Brief Reports

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Value of the Dirac-Coulomb wave function at the origin

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In several perturbative calculations, such as the Lamb shift and decay of positronium into two photons, it is necessary to calculate the wave function of the S state, or the first derivative of the P state, etc. at the origin. This value diverges for the Dirac-Coulomb wave function. A method suggested by Bethe and Salpeter is used and the result is obtained in analytically closed form. For the hydrogen atom in the ground state ($1S_{1/2}$) our result for $u^2(0)$ is equal to the traditional result, calculated by using the nonrelativistic Schrödinger wave function, multiplied by a factor slightly greater than unity, 1.000 118. For the $2S_{1/2}$ state, the multiplication factor is 1.000 004 1.

I. INTRODUCTION

In several perturbative calculations, it is necessary to use the wave function of the bound state, either in an atom or in positronium, at the origin. Practical cases in physics are the Lamb shift and the decay of positronium into two photons. In the latter case, one also needs to obtain the first derivative of the wave function for the p state, the second derivative of the d state, etc. at the origin. In all these cases, if the Dirac-Coulomb equation is used, the result diverges. Therefore so far only the nonrelativistic Schrödinger wave function has been used for these results.

This difficulty was recognized by Bethe and Salpeter[1] and explained as follows. The exact relation for the operator α acting on the bound state wave function u is

$$\alpha u = \frac{c}{mc^2+E+e\phi}[\pi + i\pi\times\sigma + mc(1-\beta)\alpha]u \ , \quad (1.1)$$

where

$$\pi = \mathbf{p} + e\,\mathbf{A}/c \ , \quad (1.2)$$

$$\sigma_i = -i\alpha_k\alpha_l \quad (i,k,l = \text{cycl. perm. } 1,2,3) \ . \quad (1.3)$$

For small distances of r, the $e\phi$ term on the denominator of (1.1) is quite large, and one has to replace $u^2(0)$ by the integral

$$u^2(\rho_0) = -\int_0^\infty d\rho \left[1+\frac{Z\alpha^2}{2\rho}\right]^{-1} \frac{d}{d\rho}u^2(\rho) \ , \quad (1.4)$$

where ρ is the radial distance in atomic units. Bethe and Salpeter then indicated that the error committed when one replaces the Dirac wave function by the Schrödinger wave function is of the order $(Z\alpha)^2\ln(Z\alpha)$. However, they did not calculate the exact value in Eq. (1.4).

In a previous paper, Wong and Yeh[2] have obtained a simplified solution to the Dirac-Coulomb equation, a result subsequently confirmed by Su.[3] We use this solution for $u(\rho)$ in Eq. (1.4) and find that the integral in Eq. (1.4) can be expressed analytically in terms of incomplete Γ functions. Thus we are able to obtain an exact value for the bound-state wave function at the origin using the relativistic Dirac-Coulomb equation. Moreover, we find that our result differs from the standard result by a factor which is extremely close to unity. For the $1S_{1/2}$ ground state of hydrogen, our factor is 1.000 118. For the $2S_{1/2}$ state, it is 1.000 004 1.

II. ANALYTIC EVALUATION OF THE DIRAC-COULOMB WAVE FUNCTION AT THE ORIGIN

In this section, we give the analytic evaluation of the value in Eq. (1.4) using the Dirac-Coulomb wave function. We shall only give the results for the S state. It is obvious how one can use the same procedure to obtain the first derivative for the p state, the second derivative for the d state, etc. Using the notation of Ref. 2, we have

$$l=0, \quad j=\tfrac{1}{2}, \quad \tilde{\omega}=-1, \quad \kappa=-1 \ , \quad (2.1)$$

$$\gamma = -(1-Z^2\alpha^2)^{1/2}, \quad \lambda=(1-Z^2\alpha^2)^{1/2}-1 \ , \quad (2.2)$$

$$\mu_1=(m^2-E^2)^{1/2}, \quad \frac{Z\alpha E}{\mu_1}=\lambda+1+n_r \quad (n_r=0,1,\ldots) \ , \quad (2.3)$$

$$E=\frac{m}{\left[1+\frac{Z^2\alpha^2}{[(1-Z^2\alpha^2)^{1/2}+n_r]^2}\right]^{1/2}} . \tag{2.4}$$

The large component ψ_l is then

$$\psi_l=\left[E\frac{\kappa}{\gamma}+m\right]^{1/2}\left[2E\frac{\kappa}{\gamma}\right]^{-1/2}R_S , \tag{2.5}$$

where R_S is the normalized Schrödinger wave function with λ replacing l, and μ_1 replacing Z/n. Explicitly,

$$\begin{aligned}R_S=&[\Gamma(2\lambda+2)]^{-1}(2\mu_1)^{3/2}[\Gamma(n_r+2\lambda+2)]^{1/2}\\&\times[2(n_r+\lambda+1)\Gamma(n_r+1)]^{-1/2}\\&\times\rho^{\lambda}e^{-\rho/2}\,{}_1F_1(-n_r,2\lambda+2,\rho) ,\end{aligned} \tag{2.6}$$

with

$$\rho=2\mu_1 r . \tag{2.7}$$

For the $1S_{1/2}$ ground state, the radial wave function u is

$$u=ce^{-r}(2r)^{\lambda},\quad c=2^{3/2}[\Gamma(2\lambda+2)]^{-1/2}(2\lambda+2)^{-1/2} , \tag{2.8}$$

where

$$c=2.000\,049\,2 \text{ for } Z=1 \text{ and } \lambda=0.000\,026\,64 . \tag{2.9}$$

Then Eq. (1.4) becomes

$$u^2(\rho_0)=c^2\Gamma(2-2y,Z\alpha^2)\Gamma(2y-1)(2y-2)e^{Z\alpha^2}(Z\alpha^2)^{2y-2}-c^2\Gamma(1-2y,Z\alpha^2)\Gamma(2y)e^{Z\alpha^2}(Z\alpha^2)^{2y-1} , \tag{2.10}$$

where $y=|\gamma|$ and

$$\Gamma(a,x)=\int_x^{\infty}e^{-t}t^{a-1}dt=\frac{e^{-x}x^a}{\Gamma(1-a)}\int_0^{\infty}\frac{e^{-t}t^{-a}}{x+t}dt \tag{2.11}$$

is an incomplete Γ function.[4]

For the hydrogen atom in the $1S_{1/2}$ state, we find that $u^2(\rho_0)$ is equal to the Schrödinger result $u^2(0)$ multiplied by a factor 1.000 118.

For the $2S_{1/2}$ state, a similar calculation has been made. We shall give only the final result

$$\begin{aligned}u^2(\rho_0)=&(2y-2)e^xx^{2y-2}\Gamma(2y-1)\Gamma(2-2y,x)+(1-3y)y^{-1}e^xx^{2y-1}\Gamma(2y)\Gamma(1-2y,x)\\&+(3/2y)e^xx^{2y}\Gamma(1+2y)\Gamma(-2y,x)-(4y^2)^{-1}e^xx^{2y+1}\Gamma(2+2y)\Gamma(-2y-1,x)\end{aligned} \tag{2.12}$$

where

$$x=1.000\,000\,684Z\alpha^2/2 . \tag{2.13}$$

Compared to the Schrödinger result, the multiplication factor is 1.000 004 1.

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