Polarized electron scattering from oriented nuclei in distorted wave method

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Expressions are developed for the differential electroexcitation cross section and the polarization of the scattered electrons in polarized electron scattering from oriented nuclei. These expressions are derived for a mixed multipole transition using the distorted-wave method. The effect of the Coulomb distortion is discussed for electric dipole transition of unoriented ^{238}U using 20 MeV partially polarized electrons.

I. INTRODUCTION

Electrons have been used successfully over the years to probe the nucleus. The roles of the electron and nucleus are going to be as significant as ever in helping us to get more insight through the nuclear structure. However, until recent years, in the vast majority of experiments, technological difficulties required averaging out the incoming and outgoing electron's spin and target orientation. This naturally reduces the amount of information that could be gained.

In recent years, because of technological advancement, polarized electron beams and oriented target nuclei are more readily available. This, in turn, requires the advancement of available theoretical calculations concerning polarization. There has been a number of excellent works on the topic of polarized electron and/or oriented nuclei (e.g., see Refs. 1–5). In 1964 Weigert and Rose completed a comprehensive work on this topic.[2] They did their calculations in plane-wave Born approximation (PWBA). However, their approach can be applied to distorted-wave methods and this is my objective in this article. I achieve this in part by using a code that calculates the electron scattering matrix elements in distorted-wave methods for finite-size nuclei.[6–8] This code has been used successfully to study electrofission of heavy nuclei with low to moderate incoming electron energy (5–200 MeV).

In Sec. II, I present the formalism which includes the derivation of the cross section and polarization of the outgoing electron. The effect of Coulomb distortion in the electric dipole transition of unoriented ^{238}U using 20-MeV, partially polarized electrons and the final remarks are presented in Sec. III.

II. FORMALISM

A. Transition matrix

Consider a process in which an electron with energy E_1, momentum $\mathbf{k}_1$, and polarization $\mathbf{P}_1$ interacts with a fixed target nucleus (the recoil effect is negligible for incoming electrons with low to moderate energies and heavy target nuclei) initially in state $\mathbf{J}_1,M_1$. As a result of the interaction, the electron scatters into the final state $\mathbf{E}_2,\mathbf{k}_2,\mathbf{P}_2$ and the nucleus by absorbing $\omega=E_1-E_2$, and angular momentum $\mathbf{L}$ transfers into the excited state $\mathbf{J}_2,M_2$. To study this process and investigate the effect of polarization, it is convenient to use the density-matrix approach and define a transition matrix A in such a way that[2,3]

$$\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)\rho(\mathbf{P}_2)=A\rho(\mathbf{P}_1)A^{\dagger}\ , \tag{1}$$

where

$$\rho(\mathbf{P})=\tfrac{1}{2}(1+\boldsymbol{\sigma}\cdot\mathbf{P}) \tag{2}$$

is the nonrelativistic density matrix, $\sigma_{i(i=1,2,3)}$ are the Pauli matrices, $\mathbf{P}$ is the polarization vector, and $\sigma(\mathbf{k}_1,\mathbf{k}_2,P_1)$ is the scattering cross section. Equation (1) and (2) imply that

$$\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)=\mathrm{Tr}[A\rho(\mathbf{P}_1)A^{\dagger}]\ , \tag{3}$$

and

$$\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)\mathbf{P}_2=\mathrm{Tr}[\boldsymbol{\sigma}A\rho(\mathbf{P}_1)A^{\dagger}]\ . \tag{4}$$

Therefore, the transition matrix A completely determines $\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)$ and $\mathbf{P}_2$.

Let a_1 and a_2 be the spinors of the incident and the outgoing electrons (see Appendix A for more detail). Then define a matrix T that transfers a_1 into a_2, namely,

$$a_2=Ta_1\ . \tag{5}$$

It is possible to relate matrices T and A and therefore rewrite Eq. (5) in terms of A:

$$\tfrac{1}{2}(1+\beta)a_2=\left[\frac{k_1(E_2+m_e)}{k_2(E_1+m_e)}\right]^{1/2}A\tfrac{1}{2}(1+\beta)a_1\ . \tag{6}$$

In the following I will find a relationship between a_2 and a_1 through solving the corresponding Hamiltonian and hence determining A through Eq. (6).

