Coulomb wave expansion in electron scattering

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(Received 19 December 1979)

Coulomb waves are the solutions of the Dirac equation with a point-charge potential and are known analytic functions (Whittaker Functions). A number of matrix elements involving two Coulomb waves can be evaluated analytically, making the Coulomb waves basis an attractive alternative to the distorted wave basis. The difference between the point-charge potential and the distributed charge potential is treated as a perturbation. Phase shifts are calculated analytically for a distribution of the form $P(x)\exp(-ax)$, where $P(x)$ is a polynomial. Also calculated are radial integrals for electric monopole and quadrupole excitations in the same approximation. Scattering cross sections are compared with the conventional distorted wave calculations. The approximation works best for large angular momentum partial waves or low momentum transfer. It could not, in general, replace distorted wave calculations for the lowest partial waves but it could serve to restrict numerical calculations to this range, or it could be used for total cross sections and calculations of radiative corrections.

[NUCLEAR REACTIONS (e, e), (e, e') $E0$, $E2$ cross sections calculated. Matrix elements involving Coulomb waves evaluated analytically.]

INTRODUCTION

The conventional method of performing phase-shift analysis of elastic scattering from a finite size nucleus is based on a numerical integration of the Dirac equation.[1,2] All matrix elements for higher multipole moments and inelastic processes are likewise the result of numerical integration[3,4] and such procedures can get lengthy, to the point of being prohibitive, in calculations demanding a large number of partial waves. In particular, in calculations of radiative corrections (bremsstrahlung) and total cross sections (virtual photon spectrum), the full distorted wave calculation has never been used. Instead calculations use the plane wave Born approximation,[5,6] Sommerfeld Maue wave function,[7] or an approximation using the electron wave functions for the Coulomb field of a point charge.[8,9] Such wave functions lead to analytic, although not always simple, amplitudes. In this work the problem of including finite nuclear size effects is tackled by expanding the electron wave function in terms of point charge solutions, which we call Coulomb waves, instead of using the actual distorted wave basis. This can be accomplished systematically by adopting the Dirac Hamiltonian with the point charge potential $V_{\rm Coul}$ as the unperturbed Hamiltonian and treating the difference between this and the potential for the actual distributed charge as a perturbation. The entire procedure is of particular value if the radial integrations, which normally are done numerically, can be carried out analytically.

The Coulomb waves are known analytic functions and we need to know integrals involving a pair of these functions for a number of different potentials or kernels. We have chosen one of these, the product of an exponential function and a polynomial, for this investigation and have indicated how results might be extended to more general shapes. We use the notation

$$U(r) = V_{\rm Coul}(r) + V(r) .$$

Thus the Dirac-Coulomb Hamiltonian

$$H_{\rm DC} = -i\vec{\alpha}\cdot\vec{\nabla} + \beta m_e + V_{\rm Coul} \tag{1}$$

is identified as the unperturbed Hamiltonian and the actual equation we wish to solve is

$$[H_{\rm DC} + V(r)]\psi(\vec{\mathbf{r}}) = 0 . \tag{2}$$

In the following section we will discuss both the formal solution

$$\psi = \psi_{\rm inc} - \int G(\vec{\mathbf{r}}, \vec{\mathbf{r}}')V(\vec{\mathbf{r}}')\psi(\vec{\mathbf{r}}')d^3r' \tag{3}$$

[where $\psi_{\rm inc}(\vec{\mathbf{r}})$ is the incoming wave function, being an appropriate eigenfunction of $H_{\rm DC}$, and $G(\vec{\mathbf{r}}, \vec{\mathbf{r}}')$ is the Green's function for the same operator], and the first Born approximation obtained by substituting $\psi_{\rm inc}(\vec{\mathbf{r}})$ for $\psi(\vec{\mathbf{r}})$ in the integral on the right-hand side (rhs) of (3).

To assess the accuracy of this wave function we compare the scattered part of the approximate wave function with the full distorted wave treatment, which can be accomplished either by looking at the elastic scattering cross section or at the phase shifts.

Now in principle $V(r)$ contains all parts of the electromagnetic interaction not explicitly included in $V_{\rm Coul}$; that is, aside from the finite size correc-

tion, it contains the contribution of higher multipole moments (for a deformed nucleus) and all inelastic interactions. It is therefore of interest to see how well these terms are represented by the approximation. We have looked at some examples of monopole excitation and quadrupole excitation.

COULOMB WAVE EXPANSION

With the Dirac Coulomb Hamiltonian in the common form [Eq. (1)], a separation of the solutions is not possible; to achieve this we first write the matrices $\vec{\alpha}$ and β as direct products

$$\vec{\alpha}=\sigma_1\otimes\vec{\sigma},\quad \beta=\sigma_3\otimes I\,.$$

Then we carry out a unitary transformation with the matrix

$$S=\tfrac{1}{2}[I\otimes(I+i\sigma_r)+\sigma_3\otimes(I-i\sigma_r)],$$

which, when applied to the Hamiltonian $H_{\rm DC}$, gives us

$$H=-i\left(\frac{d}{dr}+\frac{1}{r}\right)\sigma_2\otimes I-\frac{1}{r}\sigma_1\otimes(\vec{\sigma}\cdot\vec{\mathrm{L}}+1)$$
$$+m_e\sigma_3\otimes I+V_{\rm Coul}\,, \tag{4}$$

where $\sigma_r=\vec{\sigma}\cdot\hat{r}$. This Hamiltonian has eigenfunctions which are direct products of a two-component radial function and a two component spin-angle function (angular momentum eigenvector) written $r^{-1}u_\kappa(r)\otimes\phi_\kappa^m(\hat{r})$, where κ is the Dirac angular momentum quantum number, an eigenvalue of the operator $-(\vec{\sigma}\cdot\vec{\mathrm{L}}+1)$.

