JOURNAL OF COMPUTATIONAL PHYSICS 55, 397–407 (1984)

The Evaluation of Relativistic Oscillatory Wavefunctions on a Logarithmic Grid

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Received May 3, 1983

When calculating radial wavefunctions for use in such problems as electron scattering, the step size of a step-by-step method is severely limited by the oscillatory nature of the solution. However, the radial Schrödinger equation may be solved by computing the phase and amplitude of the oscillations; these two functions are slowly varying and permit the use of a much larger step size. In this paper it is shown how the method may be adapted to the solution of the relativistic radial Dirac equations. This method also enables oscillatory solutions over the whole radial distance to be calculated on a logarithmic grid.

1. INTRODUCTION

At present programs which solve the integro-differential equations for mixed bound-state scattering problems use a variety of different step sizes (see Burke [1]). All the bound-state calculations can be performed on a logarithmic grid but the scattering calculations use a normal radial grid in which the step size is doubled three or four times during the outward integration. Either the doubling is performed at the same place for each oscillatory eigenfunction in which case the highest frequency wave determines the step size or the doubling is performed at different places for the different eigenfunctions. In this latter case the required integrals of products of these functions cannot be evaluated without much interpolation since the discretised wavefunctions are evaluated at different points. The integral evaluation (see Walker [2]), is the time-consuming part of the calculation. It is thought that if all these calculations could be performed on the same logarithmic grid then not only would the code be easier to maintain and develop but with the reduced number of

* Supported by a grant from the Science Research Council of the United Kingdom during this work.

0021-9991/84 $3.00

grid points used by the logarithmic grid some improvement in computational speed may be obtained. The above is an ambitious objective. However, if this can be achieved it is hoped that the evaluation of scattering calculations on a logarithmic grid will be as widely used as the logarithmic grid in bound-state calculations. This paper is the very first step towards this objective in that it demonstrated the possibility of evaluating oscillatory wavefunctions on a logarithmic grid.

Trafton [3] has described a method for calculating an oscillatory solution to the radial Schrödinger equation by computing the phase and amplitude of the oscillations. These two functions vary more slowly than the original solution and thus in a numerical calculation permit the use of a much larger step size. In this paper these non-relativistic techniques are adapted for the solution of the relativistic Dirac equations. In Section 2 equations defining more slowly varying functions are obtained from the radial Dirac equations. Sections 3 and 4 discuss the numerical solution of the new equations. These equations may be conveniently solved on the same logarithmic grid as used for the calculations of bound-state eigenfunctions. Several variations of the method are possible and these are briefly compared in Sections 5 and 6. Comparisons with analytic solutions and some programming details are described in Section 7.

2. Method

The dimensionless form of the radial Dirac equation as given by Grant [4] is

$$\begin{aligned} \frac{dP}{dr} + \frac{k}{r} P + \bar{f}(r) Q = 0 \\ \frac{dQ}{dr} - \frac{k}{r} Q - \bar{g}(r) P = 0 \end{aligned} \tag{1}$$

where

$$\bar{f}(r) = \frac{1}{c} \{E - V(r) + 2c^2\}$$

$$\bar{g}(r) = \frac{1}{c} \{E - V(r)\}.$$

c is the velocity of light, E is the kinetic energy excluding the rest mass energy, $V(r)$ is the spherically symmetric potential, and k is the angular momentum quantum number. In our units $c = 137$; the quantum number k is a small integer, positive or negative.

For the oscillatory functions we are considering, the energy E is positive. For large r the solution of (1) has the asymptotic form

$$P(r) \sim N \sin\{\omega r + \eta \log(2\omega r) + \phi\} \qquad \text{as} \quad r \to \infty \tag{2}$$

with a similar form for $Q(r)$, where

$$\omega^2 = 2E + E^2/c^2$$

and

$$\eta = \frac{E}{2C}\left\{\left(\frac{E+2c^2}{E}\right)^{1/2} + \left(\frac{E}{E+2c^2}\right)^{1/2}\right\}$$

if $rV(r) \to Z$ as $r \to \infty$, while $\eta = 0$ if $rV(r) \to 0$ as $r \to \infty$. In this asymptotic form N and ϕ are unknown constants. The two boundary conditions associated with Eqs. (1) are $P(0) = 0$ and a normalization condition which specifies the value of N in (2).

