Simplified solutions of the Dirac-Coulomb equation

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With the use of a simple similarity transformation which brings the radial wave equations of the Dirac-Coulomb problem into a form nearly identical to those of the Schrödinger and Klein-Gordon equations, we derive simplified solutions to the Dirac-Coulomb equation for both the bound and continuum states following the familiar standard procedure adopted in the derivation of the conventional solutions. We show that to obtain the desired form of the second-order radial equations we can still work with a first-order partial differential equation rather than with the second-order Dirac equation widely employed in the derivation of the simplified solutions, and thus we can avoid the task of reducing the solutions of the second-order equations to those of the original Dirac equation. The transformed Dirac-Coulomb radial equations are so simple that one can apply the WKB method to them in the same way that one applies the WKB approximation to the Schrödinger radial equation, without making the further approximations commonly invoked, and the Sommerfeld-Dirac discrete spectrum follows immediately. For small $Z\alpha$, we also present approximate expressions for both the transformed and the original Dirac-Coulomb wave functions, which are valid for all energies and certainly valid in the quasirelativistic approximation which takes account of relativistic effects. The structure of these approximate expressions also suggests one of the methods to obtain relativistic approximate wave functions from the Pauli-spinor wave function for more general central potentials arising in atoms, molecules, and solids.

I. INTRODUCTION

The exact solution to the Dirac equation for an electron in a Coulomb field was first obtained by Darwin[1] and Gordon.[2] The radial part of the upper or lower component in the usual solution[3–6] can be expressed as a sum of two confluent hypergeometric functions. Instead of solving the Dirac-Coulomb equation directly, one can solve the second-order Dirac equation[7–12] which is obtained by multiplying the original equation on the left by a differential operator. The second-order equation is similar to the Klein-Gordon equation in a Coulomb field.[9–13] The latter equation can be reduced to a form nearly identical to that of the Schrödinger equation and its solution can thus be inferred from the known nonrelativistic solution.[12,13] One can also perform an analogous reduction of the second-order Dirac equation by diagonalizing this equation in a certain representation, and one thus obtains the solution in the same way as one solves the Schrödinger equation.[7–12] Since the solution to the second-order equation is not always a solution of the original Dirac-Coulomb equation, one has to find some methods to reduce solutions of the second-order equation to solutions of the original Dirac equation.[7–12] Biedenharn[8] discovered a generalized recursion operator for the radial eigenfunctions, which was utilized to reduce solutions of the second-order equation to those of the original Dirac equation for the continuum states[8] and bound states.[9] The resulting solutions are simpler than the previous ones in that each component contains only one confluent hypergeometric function.

The exact solution of the Dirac-Coulomb equation has recently been used to study the relativistic effects in bound state problems of external fields[14] and of interaction with radiation[15] and in the process of inner-shell ionization.[16] Some approximate schemes for the Dirac-Coulomb equation have also been investigated recently, which may also have relevance to relativistic calculations of systems other than the hydrogenlike atom. The variational study of the Dirac-Coulomb equation in a finite basis set[17–20] can be useful in the calculations of relativistic molecular structure. Solution to an approximate Dirac-Coulomb equation given recently is basic to the study of the relativistic wave equation for N interacting Dirac particles.[21]

In this paper we obtain simplified Dirac-Coulomb solutions by first applying a similarity transformation[13,22,23] to the Dirac-Coulomb equation. The similarity transformation is chosen so that the radial wave equations of the Dirac-Coulomb problem are simplified considerably and can be put in a form completely similar to those of the Schrödinger and Klein-Gordon equations. As a result, the solutions to these radial equations can be inferred immediately from those of the Schrödinger and Klein-Gordon equations. The resulting radial function of each of the upper and lower components contains only one confluent hypergeometric function, which is much simpler than the radial function in the usual solution, containing a sum of two confluent hypergeometric functions.[3–6] Note that throughout this paper we always study the first-order partial differential equation instead of the second-order Dirac equation.[7–12] The similarity transformation used here is fairly simple, containing no differential operator and thus does not raise the order of the Dirac equation so that the transformed Dirac-Coulomb equation under investigation remains a first-order equation. This has the advantage that we can avoid the problem of reducing the solutions of the second-order Dirac equation to those of the original Dirac equation in a certain representation, which presents a great hindrance in explicitly writing down the solutions of the Dirac-Coulomb equation in a simple form[7,11,12] and has been overcome only after the ingenious discovery by Biedenharn[8,9] of a generalized recursion operator for the radial eigenfunctions. It is evident that our method of obtaining the simplified solutions to the Dirac-Coulomb equation is simple and familiar, following the standard procedure adopted in obtaining the usual solutions.[3,4,6]

