# A Note on Dirac Central Field Wave Functions*

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A systematic treatment is developed for the discussion of the solution of the Dirac wave equation for a central field for the purposes of theories involving the finite size of the nucleus.

## I. INTRODUCTION

THERE are a number of problems for which the effect of the finite size of the nucleus is of interest.[1] In an attempt to systematize the treatment of some of these problems certain procedures for the calculation of wave functions have been developed which the author has found to be particularly useful. In view of the possible application of these procedures to other problems, it is felt to be worth while to present the following discussion.

## II. THEORY

In the representation[2] in which $j^2$ and $j_z$ are diagonal, the "small" and "large" radial functions, $u_1/r$ and $u_2/r$, respectively, are given in terms of the solutions of the differential equations,

$$du_i/dr=\alpha_{ij}u_j;\quad i,j=1,2, \tag{1}$$

sum over repeated indices implied, and

$$[\alpha_{ij}]=\begin{bmatrix}\kappa/r & -(W-1-V)\\ W+1-V & -\kappa/r\end{bmatrix}. \tag{2}$$

In Eq. (2), $W$ and $V$ are the total energy and scalar potential, respectively, and

$$\kappa=\pm(j+\tfrac{1}{2})\quad\text{for}\quad j=l\mp\tfrac{1}{2} \tag{3}$$

is a nonvanishing integer. Throughout, we use

$$\hbar=m=c=1.$$

### (A) Quadrature Solution

For an investigation of the effect of the finite size of the nucleus, it is necessary to obtain wave functions in the smeared-out nuclear charge distribution. While these are easily obtained for all of the simple models customarily used, there are certain advantages to be derived from the following more general procedure. A formal integration of (1) gives

$$u_1=r^{\kappa}\left(C_1+\int_0^r r^{-\kappa}\alpha_{12}u_2dr\right), \tag{4a}$$

$$u_2=r^{-\kappa}\left(C_2+\int_0^r r^{\kappa}\alpha_{21}u_1dr\right), \tag{4b}$$

where $C_i$ are integration constants. For $\kappa<0$, and $|\kappa|=k$, we have $C_1=0$ for the regular solution and we write (4) in the form

$$u_1=\omega_1u_2,\quad u_2=u_2^{(0)}+\omega_2u_1, \tag{4c}$$

where $u_2^{(0)}=C_2r^k$, and (4) defines the integral operators $\omega_i$. The solution of (4c), obtained by iteration, is

$$u_2=\sum_0^{\infty}(\omega_2\omega_1)^nu_2^{(0)}, \tag{5}$$

and $u_1$ is obtained from the first of (4c) or from (1). For any function $f(r)$,

$$\omega_2\omega_1f(r)=r^k\int_0^r y^k\alpha_{12}(y)\zeta(r,y)f(y)dy, \tag{5a}$$

where

$$\zeta(r,y)=\int_y^r x^{-2k}\alpha_{21}(x)dx \tag{5b}$$

is a given function once $V$ is specified.

For $\kappa>0$ we replace $\omega_2\omega_1$ by $\omega_1\omega_2$, which (with $\kappa=k$) is equivalent to interchanging[3] $\alpha_{12}$ and $\alpha_{21}$.

The solution (5) and the corresponding one for $\kappa>0$ may be applied only in those cases for which the integrals exist. In the form given, (5) is an expansion around the origin and we must make the restriction $\lim rV=0$ as $r\to0$. However, for a finite size nucleus this condition will always be fulfilled. The fact that (5) does constitute an expansion around the origin is evident if we use

$$\int_0^r f(r)dr=O(rf(r)),$$

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[1] Forbidden (zero-zero) transitions, S. D. Drell, Phys. Rev. **81**, 656A (1951); Isotope shift, G. Breit, Phys. Rev. **42**, 348 (1932); Hyperfine structure, A. Bohr and V. F. Weisskopf, Phys. Rev. **77**, 94 (1950); Electron scattering, M. E. Rose, Phys. Rev. **73**, 279 (1948); L. Acheson, Ph.D. dissertation (M.I.T.); L. R. B. Elton, Phys. Rev. **79**, 412 (1950); Effect in $\beta$-decay, M. E. Rose and D. K. Holmes (in preparation).