It is possible to eliminate Q from the two equations (1) and then transform the result into a single second-order equation to which Trafton's method [3] can be applied. The transformed equation is rather complicated, and involves the second derivative of the potential $V(r)$, so it seems preferable to apply Trafton's approach to the equations in their original form. We write

$$\begin{aligned} P(r) &= A(r)\sin\{W(r)+\phi\} \\ Q(r) &= B(r)\sin\{W(r)+\phi\} + C(r)\cos\{W(r)+\phi\} \end{aligned} \tag{3}$$

which involve four unknown functions A, B, C, and W. We substitute these expressions for P and Q into Eqs. (1), and equate the coefficients of the sin and cos terms, giving the four equations

$$\frac{dA}{dr} + \frac{k}{r}A + \bar{f}B = 0 \tag{4}$$

$$\psi A + \bar{f}C = 0 \tag{5}$$

$$\frac{dB}{dr} - \psi C - \frac{k}{r}B - \bar{g}A = 0 \tag{6}$$

$$\frac{dC}{dr} + \psi B - \frac{k}{r}C = 0 \tag{7}$$

where $\psi(r) = dW/dr$. From Eqs. (4) and (7) we easily deduce that

$$C\frac{dA}{dr} + A\frac{dC}{dr} = 0$$

so that

$$AC = \theta,$$

θ a constant, and hence from (5) that

$$\psi(r) = \frac{-\theta\bar{f}(r)}{\{A(r)\}^2}. \tag{8}$$

The function $W(r)$ is then just the integral of $\psi(r)$, as given by Eq. (8), and the phase ϕ in Eq. (3) arises from the arbitrary constant of integration. We then obtain a pair of equations for A and B

$$\begin{aligned} \frac{dA}{dr} + \frac{k}{r}A + \bar{f}B &= 0 \\ \frac{dB}{dr} - \frac{k}{r}B - \bar{g}A + \frac{\theta^2\bar{f}}{A^3} &= 0. \end{aligned} \tag{9}$$

If B is eliminated from these two equations we obtain

$$\frac{d^2A}{dr^2} - \frac{d\bar{f}}{dr}\frac{1}{\bar{f}}\frac{dA}{dr} D_1 A - \frac{[\theta\bar{f}]^2}{A^3} = 0$$

where

$$D_1 = \bar{f}\bar{g} - \frac{k(k+1)}{r^2} - \frac{k}{r\bar{f}}\frac{d\bar{f}}{dr}.$$

In the non-relativistic limit, as $c \to \infty$, this equation reduces to the amplitude equation derived by Trafton, and following Trafton's analysis we therefore use as boundary conditions for (9) that both A and B should tend to constant limits as $r \to \infty$. Then for sufficiently large r the derivatives of A will become neglegible, and we obtain an asymptotic approximation to A and from Eq. (9) the appropriate asymptotic approximation to B.

$$\begin{aligned} A(r) &\sim A_0 = \frac{(\theta\bar{f})^{0.5}}{D_1^{0.25}} \\ B(r) &\sim B_0 = \frac{-kA(r)}{r\bar{f}} \end{aligned} \qquad \text{as} \quad r \to \infty. \tag{10}$$

Taking the limit as $r \to \infty$, and using the required asymptotic form (3), we find that

$$N^4 = \theta^2(1 + 2c^2/E)$$

so that the constant θ is known in terms of the prescribed value of N.