We also consider the problem of the WKB approximation to the radial wave equations arising in the (first-order) transformed Dirac-Coulomb equation. The radial equations are so simple that the application of the WKB method to them is as elementary as the application of the WKB method to the Schrödinger radial equation,[24–27] and as a result the Sommerfeld-Dirac discrete energy spectrum follows immediately from the quantization rule. In contrast, the radial equations in the usual formulation are very complicated. In applying the WKB method to these radial equations one has to invoke further approximations, and only after that one can obtain the Sommerfeld-Dirac energy levels.[4,28,29]

From the simplified solutions to the transformed Dirac-Coulomb equation, we derive approximate expressions for both the transformed and the original Dirac-Coulomb wave functions by expanding the exact wave functions in powers of $Z\alpha$. The resulting expressions contain the Pauli approximation as the lowest-order approximation, and can also be used as quasirelativistic wave functions which take account of the relativistic effects on the wave functions. The structure of the approximate wave functions indicates how one can obtain the exact Dirac-Coulomb wave functions from the Pauli-spinor wave function, and suggests a similar procedure to find approximate relativistic wave functions[30] from the Pauli wave function for general central-potential problems, which are certainly useful in understanding relativistic effects in atoms, molecules, and solids.[19,20]

In Sec. II the Dirac-Coulomb equation is transformed under a similarity transformation. The constants in the transformation matrix are determined in such a way that the resulting radial wave equations can be put in a form completely similar to those of the Schrödinger and Klein-Gordon equations. In Sec. III we present simplified solutions of the transformed Dirac-Coulomb equation for the bound states and also the continuum states which reduce to the usual free-particle solutions for a vanishing potential. In Sec. IV we apply the WKB method to the radial wave equations obtained in Sec. II and obtain the usual discrete energy levels immediately. In Sec. V we expand the transformed and the original Dirac-Coulomb wave functions in powers of $Z\alpha$ and obtain approximate wave functions which, for small $Z\alpha$, can be used in the quasirelativistic approximation and in the relativistic case as well. Finally, in Sec. VI we summarize the results obtained in this paper.

II. THE DIRAC-COULOMB EQUATION UNDER A SIMILARITY TRANSFORMATION

We start with the Dirac equation for an electron in a stationary state of energy E in a Coulomb field,

$$H\psi=E\psi \tag{2.1}$$

with[2]

$$H=c\boldsymbol{\alpha}\cdot\mathbf{p}+\beta mc^2-Ze^2/r \tag{2.2}$$

and the Dirac matrices $\boldsymbol{\alpha}$ and β have their usual meanings. Applying a similarity transformation[13,22,23] to the Dirac-Coulomb equation, we get

$$H'\psi'=E\psi' \tag{2.3}$$

with

$$H'=SHS^{-1}\,, \tag{2.4}$$

$$\psi'=S\psi\,, \tag{2.5}$$

and

$$S=a+ib\beta\boldsymbol{\alpha}\cdot\hat{\mathbf{r}}\,, \tag{2.6}$$

where $\hat{\mathbf{r}}$ is the unit vector $\mathbf{r}/r$ and a and b are real constants to be determined. For any central potential, the solutions to (2.3) can be written in the form[5]

$$\psi'=\begin{bmatrix} iR(r)\varphi_{jm}^{l} \\ Q(r)\boldsymbol{\sigma}\cdot\hat{\mathbf{r}}\varphi_{jm}^{l}\end{bmatrix}. \tag{2.7}$$

The radial equations are then[17,18]

$$H_r'=\begin{bmatrix} R(r) \\ Q(r)\end{bmatrix}=E\begin{bmatrix} R(r) \\ Q(r)\end{bmatrix} \tag{2.8}$$

with

$$H_r'=\begin{bmatrix} mc^2\cosh\theta+\hbar c\left[\sinh\theta\left[\dfrac{d}{dr}+\dfrac{1}{r}\right]-\dfrac{Z\alpha}{r}\right] & -\left\{mc^2\sinh\theta+\hbar c\left[\cosh\theta\left[\dfrac{d}{dr}+\dfrac{1}{r}\right]-\dfrac{k}{r}\right]\right\} \\ mc^2\sinh\theta+\hbar c\left[\cosh\theta\left[\dfrac{d}{dr}+\dfrac{1}{r}\right]+\dfrac{k}{r}\right] & -\left\{mc^2\cosh\theta+\hbar c\left[\sinh\theta\left[\dfrac{d}{dr}+\dfrac{1}{r}\right]+\dfrac{Z\alpha}{r}\right]\right\}\end{bmatrix} \tag{2.9}$$