[2] M. E. Rose, Phys. Rev. **51**, 484 (1937).

[3] This is an example of the general result that changing the sign of $\kappa$ is equivalent to changing the sign of $W$ and $V$ and interchanging $u_1$ and $u_2$, as can be verified directly from (1). If we denote these operations by the operators $\Omega_\kappa$, $\Omega_W$, $\Omega_V$, and $\Omega_{12}$, respectively, acting on the 2-spinor $(u_1, u_2)$, then

$$\Omega_\kappa\Omega_W\Omega_V\Omega_{12}=1,$$

since for each operator $\Omega^2=1$, $\Omega=\Omega^{-1}$, and all of these operators commute.

where $O$ means "of order of," which will always be valid for the quadratures appearing in (5). It is now clear that the ratio of the $(n+1)$st to the $n$th term is $O(r^2)$. The convergence domain of (5) is easily established. For example, if $V$ is bounded, (5) converges as well as in the case $V=\text{const}$, and in this latter case (5) gives the power series for $r$ times the spherical bessel functions, which are the well-known solutions in this case.

Where the solutions are obtainable in the form of a power series in $r$, (5) will generate the same series but with a reordering of the terms so that each term is a polynomial with the sum of the first $m$ terms of (5) containing at least the sum of the first $m$ terms of the power series. A particularly useful feature of the series (5) is the fact that an upper limit on the error incurred in terminating the series can be obtained in almost all cases. Usually $V$ will be negative-definite, and this will almost certainly be the case over the region where (5) would be used. In that case, for the electron continuum, $(W>1)$, $\alpha_{12}$ and $\alpha_{21}$ are negative-definite and positive-definite, respectively. The series (5) is therefore alternating and, over a large domain, the absolute value of the term is monotonic decreasing so that the error is less than the first term neglected. For bound states there will always be a turning point ($\alpha_{12}=0$), but $\alpha_{12}<0$ for smaller values of $r$. In any practical case the turning point will be beyond the nuclear radius and usually far beyond it, so that the alternating character of the series (5) is retained for bound states also.

The general form of the solution (5) permits a simple examination of the effect of a coulomb field deviation on the small distance behavior of the wave functions. For the leading terms we have ($\kappa<0$)

$$u_2=C_2r^k,$$

$$u_1=-C_2r^{-k}\int_0^r(W-1-V)r'^{2k}dr'.$$

Since $|V|\gg W$, usually, we write $u_1$ in the form

$$u_1\approx C_2r^{-k}\int_0^r Vr'^{2k}dr'=\frac{C_2r^{j+\frac{1}{2}}}{2j+2}\int_0^1 Vw(x)dx, \quad (6a)$$

where we have introduced $x=r'/r$ and the normalized weight factor $w(x)=(2j+2)x^{2j+1}$, $(0\leqslant x\leqslant 1)$. Similarly, for $\kappa>0$,

$$u_1=C_1r^k,$$

$$u_2=-\frac{C_1r^{j+\frac{1}{2}}}{2j+2}\int_0^1 Vw(x)dx. \quad (6b)$$

Therefore, of the four radial functions for given $j$, two, namely, $u_1(\kappa<0)$ and $u_2(\kappa>0)$ are sensitive at small $r$ to coulomb field deviations. For the other pair, the indicial, behavior is chiefly determined by the angular momentum and not by the field $V$. Calculations of the effect of finite nuclear size in $\beta$-decay exhibit this effect rather strikingly.[1] From (6) it is clear that the short-range coulomb field deviation is important only for low angular momenta, as expected. This follows, since, for large $j$, $w\to\delta(1-x)$ and the details of the field $V$ at small $r$ become unimportant.