It is often convenient to use a numerical scheme with a gradually increasing step size as r increases. This can be achieved by making the transformation $\rho = \log r$ and using equal intervals in the variable ρ. This procedure is almost always used in the calculation of bound-state eigenfunctions for these equations, as in relativistic self-consistent field calculations. In terms of the new independent variable the equations become

$$\begin{aligned} \frac{dA}{d\rho} + kA + fB &= 0 \\ \frac{dB}{d\rho} - kB - gA + \frac{\theta^2 f}{A^3} &= 0 \end{aligned} \tag{11}$$

where $f = r\bar{f}$, $g = r\bar{g}$, and for convenience $D(r) = fg - k^2$.

Our method now is to construct a numerical solution of the amplitude equations (11) on a uniform grid in ρ, beginning from the known asymptotic form for large r and stepping inwards in the direction of decreasing ρ. This solution is then matched to a numerical solution of the original Dirac equations (1), constructed by a simple step-by-step method in the direction of increasing r. The two solutions are conveniently matched at a point near to the classical turning point, the point $r = a$ where $D(r)$ changes sign.

We denote the result of the outward integration by $P_0(r)$, $Q_0(r)$; some arbitrary normalization is chosen to define this solution. Fixing the definition of $W(r)$ in Eq. (3) by writing

$$W(r) = \int_a^r \psi(r)\, dr$$

the matching conditions require that

$$MP_0(a) = A(a) \sin \phi$$
$$MQ_0(a) = B(a) \sin \phi + C(a) \cos \phi.$$

Solution of these equations for M and ϕ then gives

$$M^2 = \frac{\theta^2}{\{C^2 P_0^2 + (AQ_0 - BP_0)^2\}_{(r=a)}}$$

and

$$\sin \phi = MP_0(a)/A(a).$$

The values of $P(r)$ and $Q(r)$ may then be tabulated over the whole range of r; in the outward integration region the functions P_0 and Q_0 are multiplied by the factor M, and outside this region P and Q are determined from Eqs. (3).

3. Solution for Large Values of r

In this section we describe an iterative scheme for the solution of Eqs. (1), which has proved satisfactory for moderately large values of r. The method is analogous to Strömgen's iteration for the non-relativistic form of the amplitude equations (see Seaton and Peach [5]). From (11) we easily construct the iterative scheme

$$B^{(n+1)} = -\left\{\frac{dA^{(n)}}{d\rho} + kA^{(n)}\right\} \Big/ f$$

$$A^{(n+1)} = \left\{\left(\frac{dB^{(n+1)}}{d\rho} - kB^{(n+1)}\right)(A^{(n)})^3 + f\theta^2\right\}^{1/4} \Big/ g^{1/4}$$

beginning with

$$A^{(0)} = \{f\theta^2/g\}^{1/4}.$$

This scheme may be written in the general form

$$\begin{aligned} B^{(n+1)} &= F(A^{(n)}, A'^{(n)}) \\ A^{(n+1)} &= G(B^{(n+1)}, B'^{(n+1)}, A^{(n)}) \end{aligned} \tag{12}$$

for the solution of

$$B = F(A, A'), \qquad A = G(B, B', A)$$

where A' denotes $dA/d\rho$, etc.

In practice the functions $A^{(n)}$ and $B^{(n)}$ will be tabulated at equal intervals in the logarithmic variable ρ, and the derivatives $A'^{(n)}$ and $B'^{(n)}$ are replaced by finite difference approximations, using central differences over most of the range and one-sided differences near the ends. The method is a natural extension of that used by Trafton, but the convergence of the iteration is analysed differently. Writing

$$\begin{aligned} \mu_m^{(n)} &= A_m^{(n)} - A_m \\ \nu_m^{(n)} &= B_m^{(n)} - B_m \end{aligned}$$

for the differences between the nth iterates and the true solution at the mth grid point, we can substitute into a Taylor series expansion of Eqs. (12) about the exact solution to obtain

$$\begin{aligned} \nu_m^{(n+1)} &= a\mu_m^{(n)} + bD(\mu_m^{(n)}) - S_m^{(n)} \\ \mu_m^{(n+1)} &= c\nu_m^{(n+1)} + dD(\nu_m^{(n+1)}) + e\mu_m^{(n)} - T_m^{(n)} \end{aligned} \tag{13}$$