The incoming wave function of Eq. (3), when expanded in terms of the product functions $u_\kappa^{\rm reg}\otimes\phi_\kappa^m(\hat{r})$, is given by

$$\psi_{\rm inc}(\vec{\mathrm{r}})=\frac{(4\pi)^{1/2}}{pr}\sum_\kappa i^l(2l+1)^{1/2}(l0\tfrac{1}{2}m\,|\,jm)$$
$$\times e^{i\delta_\kappa}u_\kappa^{\rm reg}(r)\otimes\phi_\kappa^m(\hat{\mathrm{r}})\,, \tag{5}$$

where δ_κ is the Coulomb phase shift, j is the total angular momentum, and l is the orbital angular momentum corresponding to the κth partial wave. In terms of κ

$$j=|\kappa|-\tfrac{1}{2},\quad l=\begin{cases}\kappa, & \kappa>0\\ -\kappa-1, & \kappa<0\,.\end{cases}$$

The radial function $u_\kappa^{\rm reg}(r)$ is the regular part of the Coulomb wave function and satisfies the matrix equation[10,11] derived from expression (4),

$$\frac{d}{dr}u_\kappa(r)=\left(\frac{1}{r}A-B\right)u_\kappa(r)\,, \tag{6}$$

where

$$A=\begin{bmatrix}-\kappa & e^2Z\\ -e^2Z & \kappa\end{bmatrix},\quad B=\begin{bmatrix}0 & -(E+m_e)\\ +(E-m_e) & 0\end{bmatrix}.$$

This form is referred to as the solution in the standard representation.

The part of the Green's function of Eq. (3), which we need is that for $r>r'$, and is (see Appendix A)

$$G(\vec{\mathrm{r}},\vec{\mathrm{r}}')=-\frac{i2E}{prr'}\sum_{\kappa,\mu}u_\kappa^{\rm out}(r)u_\kappa^{{\rm reg}T}(r')\otimes\phi_\kappa^\mu(\hat{r})\phi_\kappa^{\mu\,T}(\hat{r}')\,, \tag{7}$$

where $u_\kappa^{\rm out}(r)$ is the outgoing wave solution of Eq. (6), and the superscript T stands for transpose of the matrix.

DERIVATION OF THE PHASE SHIFTS

The wave function $\psi(\vec{\mathrm{r}})$ can also be expanded in terms of the Pauli spinors in a manner analogous to the Coulomb wave function $\psi_{\rm inc}(\vec{\mathrm{r}})$:

$$\psi(\vec{\mathrm{r}})=\frac{(4\pi)^{1/2}}{pr}\sum_\kappa i^l(2l+1)^{1/2}(l0\tfrac{1}{2}m\,|\,jm)$$
$$\times e^{i(\delta_\kappa+\delta_\kappa')}u_\kappa(r)\otimes\phi_\kappa^m(\hat{\mathrm{r}})\,, \tag{8}$$

where $u_\kappa(r)$ is the solution to the radial equation containing the entire potential $U(r)$. The phase shift in this expression differs from that of Eq. (5) (the Coulomb phase shift) by the additional δ_κ' which arises from the finite size of the nucleus. Substituting $\psi_{\rm inc}(\vec{\mathrm{r}})$, $G(\vec{\mathrm{r}},\vec{\mathrm{r}}')$, and $\psi(\vec{\mathrm{r}})$ from Eqs. (5), (7), and (8) in Eq. (3), we have

$$\psi(\vec{\mathrm{r}})=(4\pi)^{1/2}\sum_\kappa i^l(2l+1)^{1/2}(l0\tfrac{1}{2}m\,|\,jm)$$
$$\times e^{i\delta_\kappa}\left[\frac{u_\kappa^{\rm reg}(r)}{pr}+\frac{i2E}{pp'}e^{i\delta_\kappa'}\frac{u_\kappa^{\rm out}(r)}{r}M_E\right]$$
$$\otimes\phi_\kappa^m(\hat{\mathrm{r}})\,, \tag{9}$$

where

$$M_E=\int_0^\infty u_\kappa^{{\rm reg}T}(r')V(r')u_\kappa(r')dr'\,. \tag{10}$$

On substituting the asymptotic forms of $u_\kappa^{\rm reg}(r)$ and $u_\kappa^{\rm out}(r)$ (see Appendix A) in Eq. (9) and then equating the coefficients of the outgoing wave on either side, we are led to an expression for the shape induced phase shift

$$\delta_\kappa'=\arcsin\left(\frac{2E}{p'}M_E\right). \tag{11}$$

This result is the same as that obtained by Elton.[12] The shape induced phase shift δ_κ' cannot be determined unless we know the radial solution $u_\kappa(r)$. Evaluation of $u_\kappa(r)$ and therefore of the matrix element M_E can be done only by numerical integration. In the Coulomb wave approximation (CWA), we substitute the point Coulomb solution