and $k=\tilde{\omega}(j+\frac{1}{2})$, $\tilde{\omega}=\mp 1$ for $l=j\mp\frac{1}{2}$, and $\alpha=e^2/\hbar c$ being the fine-structure constant. Here $\cosh\theta=(a^2+b^2)/(a^2-b^2)$ and $\sinh\theta=2ab/(a^2-b^2)$ if we assume that $a^2-b^2>0$.

If one chooses

$$\tanh\theta=-Z\alpha/k \tag{2.10}$$

then the terms in the square brackets of the matrix elements $(H_r')_{11}$ and $(H_r')_{12}$ in (2.9) are proportional to those of $(H_r')_{21}$ and $(H_r')_{22}$, respectively, and one attains great simplification in solving the radial equations. In fact, one can get

$$Q(r)=\left[-E\tilde{\omega}Z\alpha/\gamma+\hbar c\left[\frac{d}{dr}+(1+\tilde{\omega}\gamma)/r\right]\right]R(r)/[mc^2+(j+\tfrac{1}{2})E/\gamma] \quad (2.11)$$

and

$$R(r)=\left[E\tilde{\omega}Z\alpha/\gamma+\hbar c\left[\frac{d}{dr}+(1-\tilde{\omega}\gamma)/r\right]\right]Q(r)/[mc^2-(j+\tfrac{1}{2})E/\gamma] \quad (2.12)$$

with $\gamma=[(j+\frac{1}{2})^2-Z^2\alpha^2]^{1/2}$. By eliminating $Q(r)$ $[R(r)]$ from the above equations one obtains the equation for $R(r)$ $[Q(r)]$

$$\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+[(E^2-m^2c^4)/\hbar^2c^2+2EZ\alpha/\hbar cr - (\gamma^2\pm\tilde{\omega}\gamma)/r^2]\right]\times\begin{Bmatrix}R(r)\\Q(r)\end{Bmatrix}=0\ , \quad (2.13)$$

where the upper (lower) sign refers to the equation for $R(r)$ $[Q(r)]$. These radial equations also arise in the second-order Dirac-Coulomb equation[7–10,31] after diagonalizing the Martin-Glauber operator.[7–10]

From Eqs. (2.5) and (2.6) it is clear that the Hermitian matrix S enables us to find a suitable linear combination of the radial functions of the upper and lower components of the usual solutions for the new radial functions of the transformed wave functions so that we can write down the transformed Dirac-Coulomb radial equations in the simple form of (2.13). The solutions of Eqs. (2.13) will be investigated in Secs. III–V. For simplicity we choose $a^2-b^2=1$ throughout this paper such that $S=1$ for $Z=0$, then we can write $a=\cosh(\theta/2)$ and $b=\sinh(\theta/2)$. The resulting similarity transformation S is then equivalent to the transformation T given by Hostler[8(b)] which was taken directly from the S operator discovered by Biedenharn[8(a)] to diagonalize the second-order Dirac-Coulomb equation.

III. SIMPLIFIED SOLUTIONS OF THE TRANSFORMED DIRAC-COULOMB EQUATION

Let us now discuss the solutions of Eqs. (2.13) for the bound states $(m^2c^4>E^2)$. Equations (2.13) can then be put in a form completely similar to the corresponding radial wave equations of the Schrödinger and Klein-Gordon equations,[9,12] and the solutions are thus given by

$$R(r)=C(s_\pm)e^{-\lambda r}(2\lambda r)^{s\pm}F(s_\pm+1-w,2s_\pm+2,2\lambda r) \quad (3.1)$$

and

$$Q(r)=C(s_\mp)e^{-\lambda r}(2\lambda r)^{s\mp}F(s_\mp+1-w,2s_\mp+2,2\lambda r)\ , \quad (3.2)$$