### (B) Normalization

For the continuum, the normalization constants $C_i$ in (5) can be determined only if (5) can be joined to the asymptotic solutions. In the case of the finite nucleus, where $V$ is a coulomb field for $r>R$ (the nuclear radius), the joining is very simple. Actually, all that is needed in this case is the ratio $\rho=u_1/u_2$ at $r=R$, and then the constants $C_i$ drop out. For bound states, the joining condition at $r=R$ fixes the eigenvalue $W$, and the normalized solutions are determined as follows. Consider two stationary-state time-dependent wave functions $\Psi_j$ and $\Psi_k$ corresponding to energies $W_j$ and $W_k$, respectively. Then

$$\operatorname{div}(\Psi_j^*\boldsymbol{\alpha}\Psi_k)+\partial(\Psi_j^*\Psi_k)/\partial t=0, \quad (7)$$

where $\boldsymbol{\alpha}$ is the usual Dirac matrix vector. Carrying out the time differentiation and inserting the time independent wave functions $\psi_j$ and $\psi_k$, we then integrate over a closed volume and obtain

$$\int\psi_j^*\alpha_n\psi_k dS=i(W_k-W_j)\int\psi_j^*\psi_k d\tau, \quad (8)$$

where $\alpha_n$ is component of $\boldsymbol{\alpha}$ along the outward normal, and $dS$ is an area element of the bounding surface. Now let $W_j=W_k+dW$ so that

$$\int\psi^*\psi d\tau=i\int(\partial\psi^*/\partial W)\alpha_n\psi dS. \quad (9)$$

On specializing to the representation used above and applying (9) to a spherical shell of radii $r_1$ and $r_2$, we get

$$\left[u_1\frac{\partial u_2}{\partial W}-u_2\frac{\partial u_1}{\partial W}\right]_{r_1}^{r_2}=\int_{r_1}^{r_2}(u_1^2+u_2^2)dr, \quad (10)$$

which can be obtained directly from (1). If we consider a solution regular at the origin (but not necessarily so at $\infty$) and take $r_1=0$, $r_2=r$, we obtain

$$u_2^2\partial\rho_L/\partial W=-\int_0^r(u_1^2+u_2^2)dr, \quad (11)$$

where $\rho=u_1/u_2$ and the subscript $L$ indicates regularity at the left end of the interval $(0, \infty)$. The left side of (11) is evaluated at $r$, and on the right side, $L$ solutions are to be understood. Next, consider a solution regular at $\infty$ (but not necessarily so at $r=0$) and take $r_1=r$, $r_2=\infty$. Then,

$$u_2^2\partial\rho_R/\partial W=\int_r^\infty(u_1^2+u_2^2)dr, \quad (12)$$

and again $R$ implies regularity at $\infty$, the left side of (12) is evaluated at $r$, and on the right side, $R$ solutions are to be understood. If $W$ is set equal to an eigenvalue $W_n$, $u_1$ and $u_2$ (with phases suitably chosen) are continuous at $r$ (but $\partial\rho_L/\partial W \neq \partial\rho_R/\partial W$), and for the normalized solution, we obtain

$$u_2^2(r)=\{[(\partial\rho_R/\partial W)-(\partial\rho_L/\partial W)]_{r,W_n}\}^{-1}, \quad (13a)$$

$$u_1^2(r)=\rho^2 u_2^2(r). \quad (13b)$$

By means of (5) and (4c) one can evaluate $\rho_L$. If an analytic solution is known for points beyond $r$ (a coulomb field solution, for example) giving $\rho_R$, the result (13) provides a relatively simple procedure for normalization and avoids the use of indefinite integrals, which often cannot be evaluated analytically. This result is also rather convenient in a simpler field $V$ (such as a coulomb field). In this case, if a solution regular at the origin is known for all $W$, the normalization integral is given by (11), with $r=\infty$ in terms of the asymptotic behavior at $\infty$, and, if a solution properly behaved at $\infty$ can be represented in analytical form for all $W$, the result (12) with $r=0$ gives the normalization in terms of the behavior of the solutions around the origin.[4]