In distorted-wave methods the Hamiltonian of the scattering process is

$$(H_e+H_N+H_{\mathrm{int}})\Psi=E\Psi\ , \tag{7}$$

where Ψ is the wave function of the electron-nucleus system, and E is the energy of the system. H_e is the Hamiltonian of the electron in the Coulomb field of the nucleus,

H_N is the nucleus Hamiltonian, and $H_{\rm int}$ represents the interaction between the electron and nucleus exclusive of the Coulomb interaction. From Eq. (7) one gets

$$(H_e-E_2)\psi_{e_2}=-H_{\rm int}\psi_{e_1}\ , \tag{8}$$

where ψ_{e_2} and ψ_{e_1} are the outgoing and incoming electron wave functions, respectively (see Appendix A). Using the Green's-function method, one can write

$$\psi_{e_2}(\mathbf{r}_2)=-\int G(\mathbf{r}_1,\mathbf{r}_2)H_{\rm int}\psi_{e_1}(\mathbf{r}_1)d\mathbf{r}_1\ , \tag{9}$$

where $G(\mathbf{r}_1,\mathbf{r}_2)$ is the Green's function satisfying the following equation:

$$(H_e-E_2)G(\mathbf{r}_1,\mathbf{r}_2)=\delta(\mathbf{r}_1,\mathbf{r}_2)I\ , \tag{10}$$

with I being a unit matrix. Using Eq. (A1) I rewrite Eq. (10) as follows:

$$[\boldsymbol{\alpha}\cdot\mathbf{k}+\beta m_e+V(r)-E_2]G(\mathbf{r}_1,\mathbf{r}_2)=\delta(\mathbf{r}_1,\mathbf{r}_2)I\ . \tag{11}$$

The solution to this equation is[9]

$$G(\mathbf{r}_1,\mathbf{r}_2)=\pi i\sum_{\kappa\mu}\psi_\kappa^\mu(\mathbf{r}_1)\phi_\kappa^{\mu\dagger}(\mathbf{r}_2)\quad \text{for } r_1>r_2\ , \tag{12}$$

and

$$G(\mathbf{r}_1,\mathbf{r}_2)=\pi i\sum_{\kappa\mu}\phi_\kappa^\mu(\mathbf{r}_1)\psi_\kappa^{\mu\dagger}(\mathbf{r}_2)\quad \text{for } r_2>r_1\ , \tag{13}$$

where ϕ is the regular solution to the Dirac equation, while ψ is, in general, a linear combination of the regular and irregular solutions (see Appendix A for more detail). Using Eqs. (9), (12), and (13), one gets the following asymptotic form for the outgoing electron wave function:

$$\psi_{\rm as}(\mathbf{r}_2)=a_2\frac{e^{ik_2r}}{r}\ , \tag{14}$$

with

$$a_2=-i\left[\frac{\pi}{k_2}\right]^{1/2}\sum_{\kappa_2\mu_2}e^{i\delta_{\kappa_2}}(-i)^{l_2}\langle\phi_{\kappa_2}^{\mu_2}|H_{\rm int}|\psi_{e_1}\rangle\begin{bmatrix}\sqrt{E_2+m_e}\,\chi_{\kappa_2}^{\mu_2}(\hat{k}_2)\\ -\sqrt{E_2-m_e}\,\chi_{\kappa_2}^{\mu_2}(\hat{k}_2)\end{bmatrix} \tag{15}$$

being the spinor of the scattered electron. Using Eqs. (A3), (A11), and (A13) in Eq. (15), one gets

$$\tfrac{1}{2}(1+\beta)a_2=\sum_{m_1m_2}c_{m_1}b_{m_1m_2}\chi^{m_2}\ , \tag{16}$$

where

$$b_{m_1m_2}=(-i)4\pi\left[\frac{\pi}{k_2}\right]^{1/2}\left[\frac{\pi}{2E_1k_1}\right]^{1/2}\sqrt{(E_2+m_e)}$$
$$\times\sum_{\substack{\kappa_1\mu_1\\ \kappa_2\mu_2}}e^{i(\delta_{\kappa_2}+\delta_{\kappa_1})}i^{l_1-l_2}C(l_1\tfrac{1}{2}j_1;\mu_1-m_1,m_1)C(l_2\tfrac{1}{2}j_2;\mu_2-m_2,m_2)Y_{l_2}^{\mu_2-m_2*}(\hat{k}_2)\left[\frac{(2l_1+1)}{4\pi}\right]^{1/2}\delta_{\mu_1m_1}\xi_{\kappa_1\kappa_2}^{\mu_1\mu_2}\ . \tag{17}$$