where $F(a,b,z)$ is the confluent hypergeometric function, $\lambda=(m^2c^4-E^2)^{1/2}/\hbar c$, $w=Z\alpha E/\hbar c\lambda$, $s_+=\gamma-1$, and $s_-=\gamma$. The upper and lower signs refer to $\tilde{\omega}=-1$ and 1, respectively. Putting $r=0$ in Eqs. (2.11) and (2.12), we obtain the relation between the integration constants:[6]

$$C(s_-)=C(s_+)(mc^2+kE/\gamma)/2\lambda\hbar c(2\gamma+1)\ . \quad (3.3)$$

The two confluent hypergeometric functions reduce to polynomials, if

$$Z\alpha E/\hbar c\lambda-(s_\pm+1)=n_r'\ , \quad (3.4)$$

where n_r' is a non-negative integer. This quantization condition yields the usual expression for the discrete energy levels:

$$E/mc^2=[1+Z^2\alpha^2/(n_r+\gamma)^2]^{-1/2}\ ,\quad n_r=0,1,2,\ldots\ . \quad (3.5)$$

It remains to determine the normalization factor $C(s_+)$ in the wave function. Using the generating function of Laguerre polynomials,[32] one can calculate the radial integrals involving two confluent hypergeometric functions and obtain the following value for the constant $C(s_+)$:

$$C(s_+)=-\tilde{\omega}[(2\lambda)^{3/2}/\Gamma(2\gamma)][\Gamma(2\gamma+n_r)E\ |\ mc^2-kE/\gamma\ |\ /n!4(n_r+\gamma)m^2c^4]^{1/2}\ . \quad (3.6)$$

The radial wave functions for the continuum states $(E^2>m^2c^4)$ can be obtained from those for the bound states, Eqs. (3.1)–(3.3), by the following substitutions:[6,9]

$$(m^2c^4-E^2)^{1/2}\to -i(E^2-m^2c^4)^{1/2}\ ,\qquad \lambda\to -ik',\quad w\to i\nu\ , \quad (3.7)$$

where $k'=(E^2-m^2c^4)^{1/2}/\hbar c$, $\nu=Z\alpha E/\hbar ck'$.

Making these substitutions in (3.1)–(3.3), we may write

$$R(r)=C'(s_\pm)e^{ik'r}(2k'r)^{s\pm}F(s_\pm+1-i\nu,2s_\pm+2,-2ik'r) \quad (3.8)$$

and

$$Q(r)=C'(s_\mp)e^{ik'r}(2k'r)^{s\mp}F(s_\mp+1-i\nu,2s_\mp+2,-2ik'r) \quad (3.9)$$

with

$$C'(s_-)=C'(s_+)(mc^2+kE/\gamma)/2k'\hbar c(2\gamma+1) \quad (3.10)$$

and $C'(s_+)$ is a normalization constant.

The simplified solutions of the radial wave functions obtained here are equivalent to those of Wong and Yeh[9] for the bound states and Biedenharn[8(a)] for the continuum states which are obtained by diagonalizing the Martin-Glauber operator arising in the second-order Dirac-Coulomb equation, and by utilizing a generalized recursion operator.[8(a),9] Substitution of the simplified solutions into Eqs. (2.11) and (2.12) will reproduce the recurrence relations for the radial functions obtained by Wong and Yeh, and Biedenharn.

For the case of a free Dirac particle, $V=0$, one can obtain[8,9] the usual radial wave functions[4] from Eqs. (3.8)–(3.10) by setting $Z=0$:

$$R(r)=A(s_\pm)j_{s_\pm}(k'r) \quad (3.11)$$

and

$$Q(r)=A(s_\pm)\tilde{\omega}\frac{k'\hbar c}{E+mc^2}j_{s_\mp}(k'r)\ , \quad (3.12)$$

where $A(s_\pm)$ are normalization constants, and $j_n(z)$ is a spherical Bessel function, since for a free particle the similarity transformation given earlier reduces to an identity transformation, $S=1$, and $\psi'=\psi$ in this case.