$\psi_{inc}(\vec{r})$ instead of $\psi(\vec{r})$ in the integral of the rhs of Eq. (3). This substitution enables us to evaluate the integral analytically and gives us a relation correct to first order in δ_κ' which, on comparing amplitudes of both sides, gives the relation

$$\tilde{\delta}_\kappa' = \tfrac{1}{2} \arctan\left(\frac{4E}{p'}\tilde{M}_E\right), \tag{12}$$

where $\tilde{M}_E$ is the modification of the matrix element M_E in the Coulomb wave approximation. Hereafter, we shall use the symbol ~ to distinguish the phase shifts and radial integrals calculated in CWA. Expressions (12) and (11) are the same to first order in δ_κ'; hence for small $\tilde{M}_E$ we can use either. Occasionally, for small values of κ, we find moderately large values of $\tilde{M}_E$ (for which the approximation is marginal); we then find that expression (12) gives better results when compared with conventional phase shift calculations. We have used expression (12) for calculating the CWA phase shifts.

CALCULATION OF THE MATRIX ELEMENTS

In the Coulomb wave approximation, we are faced with the task of evaluating

$$\tilde{M}_E = \int_0^\infty u_\kappa^{reg}(r')^T \cdot u_\kappa^{reg}(r') V(r') dr' . \tag{13}$$

For the purpose of manipulation, it is found convenient to substitute a direct product for the matrix inner product $u_\kappa^T \cdot u_\kappa$ in Eq.(13); these are related by introducing the row matrix [1 0 0 1]

$$u_\kappa^{reg}(r)^T \cdot u_\kappa^{reg}(r) = [1\ 0\ 0\ 1] \cdot [u_\kappa^{reg}(r) \otimes u_\kappa^{reg}(r)] .$$

Thus we are led to consider the 4 component column matrix

$$\mathfrak{M}_E = \int_0^\infty u_\kappa^{reg}(r) \otimes u_\kappa^{reg}(r) V(r) dr . \tag{14}$$

In this form, it is possible to use solutions of the matrix first order differential equation for the product $u_\kappa^{reg} \otimes u_\kappa^{reg}$, as discussed in Refs. 11 and 13. The function

$$w_\kappa(r) = u_\kappa^{reg}(r) \otimes u_\kappa^{reg}(r)$$

satisfies an equation of type (6) except that the matrices A and B (here called A' and B') are of order 4

$$\frac{d}{dr} w_\kappa(r) = \left(\frac{1}{r}A' - B'\right) w_\kappa(r) , \tag{15}$$

where A', B' are related to the matrices of Eq. (6) by

$$\begin{aligned} A' &= A \otimes I + I \otimes A , \\ B' &= B \otimes I + I \otimes B , \end{aligned} \tag{16}$$

It is convenient at this point to use a representation in which A' is diagonal

$$A' = \mathrm{diag}(a_1, a_2, a_3, a_4) ,$$

for then we can write a solution to Eq. (15) in the form[11]

$$w_\kappa(r) = (I + V_1 r + V_2 r^2 + \cdots) r^{A'} . \tag{17}$$

In this representation

$$r^{A'} = \mathrm{diag}(r^{a_1}, r^{a_2}, r^{a_3}, r^{a_4}) \tag{18}$$

is arranged so that the first column of w_κ is the product $u_\kappa^{reg} \otimes u_\kappa^{reg}$. Expressions for the elements of the matrices V_n are given by the recurrence relation[11]

$$\{V_n\}_{ij} = \{B' V_{n-1}\}_{ij} / (a_i - n - a_j) \tag{19}$$

with $V_0 = I$. Substituting Eq. (17) in Eq. (14) (drop the prime on A),

$$\mathfrak{M}_E = \sum_n V_n \int_0^\infty r^{(A+n)} V(r) dr . \tag{20}$$

We have chosen a charge distribution for simplicity in calculation rather than for realistic portrayal of a particular nucleus. It has the form

$$\rho_E(r) = \frac{Ze^2\Delta^3\epsilon}{4\pi} e^{-\Delta r}\left[1 + \Delta r + \tfrac{1}{3}\left(\frac{1}{8\epsilon} - 1\right)\Delta^2 r^2\right] ,$$

which gives rise to the potential

$$u(r) = -\frac{e^2 Z}{r} + V(r) ,$$

where the perturbation $V(r)$ is given by

$$V(r) = Z e^2 \Delta e^{-\Delta r}\left[\frac{1}{\Delta r} + (\tfrac{3}{4} - \epsilon) + (\tfrac{1}{4} - \epsilon)\Delta r + \tfrac{1}{3}\left(\frac{1}{8\epsilon} - 1\right)\Delta^2 r^2\right] .$$

Thus in order to find the matrix $\mathfrak{M}_E$ we need to evaluate integrals of the form

$$I_\beta = \sum_n V_n \int_0^\infty e^{-\Delta r} r^{(A+n+\beta)} dr \tag{21}$$

which leads to a matrix series, which we write as

$$I_\beta = \sum_n M_n , \tag{22}$$

where

$$M_n = V_n \Gamma(A + n + \beta + 1) \Delta^{-(A+n+\beta+1)} . \tag{23}$$

In Eq. (23), A is a diagonal matrix and Δ^{-A} has the meaning given in (18): $\Gamma(A)$ and V_n are also matrices, of course.