where

$$\begin{aligned} a &= \partial F/\partial A = -k/f \\ b &= \partial F/\partial A' = -1/f \\ c &= \partial G/\partial B = -k/4g \\ d &= \partial G/\partial B' = 1/4g \\ e &= \partial G/\partial A = 3(B' - kB)/4gA \end{aligned} \tag{14}$$

and $S_m^{(n)}$ and $T_m^{(n)}$ are sums of terms of two kinds, (i) truncation errors of the difference approximations to the derivatives and (ii) terms of second and higher order in $\nu_m^{(n)}$ and $\mu_m^{(n)}$. In Eqs. (13) D denotes the difference approximation to the derivatives A' and B'.

This system of equations, for $m = 0, 1, 2, \ldots, M$, can be written in matrix form as

$$\begin{aligned} \boldsymbol{\nu}^{(n+1)} &= K_1\boldsymbol{\mu}^{(n)} - \mathbf{S}^{(n)} \\ \boldsymbol{\mu}^{(n+1)} &= K_2\boldsymbol{\nu}^{(n+1)} + K_3\boldsymbol{\mu}^{(n)} - \mathbf{T}^{(n)} \end{aligned}$$

in an obvious notation. Here K_1 and K_2 are band matrices, where the width of the band is determined by the choice of the difference approximations; K_3 is a diagonal matrix. Eliminating $\mathbf{v}^{(n+1)}$ from these equations gives

$$\boldsymbol{\mu}^{(n+1)} = K_4 \boldsymbol{\mu}^{(n)} - \{\mathbf{T}^{(n)} + K_2 \mathbf{S}^{(n)}\}$$

and if we assume that K_1 is non-singular we can deduce that

$$\mathbf{v}^{(n+1)} = K_1 K_4 K_1^{-1} \mathbf{v}^{(n)} + K_1 K_3 K_1^{-1} S^{(n-1)} - \mathbf{S}^{(n)} - K_1 \mathbf{T}^{(n-1)}$$

where $K_4 = K_3 + K_2 K_1$. Assuming that $\mathbf{T}^{(n)}$ and $\mathbf{S}^{(n)}$ are negligible, the iteration will therefore converge if all the eigenvalues of the matrix K_4 have modulus less than unity; the other matrix, $K_1 K_4 K_1^{-1}$, clearly has the same eigenvalues as K_4.
If, for example, the derivatives in (13) are approximated by the simple 3-point central difference formula, then a general row of the matrix K_4 has five non-zero elements centred on the diagonal, these elements being

$$\frac{b_m d_{m-1}}{4h^2}, \qquad \frac{-(a_m d_m + b_m c_{m-1})}{2h}, \qquad \frac{(-b_m d_{m-1} - b_m d_{m+1} + 4h^2(a_m c_m + e_m))}{4h^2}$$

$$\frac{(a_m d_m + b_m c_{m+1})}{2h}, \qquad \frac{b_m d_{m+1}}{4h^2}.$$

With the interval size likely to be used in practice the dominant terms in this row are the terms of order $1/h^2$; retaining only these terms, applying Gerschgorin's theorem, and using the expressions (14), we find that the iteration converges if $h^2 > 1/4fg$. Since $f(r)\,g(r) \to \infty$ as $r \to \infty$, this means that the iteration will converge if r is sufficiently large. If we used a grid of equal intervals in the r variable rather than in ρ the same analysis gives the conditions $h^2 > 1/4\bar{f}\bar{g}$, which now tends to a constant limit as $r \to \infty$. Hence the iteration may only converge when the step size h is sufficiently large.

In this analysis we have ignored the effect of the one-sided difference approximation which must be used near the ends of the range, and we have neglected all except the dominant terms of order $0(1/h^2)$. A full account of more refined estimates for the spectral radius of the matrix K_4 is given by Turner [6]. Although no simple practical estimate has been found, practical results show that the method does converge well for large values of r, but fails in the region of the classical turning point.