IV. THE WKB APPROXIMATION TO THE RADIAL WAVE EQUATIONS

We have solved the radial wave equations (2.13) for the bound states and obtained the usual expression (3.5) for the discrete energy levels. We can also obtain these discrete energy levels by applying the WKB approximation to the same radial wave equations. The quantization rule for these radial equations, after taking account of the Langer-Kemble modification,[24–27] is

$$\int_{r_1}^{r_2} k_r dr=(n_r'+\tfrac{1}{2})\pi,\quad n_r'=0,1,2,\ldots \quad (4.1)$$

with r_1 and r_2 being the classical turning points and

$$k_r=[(E^2-m^2c^4)/\hbar^2c^2 +2EZ\alpha/\hbar cr-(\gamma\pm\tilde{\omega}/2)^2/r^2]^{1/2}\ , \quad (4.2)$$

which gives rise to

$$E/mc^2=[1+Z^2\alpha^2/(n_r'+\tfrac{1}{2}+\gamma\pm\tilde{\omega}/2)^2]^{-1/2}\ . \quad (4.3)$$

The above expression can be summarized as

$$E/mc^2=[1+Z^2\alpha^2/(n_r+\gamma)^2]^{-1/2},\quad n_r=0,1,2,\ldots \quad (4.4)$$

which is identical to (3.5). It is the radial wave equations in the representation defined by the similarity transformation S that make our calculations straightforward and completely similar to those employed in the WKB approximation to the Schrödinger radial equation, which give rise to the Bohr energy levels.[25,26] On the contrary, if one starts with the usual radial equation for the upper component, which is rather complicated, one has to make various approximations by dropping certain terms[4,28,29] to obtain the Sommerfeld-Dirac fine-structure levels (4.4).

V. APPROXIMATE DIRAC-COULOMB WAVE FUNCTIONS FOR SMALL $Z\alpha$

We can expand the radial functions $R(r)$ and $Q(r)$ in powers of $Z\alpha$. For $\tilde{\omega}<0$ ($l=j-\frac{1}{2}$), we have

$$R(r)=C[-2k+\lambda\hbar cZ\alpha/(mc^2+E)+3Z^2\alpha^2/4k+\cdots]\times e^{-\lambda r}(2\lambda r)^{\gamma-1}F(\gamma-w,2\gamma,2\lambda r) \quad (5.1)$$

and

$$Q(r)=C(-2k)[(mc^2-E-mc^2Z^2\alpha^2/2k^2+\cdots)/2\lambda\hbar c(-2k+1)]\times e^{-\lambda r}(2\lambda r)^{\gamma}F(\gamma+1-w,2\gamma+2,2\lambda r) \quad (5.2)$$

and for $\tilde{\omega}>0$ ($l=j+\frac{1}{2}$), we have

$$R(r)=[C/(2k+1)](k\{1+[-\tfrac{3}{4}+(4k+1)/(2k+1)-mc^2/(mc^2+E)]Z^2\alpha^2/2k^2+\cdots\} -[Z\alpha(mc^2+E)/2\lambda\hbar c]\{1+[-\tfrac{1}{4}+(4k+1)/(2k+1)-mc^2/(mc^2+E)]Z^2\alpha^2/2k^2+\cdots\})\times e^{-\lambda r}(2\lambda r)^{\gamma}F(\gamma+1-w,2\gamma+2,2\lambda r)\ , \quad (5.3)$$

and

$$Q(r)=C[2k\lambda\hbar c/(mc^2+E)-Z\alpha+\cdots]e^{-\lambda r}(2\lambda r)^{\gamma-1}\times F(\gamma-w,2\gamma,2\lambda r)\ , \quad (5.4)$$

with $\gamma=|k|(1-Z^2\alpha^2/2k^2+\cdots)$ to be substituted in the exponent of $2\lambda r$ and in the confluent hypergeometric functions, and C being a common normalization factor. For bound states, one can write $w-\gamma=n_r=0,1,2,\ldots$ in the above expressions, which are also valid for the continuum states by making the substitutions (3.7). For small $Z\alpha$, the leading terms in $R(r)$ in the nonrelativistic limit give rise to the Pauli-spinor wave functions for both the bound states[33] and the continuum states,[13] since in this limit $S\approx 1$ and $\psi'\approx\psi$. In this way the simplified solutions ψ' lead directly to the Pauli approximation.