We need to consider only the first column of the matrices M_n and for these we can establish the recurrence relation

$$(M_n)_{i1} = \frac{(a_1 + n + \beta)}{\Delta} (B M_{n-1})_{i1} . \tag{24}$$

The matrices we are dealing with at this point are of order 4 and are complex. Transforming back to the standard representation, we render A, B, and M_n all real (see Appendix B). In this representation A and B have two identical rows and columns; thus the order of the matrices under consideration can be reduced to 3. The final expression for the column M_n is given by (see Appendix B)

$$M_N = \frac{(2\gamma+n+\beta)}{\Delta(2\gamma+n)}\left[-\frac{1}{2\gamma n}\underline{X}+\frac{1}{2\gamma(4\gamma+n)}\underline{Y}-\underline{Z}\right]M_{n-1}\,, \tag{25}$$

where

$$M_0 = N\frac{\Gamma(2\gamma+\beta+1)}{\Delta^{2\gamma+\beta+1}}(E_\kappa - m\gamma)^2\begin{pmatrix}\kappa-\gamma\\ 2e^2Z\\ \kappa+\gamma\end{pmatrix},$$

$$\gamma = [\kappa^2-(e^2Z)^2]^{1/2}\,,$$

$$N = \frac{e^{\eta\pi}}{4E}\frac{|\Gamma(\gamma+i\eta)|^2(2p)^{2\gamma}}{(E\kappa-m\gamma)[\Gamma(2\gamma+1)]^2}\,,\quad \eta = Ze^2E/p\,.$$

The 3×3 matrices $\underline{X}$, $\underline{Y}$, and $\underline{Z}$, also functions of E, m_e, κ, Z, etc., are given explicitly in Appendix B.

To sum the matrix series of Eq. (22), we apply a technique to speed up convergence similar to the one discussed by Shanks[14] adapted here for matrix series. If we denote the sum of n terms by S_n,

$$S_n = \sum_{i=0}^{n-1} M_i$$

and successive terms are related by

$$M_i = R_i M_{i-1}\,,$$

then a faster converging sequence S_n', with the same limit as S_n for $n\to\infty$, is given by

$$S_n' = S_{n-1} + (I-R_n)^{-1}M_n\,.$$

From the expression for M_n it can be seen that convergence is slower the larger the values of a_1 and β. Typically we find that the use of S_n' reduces by 20—25% the number of terms required to achieve a given precision.

Convergence should in general be further enhanced by applying the technique for a second time. Denoting this new sum by S_n'' we find for the same cases that S_n'' converges to the same accuracy with a further 20% reduction in the number of terms. On close inspection this second application of the convergence technique, in our case, is technically invalid as it involves the inversion of a singular matrix which was achieved only through a fortuitous sequence of events in the computer. We have observed, however, that the addition of small but arbitrary quantities to break the singularity does not change the limit of S_n'' as $n\to\infty$. We have been unable to match the computer's success with analytical arguments.

Using Eq. (21) for the integral I_β, the expression for the radial integral $\tilde{M}_E$ is given by

$$\tilde{M}_E = e^2Z[1\ \ 0\ \ 1]\left[I_{-1}+(\tfrac{3}{4}-\epsilon)\Delta I_0+(\tfrac{1}{4}-\epsilon)\Delta^2 I_1 + \tfrac{1}{3}\left(\frac{1}{8\epsilon}-1\right)\Delta^3 I_2\right]\,. \tag{26}$$

In fact, we can express $\tilde{M}_E$ in terms of the I_{-1} alone, since the I_β are found to be related by the recurrence relation

$$I_{\beta+1} = (B+\Delta)^{-1}(A+\beta+1)I_\beta\,. \tag{27}$$

Substituting the value of $\tilde{M}_E$ in Eq. (12) we get the shape-induced phase shifts.

In the form given above the series S_n does not converge for $E \geq \Delta/2$. Therefore, for higher energies, it will be necessary to do analytic continuation of the integrand of I_β. To simplify calculations we have neglected the mass of the electron compared with its kinetic energy. We then have to calculate phase shifts for positive κ values only, since $\delta_\kappa' = \delta_{-\kappa}'$. The differential cross section for the elastic case is calculated from[15]

$$\frac{d\sigma}{d\Omega} = |\psi_{\text{out}}^*|^2\left(1+\tan^2\frac{\theta}{2}\right), \tag{28}$$

where

$$\psi_{\text{out}}^* = \frac{1}{2p}\sum_{\kappa>0}|\kappa|\,e^{i2(\delta_\kappa+\delta_\kappa')}[P_\kappa(\cos\theta)+P_{\kappa-1}(\cos\theta)] \tag{29}$$

and $P_\kappa(\cos\theta)$ is the Legendre function corresponding to the κth partial wave. To check our results we have obtained the expression for the radial integral M_E of Eq. (10) by numerical integration in the distorted-wave Born approximation (DWBA) and from there calculated the shape induced phase shifts δ_κ' and the cross section $d\sigma/d\Omega$.

We have also performed calculations of the inelastic scattering cross section for the case of electric monopole and quadrupole excitations, evaluating both the phase shifts and the radial integrals in the Coulomb wave approximation. We have considered transition charge distributions in each case derived from the ground state charge distribution $\rho_E(r)$

$$\rho_M(r) = \frac{d\rho_E(r)}{d\Delta} - \text{monopole}\,,$$

$$\rho_Q(r) = \frac{d\rho_E(r)}{dr} - \text{quadrupole}\,.$$

To simplify numerical procedures we have neglected the energy loss ω.[16] This enables us to evalu-

TABLE I. Comparison of shape induced phase shifts in CW and DW approximations for electron energy $E = 70$ MeV; precision is one part in 10^5.