4. Solution near the Classical Turning Point

The iterative scheme described in the previous section is used to provide a solution of the amplitude equations for moderately large values of r. This solution is then used as an initial value for the inward integration of Eq. (11) towards the classical turning

point. It is well known that the use of standard explicit differences schemes for the solution of the non-relativistic amplitude equation is unstable except for small step sizes; similar problems are encountered with the solution of the relativistic equations. Faisal [7] has used a Newton method for the nonrelativistic equation, and the following scheme gives a similar method for the solution of Eq. (11).

$$\begin{aligned} A'^{(n)} + kA^{(n)} + fB^{(n)} &= 0 \\ B'^{(n)} - kB^{(n)} - \{g + 3f\theta^2/[A^{(n-1)}]^4\} A^{(n)} + 4f\theta^2/[A^{(n-1)}]^3 &= 0. \end{aligned} \tag{15}$$

At each level of iteration these equations are linear and are easily solved; the integration can proceed over a group of three or four grid points at a time, convergence at these points then being obtained before proceeding to the next group. This scheme may be used to continue the solution inwards to the classical turning point, or just beyond it if required. This is sufficient to permit matching to the outward integration.

We shall now discuss briefly the convergence of this discrete Newton iteration. Given an initial estimate $\hat{A}^{(0)}$ to the solution of the general system of non-linear equations $\mathbf{F}(\hat{\mathbf{A}}) = \mathbf{0}$, the Newton process may be written

$$\hat{\mathbf{A}}^{(n+1)} = \hat{\mathbf{A}}^{(n)} - [J(\hat{\mathbf{A}}^{(n)})]^{-1} \cdot \mathbf{F}(\hat{\mathbf{A}}^{(n)})$$

where J is the Jacobian of the system. This leads to the relation

$$\|\hat{\mathbf{A}}^{(n+1)} - \hat{\mathbf{A}}\| \leqslant \|\hat{C}^{(n)}\| \, \|\hat{\mathbf{A}}^{(n)} - \hat{\mathbf{A}}\|$$

where

$$\hat{C}^{(n)} = I - [J(\hat{\mathbf{A}}^{(n)})]^{-1} J(\hat{\boldsymbol{\xi}})$$

and $\hat{\boldsymbol{\xi}}$ lies between $\hat{\mathbf{A}}$ and $\hat{\mathbf{A}}^{(n)}$. The process will therefore converge provided that $\|\hat{C}^{(n)}\| < 1$. Consider the convergence of (15) at the $(m+1)$st grid point, so that

$$\hat{\mathbf{A}} = \begin{pmatrix} A_{m+1} \\ B_{m+1} \end{pmatrix}$$

and

$$\hat{C}^{(n)} = \alpha \begin{pmatrix} Hf & 0 \\ -(1+Hk) & 0 \end{pmatrix}$$

where

$$\alpha = \frac{-3Hf\theta^2 \left\{ \dfrac{1}{\xi^4} - \dfrac{1}{[A^{(n)}]^4} \right\}}{1 + H^2 D(r) + \dfrac{36H^2 f^2 \theta^2}{[A^{(n-1)}]^5}}$$

and $H = h\beta_0$, β_0 being the leading coefficient in the implicit difference scheme used for the numerical solution of (15). The value of α may be estimated by using the WKB approximation in the denominator, giving

$$\alpha \sim \frac{-3Hf\theta^2}{A^4 + 4H^2f^2\theta^2}\left[\frac{A^4}{\xi^4} - 1\right] = 0\left(\frac{1}{f}\right).$$

Thus given any reasonable initial estimate, the eigenvalues of $\hat{C}^{(n)}$ have modulus less than unity, and the Newton iteration converges.

If we solve (15) by the fourth-order Adams–Moulton process, the standard stability theory (see, for example, Lambert [8]) restricts the size of interval which can be used by requiring that $hD(\rho) < 5$. To use a reasonable sized step, such as $h = 0.05$, we are therefore restricted to the region $D < 100$. Close to the classical turning point there is no difficulty, since $D(\rho)$ is small, but for large r, $D(\rho)$ increases. But in this region the solution of the amplitude equations varies very slowly, and use of the trapezium rule was found to give more than adequate accuracy; the trapezium rule is unconditionally stable for any interval size.