We can also obtain the approximate wave function ψ for the original Dirac-Coulomb equation (2.1) for small $Z\alpha$. We first present the exact expressions for $g(r)$ and $f(r)$, the radial functions of the upper and lower components of $\psi=S^{-1}\psi'$:

$$g(r)=Ce^{-\lambda r}(2\lambda r)^{\gamma-1}[\gamma-k+Z\alpha\lambda\hbar c/(mc^2+E)]$$
$$\times\{F(\gamma-w,2\gamma,2\lambda r)-[(mc^2\gamma+kE)Z\alpha/2\lambda\hbar c\gamma(2\gamma+1)(\gamma-k)](2\lambda r)F(\gamma+1-w,2\gamma+2,2\lambda r)\} \quad (5.5)$$

and

$$f(r)=C[(mc^2-E)/\lambda\hbar c]e^{-\lambda r}(2\lambda r)^{\gamma-1}[\gamma+k-Z\alpha(mc^2+E)/\lambda\hbar c]$$
$$\times\{F(\gamma-w,2\gamma,2\lambda r)+[(mc^2\gamma+kE)Z\alpha/2\lambda\hbar c\gamma(2\gamma+1)(\gamma+k)](2\lambda r)F(\gamma+1-w,2\gamma+2,2\lambda r)\}\ , \quad (5.6)$$

where C is a common normalization factor. These expressions are equivalent to the usual results for the radial functions.[1-6] These expressions, being written for the bound states with $w-\gamma=n_r=0,1,2,\ldots$, are also valid for the continuum states if one makes the substitutions (3.7). From the leading terms of $g(r)$ in (5.5) one immediately obtains the Pauli-spinor wave functions for both bound and continuum states and for $\tilde{\omega}=\mp 1$, if small $Z\alpha$ is assumed and the nonrelativistic limit is taken, since in each case the leading term in $g(r)$ involves only one confluent hypergeometric function. The solutions ψ written in this form thus lead directly to the Pauli approximation. On the contrary, the usual expression for $g(r)$ in the conventional solutions involves two confluent hypergeometric functions with coefficients of comparable magnitude,[1-6] and therefore one cannot immediately obtain the Pauli-spinor wave functions from the usual solutions in the nonrelativistic limit.

The approximate expressions for $g(r)$ and $f(r)$ for small $Z\alpha$ are given, for $\tilde{\omega}<0$ ($l=j-\frac{1}{2}$) for instance, by

$$g(r)\approx Ce^{-\lambda r}(2\lambda r)^{\gamma-1}\{[-2k+Z\alpha\lambda\hbar c/(mc^2+E)+Z^2\alpha^2/2k]F(\gamma-w,2\gamma,2\lambda r)$$
$$-[Z\alpha(mc^2-E-mc^2Z^2\alpha^2/2k^2)/2\lambda\hbar c(-2k+1)](2\lambda r)F(\gamma+1-w,2\gamma+2,2\lambda r)\} \quad (5.7)$$

and

$$f(r)\approx Ce^{-\lambda r}(2\lambda r)^{\gamma-1}\{-Z\alpha F(\gamma-w,2\gamma,2\lambda r)$$
$$-k[(mc^2-E-mc^2Z^2\alpha^2/2k^2)/\lambda\hbar c(-2k+1)](2\lambda r)F(\gamma+1-w,2\gamma+2,2\lambda r)\} \quad (5.8)$$

with $\gamma=-k(1-Z^2\alpha^2/2k^2+\cdots)$ to be substituted above. These approximate formulas can be obtained from Eqs. (5.5) and (5.6) or from the following relations:

$$g(r)\approx(1+Z^2\alpha^2/8k^2)R(r)+(Z\alpha/2k)Q(r)\ , \quad (5.9)$$

$$f(r)\approx(Z\alpha/2k)R(r)+(1+Z^2\alpha^2/8k^2)Q(r)\ , \quad (5.10)$$

and Eqs. (5.1) and (5.2). From the above relations and Eqs. (5.3) and (5.4) we can similarly write down the approximate expressions for $\tilde{\omega}>0$ ($l=j+\frac{1}{2}$).

The approximate expressions for $g(r)$ and $f(r)$ give the wave function ψ with relativistic corrections. The behavior of $g(r)$ near the origin $r=0$ is proportional to $r^{\gamma-1}$ or r^{γ} for $\tilde{\omega}=-1$ or 1, which is a modification of the nonrelativistic behavior $\sim r^l$ since $\gamma=(l+1)[1-Z^2\alpha^2/2(l+1)^2+\cdots]$ for $\tilde{\omega}=-1$ and $\gamma=l(1-Z^2\alpha^2/2l^2+\cdots)$ for $\tilde{\omega}=1$. This behavior can easily be deduced from the usual equations[4] for $g(r)$ and $f(r)$,

$$\left[E-mc^2+\frac{Ze^2}{r}\right]g(r)=-\hbar c\left[\frac{d}{dr}+\frac{1}{r}(1-k)\right]f(r)\ , \quad (5.11)$$