	$Z = 20$		$Z = 82$	
κ	CWA	DWBA	CWA	DWBA
1	$-6.065\,73 \times 10^{-2}$	$-5.720\,55 \times 10^{-2}$	$-4.992\,16 \times 10^{-1}$	$-4.975\,35 \times 10^{-1}$
2	$-8.075\,33 \times 10^{-3}$	$-7.940\,07 \times 10^{-3}$	$-8.055\,85 \times 10^{-2}$	$-7.223\,32 \times 10^{-2}$
3	$-1.114\,04 \times 10^{-3}$	$-1.109\,09 \times 10^{-3}$	$-1.078\,59 \times 10^{-2}$	$-1.045\,35 \times 10^{-2}$
4	$-1.499\,61 \times 10^{-4}$	$-1.497\,89 \times 10^{-4}$	$-1.435\,87 \times 10^{-3}$	$-1.424\,23 \times 10^{-3}$
5	$-1.960\,72 \times 10^{-5}$	$-1.960\,18 \times 10^{-5}$	$-1.870\,57 \times 10^{-4}$	$-1.866\,64 \times 10^{-4}$
6	$-2.497\,77 \times 10^{-6}$	$-2.497\,65 \times 10^{-6}$	$-2.380\,84 \times 10^{-5}$	$-2.379\,56 \times 10^{-5}$
7	$-3.112\,11 \times 10^{-7}$	$-3.112\,15 \times 10^{-7}$	$-2.967\,15 \times 10^{-6}$	$-2.966\,76 \times 10^{-6}$
8	$-3.805\,32 \times 10^{-8}$	$-3.805\,41 \times 10^{-8}$	$-3.630\,61 \times 10^{-7}$	$-3.630\,57 \times 10^{-7}$
9	$-4.578\,85 \times 10^{-9}$	$-4.579\,10 \times 10^{-9}$	$-4.372\,67 \times 10^{-8}$	$-4.372\,76 \times 10^{-8}$
10	$-5.434\,40 \times 10^{-10}$	$-5.434\,85 \times 10^{-10}$	$-5.194\,57 \times 10^{-9}$	$-5.194\,90 \times 10^{-9}$

ate the cross section for monopole scattering by an expression which is analogous to Eq. (28), but now the scattering amplitude ψ^{+}_{out} becomes

$$\psi^{+}_{\text{out}} = \frac{1}{2p} \sum_{\kappa>0} |\kappa| \tilde{M}_{M\kappa} e^{i2(\delta_\kappa + \tilde{\delta}'_\kappa)} [P_\kappa(\cos\theta) + P_{\kappa-1}(\cos\theta)] ,$$

where $\tilde{M}_{M\kappa}$ is the radial integral for the κth partial wave. The radial integrals are determined from expression (13) for $\tilde{M}_E$ but using the monopole potential V_M instead of $V(r)$. To obtain radial integrals for the quadrupole scattering, the quadrupole potential V_Q is used instead of $V(r)$. The quadrupole cross section is calculated using standard techniques and the sum given by Griffy *et al.*[3]

As stated earlier, we do not get convergence for $E \geq \Delta/2$. Since we are concerned to see what happens at higher energies, we have used numerical methods rather than analytic continuation to evaluate radial integrals at 200 MeV. For this and for the comparable DWBA calculations, we have used the technique of Runge Kutta Gill for numerical integration.[17]

RESULTS AND DISCUSSIONS

We have done a number of calculations for the values of the size parameter $\Delta = 200$ MeV and $\epsilon = 0.1$. Tables I and II compare the shape-induced phase shifts obtained in the CWA for two values of atomic number to those obtained by DW calculations. Figure 1 shows the elastic cross section (divided by the Mott cross section) obtained using these phase shifts. The effect of CWA is to decrease the form factor at backward angles which can be traced to the first two phase shifts; by replacing these with the corresponding DW phase shifts, we can get the two curves to agree. This is consistent with the observations of Elton[12] and

TABLE II. Comparison of shape induced phase shifts in CW and DW approximations for electron energy $E = 200$ MeV; precision is one part in 10^5.

	$Z = 20$		$Z = 82$	
κ	CWA	DWBA	CWA	DWBA
1	$-1.765\,79 \times 10^{-1}$	$-1.724\,96 \times 10^{-1}$	$-6.238\,75 \times 10^{-1}$	$-1.025\,52$
2	$-7.439\,36 \times 10^{-2}$	$-7.236\,48 \times 10^{-2}$	$-3.843\,14 \times 10^{-1}$	$-4.065\,92 \times 10^{-1}$
3	$-3.373\,70 \times 10^{-2}$	$-3.312\,20 \times 10^{-2}$	$-1.972\,09 \times 10^{-1}$	$-1.883\,48 \times 10^{-1}$
4	$-1.549\,44 \times 10^{-2}$	$-1.532\,76 \times 10^{-2}$	$-9.284\,40 \times 10^{-2}$	$-8.868\,64 \times 10^{-2}$
5	$-7.097\,37 \times 10^{-3}$	$-7.054\,86 \times 10^{-3}$	$-4.263\,14 \times 10^{-2}$	$-4.138\,74 \times 10^{-2}$
6	$-3.226\,85 \times 10^{-3}$	$-3.216\,49 \times 10^{-3}$	$-1.937\,15 \times 10^{-2}$	$-1.904\,81 \times 10^{-2}$
7	$-1.454\,22 \times 10^{-3}$	$-1.451\,79 \times 10^{-3}$	$-8.728\,45 \times 10^{-3}$	$-8.650\,01 \times 10^{-3}$
8	$-6.495\,76 \times 10^{-4}$	$-6.490\,20 \times 10^{-4}$	$-3.900\,53 \times 10^{-3}$	$-3.882\,30 \times 10^{-3}$
9	$-2.877\,18 \times 10^{-4}$	$-2.875\,94 \times 10^{-4}$	$-1.729\,11 \times 10^{-3}$	$-1.725\,00 \times 10^{-3}$
10	$-1.264\,47 \times 10^{-4}$	$-1.264\,20 \times 10^{-4}$	$-7.607\,00 \times 10^{-4}$	$-7.597\,98 \times 10^{-4}$