5. An Alternative Transformation

An alternative pair of amplitude equations, instead of (9), may be obtained by writing

$$\begin{aligned} P(r) &= \hat{B}(r)\sin\{\hat{W}(r) + \hat{\phi}\} + \hat{C}(r)\cos\{\hat{W}(r) + \hat{\phi}\} \\ Q(r) &= \hat{A}(r)\sin\{\hat{W}(r) + \hat{\phi}\}. \end{aligned} \tag{16}$$

As before, $\hat{\phi}$ is an arbitrary phase, and $\hat{A}$, $\hat{B}$, $\hat{C}$, and $\hat{W}$ are unknown functions. Equation (3) will be referred to as the P-transformation, and Eq. (16) as the Q-transformation. The Q-transformation yields equations similar to those obtained from the P-form, and may be obtained very simply by the following interchange:

$$\begin{aligned} k &\leftrightarrow -k \\ f &\leftrightarrow -g \\ g &\leftrightarrow -f. \end{aligned} \tag{17}$$

This interchange leaves much of the previous analysis unaltered. The difference between the two forms of the transformation is most evident in the analysis of the Newton iteration in the previous section. In the Q-form of the analysis the non-zero off-diagonal element of $\hat{C}^{(n)}$ is of order $1/g$, and is thus a factor of about c^2 larger than in the P-form. The order of the diagonal element is unaltered, and both schemes have about the same region of convergence. However, the P-form scheme initially converges faster than the Q-form, and in practice it has been found that the Q-form often requires one extra iteration to obtain the same relative tolerance.

6. Smoother Variable Transformation

Following the analysis of Trafton [3] we have considered the use of the transformation from the amplitudes A, B to the "smoother" variables y, z, where

$$A = A_0 y, \qquad B = B_0 z$$

and A_0, B_0 are asymptotic forms of A and B as in (10). Substituting these into (11) we obtain a new pair of equations for y and z, which can be solved by the same methods as already described; further details may be found in Turner [6]. Although the new variables y and z vary more slowly than A and B for large values of r, the transformation does not seem to offer any real advantage. The number of Newton iterations for convergence has been found in practice to be the same as for the original variables A and B.

7. Results and Conclusions

In this section we first give some further details of the calculations. Initial values for the outward integration are obtained from a power series solution; the outward integration then uses the fourth-order Adams–Moulton method. Since the solution is monotonic in this region, accuracy is easily checked by the evaluation of a difference correction at the outermost point; if the accuracy is inadequate, the difference correction can be applied to the solution as necessary. For small values of the angular quantum number $|k| < 10$, it was found convenient to continue the outward integration just into the oscillatory region, but for larger values it is best to stop before the oscillatory region is reached. This choice seems to minimize the order of approximation used by both the outward integration and the inward solution. The solution for larger values of r was obtained as described in Sections 3 and 4, using the P-form of the transformation. The evaluation of $W(r)$, as the integral of $\psi(r)$ to use in (3), was performed by using the fourth-order formula discussed by Mayers and O'Brien [9]. In parts of the region where a higher-order method is used for the inward integration an integration method of the same order is used for the evaluation of this integral.

The results of the calculations have been checked by comparison with Darwin's analytic solution (see Flügge [10]), for the Coulomb scattering problem. We used asymptotic approximations for evaluating the complex confluent hypergeometric functions which define the solution. Buhring [11] has obtained a real asymptotic approximation to the problem, which has been related to the complex solution by Johnson and Cheng [12]. Since the result must be real, the complex series has the advantage that the size of the imaginary part of the result gives a useful check on its accuracy. Results for small values of r were checked by use of the power series form of the hypergeometric functions. We have calculated wavefunctions and phase shifts for a variety of different energies and angular momenta. An accuracy of six or seven

significant figures in the wavefunction, and about one fewer in the phase shift, has been obtained without any difficulty.

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