In Eq. (17), $C(\cdots)$ is the Clebsch-Gordan coefficient and

$$\xi_{\kappa_1\kappa_2}^{\mu_1\mu_2}=\langle\phi_{\kappa_2}^{\mu_2}|H_{\rm int}|\phi_{\kappa_1}^{\mu_1}\rangle\ . \tag{18}$$

Also, in Eq. (17), I have assumed that the incident beam is along the z axis and therefore replaced $Y_{l_1}^{\mu_1-m_1*}(\hat{k}_1)$ with $\sqrt{(2l_1+1)/(4\pi)}\delta_{\mu_1m_1}$.

Following the works by Zamani-Noor and Onley,[6] Zamani-Noor,[8] Gargaro and Onley,[10] and Gargaro[11], I expand the right-hand side of Eq. (18) and write

$$\xi_{\kappa_1\kappa_2}^{\mu_1\mu_2}=4\pi\omega\alpha^{1/2}\sum_{LM}(-1)^{j_1+1/2}\left[\frac{2j_1+1}{4\pi}\right]^{1/2}C(j_1j_2L;-\tfrac{1}{2},\tfrac{1}{2})C(j_1Lj_2;\mu_1M\mu_2)$$
$$\times[R^{EL}(\kappa_1,\kappa_2)N^{EL}(\omega)+R^{ML}(\kappa_1,\kappa_2)N^{ML}(\omega)]\ , \tag{19}$$

where $R^{EL}(\kappa_1,\kappa_2)$ and $R^{ML}(\kappa_1,\kappa_2)$ are the radial integrals for electric and magnetic transitions, respectively (see Appendix B for more detail), while $N^{EL}(\omega)$ and $N^{ML}(\omega)$ are the reduced nuclear matrix elements for electric and magnetic transitions, respectively, and α is the fine structure constant. Using Eq. (19), I rewrite Eq. (17) as follows:

$$b_{m_1m_2}=(-i)8\pi^{5/2}\left[\frac{E_2+m_e}{2E_1k_1k_2}\right]^{1/2}\sum_{\substack{\kappa_1\kappa_2\\LM}} e^{i(\delta_{\kappa_2}+\delta_{\kappa_1})}i^{l_1-l_2}(-1)^{(j_1+1/2)}\sqrt{(2j_1+1)(2l_1+1)}$$
$$\times Y_{l_2}^{m_1+M-m_2*}(\hat{k}_2)C(l_1\tfrac{1}{2}j_1;0,m_1)C(l_2\tfrac{1}{2}j_2;m_1+M-m_2,m_2)C(j_1j_2L;-\tfrac{1}{2},\tfrac{1}{2})$$
$$\times C(j_1Lj_2;m_1,M)C(J_1LJ_2;M_1,M)[R^{EL}(\kappa_1,\kappa_2)N^{EL}(\omega)+R^{ML}(\kappa_1,\kappa_2)N^{ML}(\omega)]\ . \tag{20}$$

Now that $b_{m_1m_2}$ has been evaluated in terms of calculable terms, namely, the electron radial integrals and nuclear matrix elements, I use Eqs. (6) and (16) to write

$$\sum_{m_1m_2} c_{m_1}b_{m_1m_2}\chi^{m_2}=\left[\frac{k_1(E_2+m_e)}{k_2(E_1+m_e)}\right]^{1/2}\times A\left[\frac{E_1+m_e}{2E_1}\right]^{1/2}\sum_{m_1}c_{m_1}\chi^{m_1}\ , \tag{21}$$

with the following result for A:

$$A=\left[\frac{2E_1k_2}{k_1(E_2+m_e)}\right]^{1/2}\begin{bmatrix}b_{++} & b_{-+}\\ b_{+-} & b_{--}\end{bmatrix}\ , \tag{22}$$

where $+$ stands for $+\frac{1}{2}$ and $-$ stands for $-\frac{1}{2}$. Using Eq. (22) in Eqs. (3) and (4) will determine the cross section and polarization of the scattered electron completely.