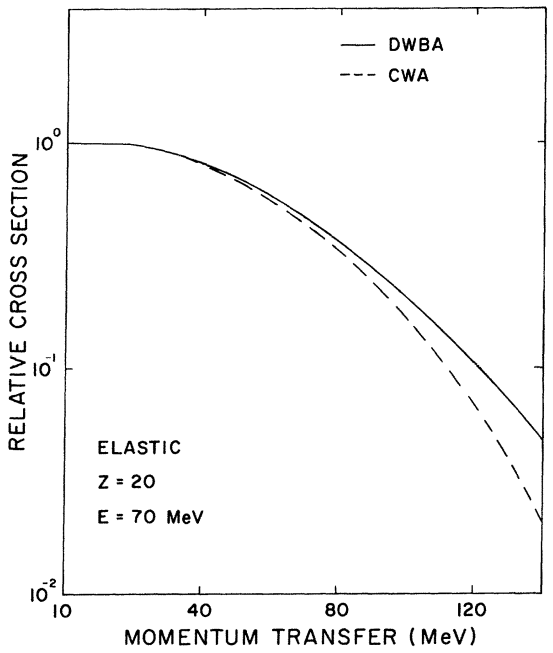

FIG. 1. Elastic electron scattering calculated using Coulomb wave (CW) and distorted wave (DW) approximations. Target is a fictitious nucleus with $Z=20$ having charge distribution ρ_E in text. Incident energy is 70 MeV.

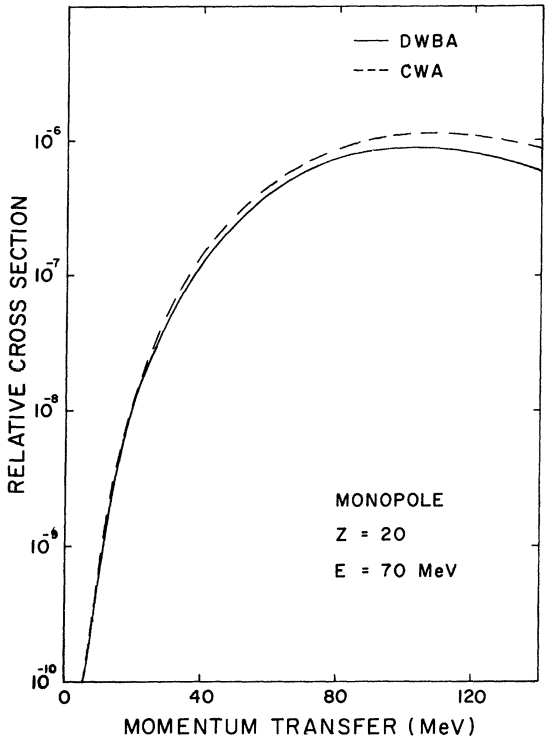

FIG. 2. Monopole inelastic electron cross section calculated in CW and DW approximations. Target as described in Fig. 1 having transition charge density ρ_M in text. Incident energy is 70 MeV, excitation energy is neglected.

Acheson[18] for lower energy electrons that the first one or two phase shifts must be evaluated exactly. However, for processes in which low momentum transfer is dominant, such as total cross section, the approximation should be adequate.

This approximation does not always give as good results for the elastic cross section at higher energies. The particular charge distribution that we are using has the unusual property of producing a smoothly decreasing cross section as a function of angle, and the CWA is unable to maintain this and tends to a diffraction pattern, which is a more common behavior.

Figures 2 and 3 display the behavior of the monopole cross section for different values of energy. In both cases, the CWA cross section gives fairly good agreement with the DWBA cross section. At lower energies, for $Z=20$ it is observed that if we replace the CWA phase shifts by the DW phase shifts the cross section does not change significantly. This implies that the difference between the two curves is due to the difference between the radial integrals $\tilde{M}_M$ and M_M, calculated in the CWA and DWBA, respectively.

Also shown is a curve for quadrupole scattering of 70 MeV electrons (Fig. 4). There seems to be rather good agreement between the two curves for any Z. Again, the difference we observe is a consequence of using the approximate radial integrals $\tilde{M}_Q$ and is relatively insensitive to the phase shifts.

CONCLUSIONS

A general observation is that the first few phase shifts and radial integrals do not agree well with the corresponding DWBA quantities and we would have to make special provisions for these in calculating angular distributions. However, we are not advocating these approximate wave functions for this purpose for which many better calculations already exist.