$$\left[E+mc^2+\frac{Ze^2}{r}\right]f(r)=\hbar c\left[\frac{d}{dr}+\frac{1}{r}(1+k)\right]g(r)\ , \quad (5.12)$$

by neglecting the terms $E\pm mc^2$ compared to the potential term $|V|=Ze^2/r$. The asymptotic behavior of $g(r)$ and $f(r)$ is roughly given by $e^{-\lambda r}$ and $e^{\pm ik'r}$ for the bound and continuum states with $\lambda=(m^2c^4-E^2)^{1/2}/\hbar c$ and $k'=(E^2-m^2c^4)^{1/2}/\hbar c$ which are modifications of the nonrelativistic expressions, since in the latter cases $\lambda=(-2mE)^{1/2}/\hbar$ and $k'=(2mE)^{1/2}/\hbar$. These asymptotic expressions can also be deduced from Eqs. (5.11) and (5.12) by neglecting the potential term and the $(1/r)(1\mp k)$ terms compared to the other terms.

If one starts with the Pauli-spinor wave function, determines the small component by (5.12) in the limit of $Ze^2/r \ll mc^2$, and takes account of the relativistic corrections near the origin and at infinity, one will make the following substitutions: $l\to\gamma-1$ for $\tilde{\omega}<0$, $l\to\gamma$ for $\tilde{\omega}>0$, and $(-2mE)^{1/2}r/\hbar\to(m^2c^4-E^2)^{1/2}r/\hbar c$ in the radial wave functions and obtain two confluent hypergeometric functions as suggested in Eqs. (5.1) and (5.3). Motivated by these arguments one may be able to find the exact solutions or better approximate solutions more easily. A similar procedure or its variant is expected to be applicable also in other relativistic central-potential problems.

VI. CONCLUSIONS

In this paper we have solved the first-order transformed Dirac-Coulomb equation and obtained simplified solutions for the bound states and also the continuum states which reduce to the usual free-particle solutions when the Coulomb potential is turned off. We also show that the transformed Dirac-Coulomb radial equations are so simple that we can apply the WKB approximation to them in a fashion similar to that used to apply the WKB approximation to the Schrödinger radial equation, and the Sommerfeld-Dirac discrete spectrum follows immediately. In contrast, the radial equations in the usual formulation are very complicated. One has to make further approximations in applying the WKB method to these radial equations, and only after that one can obtain the Sommerfeld-Dirac energy levels. We have also given approximate expressions for both the transformed and the original Dirac-Coulomb wave functions which are valid for small $Z\alpha$ and for all energies.

In solving the *second-order* Dirac-Coulomb equation, many authors also got the radial wave equations[7–12,31] in the form of Eq. (2.13) after diagonalizing the operator introduced by Martin and Glauber[7–10] in four-component form[7–10] (or in two-component form[11,12]), especially in the representation defined by the transformation operator S found by Biedenharn.[8,9,31]

The simplified solutions for the *second-order* Dirac-Coulomb equation can then be obtained easily. Afterward one has to utilize Biedenharn's generalized recursion operator for the radial eigenfunctions[8,9] to obtain the simplified solutions to the original first-order Dirac-Coulomb equation, which were obtained by Biedenharn for the continuum states[8,9] and by Wong and Yeh for the bound states.[9] In this paper we first apply a similarity transformation to the Dirac-Coulomb equation. The constants in the transformation matrix for the similarity transformation are chosen so that the resulting radial wave equations can be put in a desired simple form. The transformation matrix obtained in this way, which happens to be proportional to the simplified form of the Biedenharn S operator[8,9] utilized to diagonalize the *second-order* Dirac-Coulomb equation, enables us immediately to obtain the simplified solutions of the *first-order* transformed Dirac-Coulomb equation. Therefore we can avoid the task of reducing the solutions of the *second-order* equation to those of the original Dirac-Coulomb equation.

It is clear that to bring the radial wave equations, second-order in coordinates, into a form completely similar to the corresponding radial wave equations of the Schrödinger and Klein-Gordon equations, we need not first transform the Dirac-Coulomb equation into a second-order equation. Since we originally have two coupled first-order equations for the two radial functions of the upper and lower components, by eliminating one radial function in favor of the other we can obtain the desired form of the second-order radial equations in the representation defined by the similarity transformation given in Sec. II.