B. Cross section

To calculate the cross section for nuclear transition $J_1\rightarrow J_2$, one basically has to evaluate terms of the following type [see Eqs. (3) and (22)]:

$$Z_{J_1m_1m_1'}^{J_2m_2m_2'}=\frac{2E_1k_2}{k_1(E_2+m_e)}\sum_{M_1M_2}w_{M_1}b_{m_1m_2}b^*_{m_1'm_2'}\ , \tag{23}$$

where w_{M_1} is the probability of sublevel M_1 being occupied. If w_{M_1} is the same for all M_1 values, then the target nucleus is unoriented; otherwise, the target is oriented. To perform the sum over M_1 and M_2, we write w_{M_1} in terms of statistical tensors f_I, which were first introduced by Fano.[12] In what follows I assume that the oriented nucleus is axially symmetric with the symmetry axis being the spin quantization axis. Hence[13]

$$w_{M_1}=\sum_I f_I(2I+1)^{1/2}C(J_1IJ_1;M_10)\ . \tag{24}$$

An oriented target is defined to be aligned if $w_{M_1}=w_{-M_1}$; otherwise, it is polarized. Therefore, from Eq. (24) it follows that even values of I ($I\neq0$) represent the contribution from alignment of the nuclei, while odd contributions represent the polarization of the nucleus. For $I=0$, $f_0=1/(2J_1+1)$, which is always present. Inserting Eq. (24) into Eq. (23) and using Eq. (20), one can sum over M_1 and M_2 to get

$$Z_{J_1m_1m_1'}^{J_2m_2m_2'}=\frac{64\pi^5\omega^2\alpha}{k_1}\sum_{\substack{\kappa_1\kappa_2\\\kappa_1'\kappa_2'\\LL'\\M\\I}}(-)^{J_2-J_1}(2J_2+1)\sqrt{2J_1+1}(-)^Mf_IW(J_1J_1LL';IJ_2)C(LL'I;M,-M)$$
$$\times e^{i(\delta_{\kappa_2}+\delta_{\kappa_1})}i^{l_1-l_2}(-)^{j_1+1/2}\sqrt{(2j_1+1)(2l_1+1)}Y_{l_2}^{m_1+M-m_2^*}(\hat{k}_2)$$
$$\times e^{-i(\delta_{\kappa_2'}+\delta_{\kappa_1'})}(-i)^{l_1'-l_2'}(-)^{j_1'+1/2}\sqrt{(2j_1'+1)(2l_1'+1)}Y_{l_2'}^{m_1'+M-m_2'}(\hat{k}_2)$$
$$\times C(l_1\tfrac{1}{2}j_1;0,m_1)C(l_2\tfrac{1}{2}j_2;m_1+M-m_2,m_2)C(j_1j_2L;-\tfrac{1}{2},\tfrac{1}{2})C(j_1Lj_2;m_1,M)$$
$$\times C(l_1'\tfrac{1}{2}j_1';0,m_1')C(l_2'\tfrac{1}{2}j_2';m_1'+M-m_2',m_2')C(j_1'j_2'L';-\tfrac{1}{2},\tfrac{1}{2})C(j_1'L'j_2';m_1',M)$$
$$\times[R^{EL}(\kappa_1,\kappa_2)N^{EL}(\omega)+R^{ML}(\kappa_1,\kappa_2)N^{ML}(\omega)]$$
$$\times[R^{EL'*}(\kappa_1',\kappa_2')N^{EL'*}(\omega)+R^{ML'*}(\kappa_1',\kappa_2')N^{ML'*}(\omega)]\ . \tag{25}$$