### (C) Phase Shifts

We again consider the situation in which $V=V_0(r)$ (a coulomb field, say) for $r>R$ and $V=V_1(r)$ for $r<R$. Then, of course, the wave functions for $r>R$ are completely determined in terms of the phase shifts for each partial wave (labeled by $\kappa$). The regular and irregular solutions of (1) for $V=V_0$ are denoted by $v_i$ and $\bar{v}_i$, respectively. Then the integral equation obtained by use of the Green function for (1) is, with $P(r)=V-V_0$,

$$u_i=v_i\left[1-\int_r^\infty \bar{v}_j(r')u_j(r')P(r')dr\right] - \bar{v}_i\int_0^r v_j(r')u_j(r')P(r')dr'$$

$$=v_i-\int_0^\infty G_{ij}(r,r')u_j(r')P(r')dr' \quad (14)$$

subject to the normalization condition

$$v_1\bar{v}_2-v_2\bar{v}_1\equiv 1. \quad (15)$$

In (14), the Green function (matrix) is

$$G_{ij}(r,r')=v_i(r)\bar{v}_j(r'), \quad r'>r$$
$$=\bar{v}_i(r)v_j(r'), \quad r>r'. \quad (16)$$

The properly normalized solutions $v_i$ and $\bar{v}_i$ have the asymptotic behavior

$$v_1\to[(W-1)/p]^{\frac{1}{2}}\sin\xi, \quad \bar{v}_1\to[(W-1)/p]^{\frac{1}{2}}\cos\xi,$$
$$v_2\to-[p/(W-1)]^{\frac{1}{2}}\cos\xi, \quad \bar{v}_2\to[p/(W-1)]^{\frac{1}{2}}\sin\xi, \quad (17)$$

where $p=(W^2-1)^{\frac{1}{2}}$ is the electron momentum and $\xi$ is the total phase.[5] For $u_i$, the asymptotic behavior is taken to be

$$u_1\to[(W-1)/p]^{\frac{1}{2}}(\sin\xi+\tan\delta\cos\xi),$$
$$u_2\to-[p/(W-1)]^{\frac{1}{2}}(\cos\xi-\tan\delta\sin\xi). \quad (18)$$

It follows from (14), (17), and (18) that[6]

$$\tan\delta=-\int_0^\infty v_j(r')u_j(r')P(r')dr'. \quad (19)$$

In this form the phase shift, $\delta$, is not stationary with respect to variations $\delta u_i$. To obtain the phase shift from a variation principle, we proceed in complete analogy with Schwinger's derivation of the corresponding nonrelativistic phase shift.[7] The final result for the relativistic generalization of Schwinger's variation principle is

$$-\cot\delta=\frac{\int_0^\infty drP(r)u_j(r)u_j(r)+\int_0^\infty dr\int_0^\infty dr'P(r)u_i(r)G_{ij}(r,r')u_j(r')P(r')}{\left[\int_0^\infty drP(r)u_j(r)v_j(r)\right]^2}. \quad (20)$$

A more convenient form of variation principle is obtained by putting (1) in hamiltonian form. Then, with the normalization (18) and the regularity condition $u_i(0)=0$, we find that

$$F[u]=\tan\delta-\int_0^\infty u_i\gamma_{ij}[(du_j/dr)-\alpha_{jk}u_k]dr \quad (21)$$

is stationary for the correct wave function. In (21)

$$(\gamma_{ij})=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}.$$

More specific results can be obtained in analogy with the treatment of corresponding nonrelativistic problems.[8]

[4] A corresponding result for the nonrelativistic case has been given by W. Furry, Phys. Rev. **71**, 360 (1937).

[5] Defined for coulomb fields in reference 2.

[6] A similar result has been obtained by G. Parzen, Phys. Rev. **80**, 261 (1950).

[7] J. M. Blatt and J. D. Jackson, Phys. Rev. **76**, 18 (1949). The difference between our result (20) and their result (2.11) arises from the different definitions of the Green function.

[8] T. Kato, Phys. Rev. **80**, 475 (1950).