-^* is the Hermitian conjugate of u_-.

Therefore according to (4.1), we find

$$\mid u_+ \rangle = N_+ \begin{bmatrix} i(E\kappa/\gamma - m_0)^{1/2}\phi_{|\gamma|-1}\chi_{-\kappa}^m(+1) \\ (E\kappa/\gamma + m_0)^{1/2}\phi_{|\gamma|}\chi_\kappa^m(+1) \end{bmatrix} , \tag{4.2}$$

where we have used m to denote the magnetic quantum number and m_0 to denote the mass of the electron with

$$u_-^* = [-N_- i(E\kappa/\gamma - m_0)^{1/2}\phi_{|\gamma|}\chi_{-\kappa}^m(-1),\ -N_-(E\kappa/\gamma + m_0)^{1/2}\phi_{|\gamma|-1}\chi_\kappa^m(-1)] , \tag{4.3}$$

where the $\pm$ signs refer to $\tilde{\omega}=\pm 1$, respectively.

Finally, we find

$$\langle u_-^* \mid eFz \mid u_+ \rangle = eF\left[\int r^3 dr \left[N_+ N_-(E\kappa/\gamma - m_0)\phi_{|\gamma|}\phi_{|\gamma|-1} \int \cos\theta \chi_{-\kappa}^{*m}(-1)\chi_{-\kappa}^m(+1)d\omega \right] - \int r^3 dr N_+ N_-(m_0 + E\kappa/\gamma)\phi_{|\gamma|}\phi_{|\gamma|-1} \int \cos\theta \chi_\kappa^{*m}(-1)\chi_\kappa^m(+1)d\omega \right] . \tag{4.4}$$

The angular integrals can be readily evaluated with the value $m/[2j(j+1)]$ for both terms. Before evaluating the radial integrals in (4.4), let us compare our results with the Pauli approximation. It can be easily seen that, of the two terms in (4.4), the largest term is the second one since it contains the factor $(m_0+E\kappa/\gamma)$. The radial functions $\phi_{|\gamma|}$ and $\phi_{|\gamma|-1}$ reduce to $R_{n,j,+1/2}$ and $R_{n,j-1/2}$, respectively, if one replaces $|\gamma| = [(j+\frac{1}{2})^2 - \alpha^2 Z^2]^{1/2}$ by $j+\frac{1}{2}$. Thus the second term reproduces the Pauli approximation result [Eq. (55.2) of Ref. 6]. The other term is a further improved correction over the Pauli approximation due to the small component. The radial integral can be easily evaluated with the following result:

$$\int r^3 dr\, \phi_{|\gamma|}\phi_{|\gamma|-1} = -6(2\mu)^{-4}[(n-|\gamma|)!][(n-|\gamma|+1)!]^{1/2}[(n-|\gamma|-1)!]^{1/2}(n^2-\gamma^2)^{1/2} . \tag{4.5}$$

The final expression for (4.4) is

$$\langle u_-^* \mid eFz \mid u_+ \rangle = eFN_+N_-[m/j(j+1)](2\mu)^{-4}2m_0 6[(n-|\gamma|)!] \times [(n-|\gamma|+1)!]^{1/2}[(n-|\gamma|-1)!]^{1/2}(n^2-\gamma^2)^{1/2} = \epsilon_m . \tag{4.6}$$

As we have pointed out in Sec. II, the terms $(n-|\gamma|)$, etc., are all non-negative integers connected with the radial quantum number n_r. In fact, in the present case, we have

$$n_r(+) = n - |\gamma| - 1 , \tag{4.7}$$

$$n_r(-) = n_r(+) + 1 , \tag{4.8}$$

where $n_r(+)$ and $n_r(-)$ refer to the cases $\tilde{\omega}=+1$ and $\tilde{\omega}=-1$, respectively.

The eigenvalues of the perturbing energy are equal to

$$\pm\epsilon_m . \tag{4.9}$$

Thus each fine-structure level is split by the electric field into $2j+1$ equidistant terms labeled by $m=-j,\ldots,+j$. The separation of neighboring terms is given by ϵ_m/m as is (4.6).

V. CONCLUSIONS

We have shown that an exact treatment of relativistic effects for bound electrons in hydrogenlike atoms can be carried out. In this paper, we have discussed the Zeeman effect and the Stark effect, where the external fields are weak compared to fine-structure levels. We have carried out an exact calculation in first-order perturbation theory. In principle, this calculation can be carried out to any higher orders. In the following paper, we shall discuss interaction of the bound electron with radiation in an exact, relativistic way.

One interesting observation we would like to make with regard to our work is that "relativity" is not necessarily synonymous with "high energy." In our treatment of the bound electron, we have used the manifestly covariant formalism required by relativity, which is the only exact way to deal with the spin of the electron, and yet the energy need not be high at all. Moreover, the external fields, in either the Zeeman effect or the Stark effect, are "weak" compared with fine structure, so that perturbation theory can be used.

In our calculation for the Stark effect, we have used the simplified solution of the Dirac-Coulomb equation obtained by Wong and Yeh. This solution has the advantage that it contains the Pauli approximation automatically, in the limit when (1) the small component is neglected and (2) $(l^2-\alpha^2 Z^2)^{1/2}$ is replaced by l. Our result for the Stark effect in (4.6) shows that the exact calculation is just as simple as the Pauli approximation.

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