Our approximation provides a method of evaluating the phase shifts and the radial integrals, particularly for large partial waves, where DWBA calculations sometimes run into problems with convergence and matching of wave functions with asymptotic wave functions, etc. It also leads to good results for forward scattering and could conceivably be used for determining the total cross sections.

An advantage of having analytic expressions for phase shifts and matrix elements is the possibility of exploiting expressions for their dependence

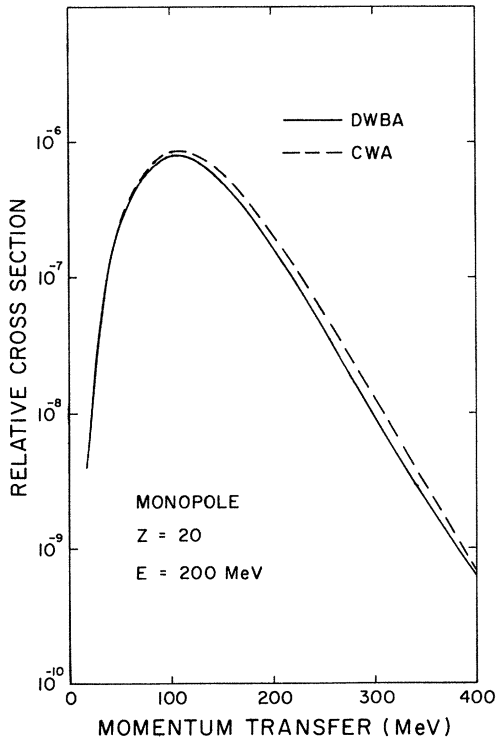

FIG. 3. Monopole scattering as in Fig. 2, but at higher energy.

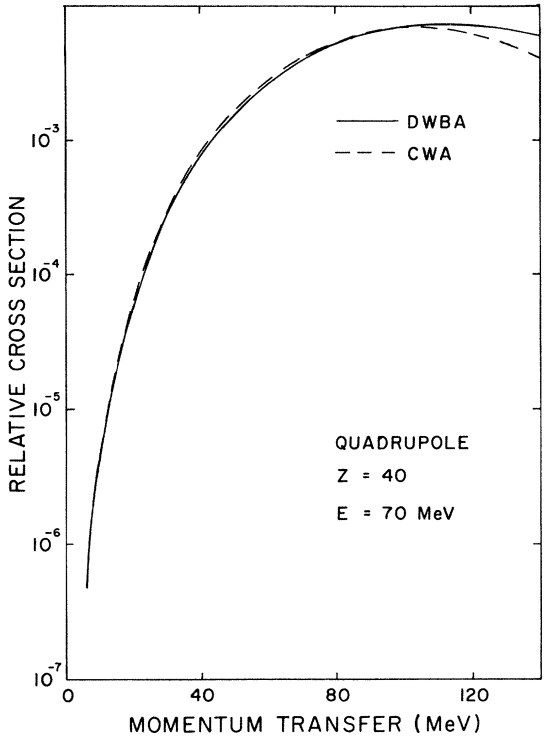

FIG. 4. Quadrupole inelastic scattering calculated in CW and DW approximations. For incident energy $E=70$ MeV and any Z, agreement is as good or better or better than shown here for $Z=40$. Transition charge is ρ_Q in text.

on physical parameters, particularly the energy and the size parameter Δ. In the limit $m_e \to 0$, the matrix I_β satisfies a first order differential equation[13]

$$\frac{dI_\beta}{dE} = TI_\beta ,$$

where

$$T = \left[\frac{A}{E} - B(B+\Delta)^{-1}(A+\beta+1)\right] .$$

Elton[12] has made use of expressions for the energy derivative of the shape induced phase shifts $[d\zeta_n/dE)$ in his notation] to derive the phase shift at one energy from that at another. The present treatment extends this possibility to matrix elements of any multipole order.

We do not consider that the ability to obtain an analytic expression is necessarily restricted to charge distribution used here, although the form $e^{-\Delta r}P(r)$, where P is any polynomial, is a good candidate for model independent analysis. It is unlikely that for any distribution a single expression can be written to cover all ranges of energy. The series we have use, for example, do not converge for $E \geq \Delta/2$ and a high energy expansion would obviously be desirable.

We are grateful to Dr. L. E. Wright for assistance, particularly with the phase shift analysis program. Calculations described herein were carried out on the Ohio University IBM 370/158 computer. This work was supported by the U.S. Department of Energy and by the Ohio University Research Committee.

APPENDIX A: MATRIX GREEN'S FUNCTION

The radial equation resulting from applying the transformed Hamiltonian H of Eq. (4) to the separated solution $u_\kappa(r)\otimes\phi_\kappa^m(\hat{r})$ is

$$\left[-i\sigma_2\frac{d}{dr} + \frac{\kappa}{r}\sigma_1 + m\sigma_3 + V(r)\right]u_\kappa(r) = Eu_\kappa(r) . \quad \text{(A1)}$$

Inserting the Coulomb potential for $V(r)$, we can rewrite the operator more compactly in terms of the matrices A and B of Eq. (5), and the equation for its Green's function $G(r,r')$ is

$$-i\sigma_2\left(\frac{d}{dr} - \frac{1}{r}A + B\right)G(r,r') = \delta(r-r') . \quad \text{(A2)}$$