From the simplified solutions to the transformed Dirac-Coulomb equation we obtain Eqs. (5.5) and (5.6), the solutions to the Dirac-Coulomb equation in the conventional representation. Each of the upper and lower components of the solutions contains two confluent hypergeometric functions like the usual solutions. Nevertheless, only the first (second) coefficient in (5.5) for the upper large component is important for $l=j-\frac{1}{2}$ ($l=j+\frac{1}{2}$) in the Pauli approximation for small $Z\alpha$. In contrast, both coefficients in the conventional solutions[1–6] are of comparable magnitude in the same approximation. Consequently the solutions given in Eqs. (5.5) and (5.6) are more suitable than those given in the usual form[1–6] for obtaining the approximate wave functions (5.7) and (5.8) for small $Z\alpha$ and for all energies, which take into account the relativistic effects and go beyond the Pauli approximation. The structure of these approximate wave functions also suggests one of the methods to obtain the approximate relativistic wave functions for general central-potential problems arising in atoms, molecules, and solids,[19,20] which may complement the perturbation approach to the general central-potential problems[30] and shed some interesting light on the approximate methods used in the problems of atoms, molecules, and solids[17–20] and of N interacting Dirac particles.[21]

[1] C. G. Darwin, Proc. R. Soc. London, Ser. A **118**, 654 (1928).
[2] W. Gordon, Z. Phys. **48**, 11 (1928).
[3] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer, Berlin, 1957).
[4] M. E. Rose, *Relativistic Electron Theory* (Wiley, New York, 1961).
[5] C. Itzykson and J.-B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).
[6] V. B. Berestetskii, E. M. Lifshitz, and L. P. Pitaevskii, *Quantum Electrodynamics* (Pergamon, Oxford, 1982).
[7] P. C. Martin and R. J. Glauber, Phys. Rev. **109**, 1307 (1958).
[8] (a) L. C. Biedenharn, Phys. Rev. **126**, 845 (1962); (b) L. Hostler, J. Math. Phys. **5**, 591 (1964).
[9] M. K. F. Wong and H. Y. Yeh, Phys. Rev. D **25**, 3396 (1982).
[10] G. Baym, *Lectures on Quantum Mechanics* (Benjamin, New York, 1969).
[11] P. R. Auvil and L. M. Brown, Am. J. Phys. **46**, 679 (1978).
[12] M. D. Scadron, *Advanced Quantum Theory* (Springer, New York, 1979).
[13] L. I. Schiff, *Quantum Mechanics,* 3rd ed. (McGraw-Hill, New York, 1968).
[14] M. K. F. Wong and H. Y. Yeh, Phys. Rev. A **27**, 2300 (1983).
[15] M. K. F. Wong and H. Y. Yeh, Phys. Rev. A **27**, 2305 (1983).
[16] C. V. Sheth, Phys. Rev. A **29**, 1151 (1984).
[17] G. W. F. Drake and S. P. Goldman, Phys. Rev. A **23**, 2093 (1981).
[18] I. P. Grant, Phys. Rev. A **25**, 1230 (1982).
[19] *Relativistic Effects in Atoms, Molecules, and Solids,* edited by G. Malli (Plenum, New York, 1983).
[20] *Proceedings of the Symposium on Relativistic Effects in Quantum Chemistry, Turku, 1982,* edited by P. Pyykkö [Int. J. Quantum Chem. **25** (1984)].
[21] G. Hardekopf and J. Sucher, Phys. Rev. A **30**, 703 (1984).
[22] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, Mass., 1980).
[23] J. Mathews and R. L. Walker, *Mathematical Methods of Physics* (Benjamin, New York, 1970).
[24] R. E. Langer, Phys. Rev. **51**, 669 (1937).
[25] E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* (McGraw-Hill, New York, 1937).
[26] A. B. Migdal, *Qualitative Methods in Quantum Theory* (Benjamin, Reading, Mass., 1977).
[27] M. V. Berry and K. E. Mount, Rep. Prog. Phys. **35**, 315 (1972).

[28]R. J. Bessey, Thesis, University of Michigan, 1942.
[29]R. H. Good, Jr., Phys. Rev. **90**, 131 (1953); **94**, 931 (1954).
[30]C. K. Au and G. W. Rogers, Phys. Rev. A **22**, 1820 (1980); C. K. Au, *ibid.* **23**, 2068 (1981).
[31]M. J. Cunningham, J. Math. Phys. **13**, 1108 (1972).
[32]P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 1.
[33]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics,* 3rd ed. (Pergamon, Oxford, 1977).