The Green's function with the boundary conditions

we require must have the form

$$G(r,r')=a_\kappa[u_\kappa^{\mathrm{reg}}(r)u_\kappa^{\mathrm{out}\,T}(r')\mathfrak{U}(r'-r) + u_\kappa^{\mathrm{out}}(r)u_\kappa^{\mathrm{reg}\,T}(r')\mathfrak{U}(r-r')], \quad \text{(A3)}$$

where $\mathfrak{U}(r'-r)$ is the Heaviside step function

$$\mathfrak{U}(r'-r)=1 \text{ for } r'>r$$
$$=0 \text{ for } r'<r,$$

and u_κ^{reg} and u_κ^{out} are solutions of Eq. (1a) with the asymptotic forms

$$u_\kappa^{\mathrm{reg}}(r)\sim\frac{1}{(2E)^{1/2}}\begin{bmatrix}(E+m)^{1/2}\cos(pr+\Delta)\\ -(E-m)^{1/2}\sin(pr+\Delta)\end{bmatrix} \quad \text{(A4)}$$

and

$$u_\kappa^{\mathrm{out}}(r)\sim\frac{1}{(2E)^{1/2}}\begin{bmatrix}(E+m)^{1/2}e^{i(pr+\Delta)}\\ i(E-m)^{1/2}e^{i(pr+\Delta)}\end{bmatrix}, \quad \text{(A5)}$$

where

$$\Delta=\eta\ln 2pr+\delta_\kappa-\tfrac{1}{2}(l+1)\pi,$$
$$\eta=e^2ZE/p.$$

Inserting Eq. (3a) into Eq. (2a) and integrating with respect to r, we get

$$-i\sigma_2 a_\kappa[u_\kappa^{\mathrm{reg}}(r)u_\kappa^{\mathrm{out}\,T}(r)-u_\kappa^{\mathrm{out}}(r)u_\kappa^{\mathrm{reg}\,T}(r)]=I. \quad \text{(A6)}$$

Substituting Eqs. (4a) and (5a) in Eq. (6a), we get

$$a_\kappa=-\frac{2iE}{p}.$$

APPENDIX B: SOME DETAILS OF MATRIX MANIPULATIONS

Expression (19) is only valid in a representation with matrix A diagonal (17). To transform it we must restrict ourselves to the first column (which is all that is required)

$$\{V_n\}_{i1}=\frac{1}{a_i-n-a_1}\{BV_{n-1}\}_{i1}, \quad \text{(B1)}$$

where

$$a_1=-a_4=2\gamma,\quad a_2=a_3=0,$$

and

$$\gamma=[\kappa^2-(e^2Z)^2]^{1/2}.$$

This can be written in the form of an ordinary matrix product

$$\{V_n\}_{i1}=[A-(n-a_1)I]^{-1}(BV_{n-1})_{i1}$$

which can then be subjected to a similarity transformation in the standard way. Using the transformation matrix

$$C=c\otimes c$$

with

$$c=\begin{bmatrix}(E\kappa-m\gamma)(\kappa-\gamma)^{1/2} & p(\eta+i\gamma)(\kappa+\gamma)^{1/2}\\ (E\kappa-m\gamma)(\kappa+\gamma)^{1/2} & p(\eta+i\gamma)(\kappa-\gamma)^{1/2}\end{bmatrix}$$

we get in the new representation

$$V_n'=Q_nV_{n-1}',$$

where Q_n has the explicit n dependence

$$Q_n=\frac{1}{(2\gamma+n)}\left[-\frac{1}{2\gamma n}D_1+\frac{1}{2\gamma(4\gamma+n)}D_2-D_3\right]. \quad \text{(B2)}$$

In our case, the expressions for D_1, etc., show that each of these matrices has its second columns identical with the third column and the second rows identical with the third row; consequently, each can be reduced to a 3×3 form, for example,

$$D_1=\begin{bmatrix}1&0&0\\0&1&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}-2cad & -a^2e+c^2d & 2cae\\ -2c^2d & -cae+cdb & 2c^2e\\ -2cbd & -c^2e+b^2d & 2cbe\end{bmatrix}\begin{bmatrix}1&0&0&0\\0&1&1&0\\0&0&0&1\end{bmatrix}, \text{etc.},$$

where

$$a=\kappa-\gamma,\quad b=\kappa+\gamma,\quad c=e^2Z,$$
$$d=E-m_e,\quad e=E+m_e.$$

The entire Eq. (2b) can then be reduced to the 3×3 form

$$V_n'=\frac{1}{2\gamma+n}\left[-\frac{1}{2\gamma n}\underline{X}+\frac{1}{2\gamma(4\gamma+n)}\underline{Y}-\underline{Z}\right]V_{n-1}',$$

where

$$V_0'=(E\kappa-m\gamma)^2\begin{bmatrix}\kappa-\gamma\\ 2e^2Z\\ \kappa+\gamma\end{bmatrix},$$

$$\underline{X}=\begin{pmatrix} a \\ 2c \\ b \end{pmatrix}(-2cd \;\; bd-ae \;\; 2ce),$$

$$\underline{Y}=\begin{pmatrix} b \\ 2c \\ a \end{pmatrix}(-2cd \;\; ad-be \;\; 2ce),$$

$$\underline{Z}=\begin{bmatrix} 0 & -e & 0 \\ 2d & 0 & -2e \\ 0 & d & 0 \end{bmatrix}.$$

This if the form used in Eq. (25)

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