For an unoriented target, only the $I=0$ term will contribute and Eq. (25) for each multipole transition L simplifies to

$$Z^{J_2 m_2 m_2'(\lambda L)}_{J_1 m_1 m_1'} = \frac{64\pi^5\omega^2\alpha}{k_1}\frac{(2J_2+1)}{(2J_1+1)}\frac{1}{(2L+1)}|N^{\lambda L}(\omega)|^2 \times \sum_M \left| \sum_{\kappa_1\kappa_2} e^{i(\delta_{\kappa_2}+\delta_{\kappa_1})} i^{l_1-l_2}(-)^{j_1+1/2}\sqrt{(2j_1+1)(2l_1+1)}\,Y^{m_1+M-m_2^*}_{l_2}(\hat{k}_2) \times C(l_1\tfrac{1}{2}j_1;0,m_1)C(l_2\tfrac{1}{2}j_2;m_1+M-m_2,m_2)C(j_1j_2L;-\tfrac{1}{2},\tfrac{1}{2})C(j_1Lj_2;m_1,M) \times R^{\lambda L}(\kappa_1,\kappa_2)\right|^2 , \tag{26}$$

where λ stands for the type of transition (i.e., $\lambda=E$ for electric transition, $\lambda=M$ for magnetic transition). Using Eqs. (3), (20), and (25), I calculate the cross section with the following result:

$$\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)=[(P_{1x}-iP_{1y})(Z^{J_2 + -}_{J_1 + +}+Z^{J_2 + -}_{J_1 - -})+(P_{1x}+iP_{1y})(Z^{J_2 - +}_{J_1 + +}+Z^{J_2 - +}_{J_1 - -}) + P_{1z}(Z^{J_2 + +}_{J_1 + +}-Z^{J_2 + -}_{J_1 + -}+Z^{J_2 - +}_{J_1 - +}-Z^{J_2 - -}_{J_1 - -})+(Z^{J_2 + +}_{J_1 + +}+Z^{J_2 - -}_{J_1 + +}+Z^{J_2 + +}_{J_1 - -}+Z^{J_2 - -}_{J_1 - -})] . \tag{27}$$

The terms involving $(P_{1x}\mp iP_{1y})$ represent the effect of the transverse polarization on the cross section, while the coefficient of P_{1z} represent that of longitudinal polarization. The last term is the cross section for unpolarized electron beam.

C. Polarization of the scattered electron

The polarization of the scattered electron can be calculated by using Eqs. (4), (23), and (25) with the following results:

$$\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)(P_{2x}-iP_{2y})=[(P_{1x}-iP_{1y})Z^{J_2 + -}_{J_1 + -}+(P_{1x}+iP_{1y})Z^{J_2 - +}_{J_1 + -}+P_{1z}(Z^{J_2 + +}_{J_1 + -}-Z^{J_2 - -}_{J_1 + -})+(Z^{J_2 + +}_{J_1 + -}+Z^{J_2 - -}_{J_1 + -})] , \tag{28}$$

$$\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)(P_{2x}+iP_{2y})=[(P_{1x}-iP_{1y})Z^{J_2 + -}_{J_1 - +}+(P_{1x}+iP_{1y})Z^{J_2 - +}_{J_1 - +}+P_{1z}(Z^{J_2 + +}_{J_1 - +}-Z^{J_2 - -}_{J_1 - +})+(Z^{J_2 + +}_{J_1 - +}+Z^{J_2 - -}_{J_1 - +})] , \tag{29}$$

and

$$\sigma(\mathbf{k}_1,\mathbf{k}_2,\mathbf{P}_1)P_{2z}=[(P_{1x}-iP_{1y})(Z^{J_2 + -}_{J_1 + +}-Z^{J_2 + -}_{J_1 - -})+(P_{1x}+iP_{1y})(Z^{J_2 - +}_{J_1 + +}-Z^{J_2 - +}_{J_1 - -}) + P_{1z}(Z^{J_2 + +}_{J_1 + +}-Z^{J_2 - -}_{J_1 + +}-Z^{J_2 + +}_{J_1 - -}+Z^{J_2 - -}_{J_1 - -})+(Z^{J_2 + +}_{J_1 + +}+Z^{J_2 - -}_{J_1 + +}-Z^{J_2 + +}_{J_1 - -}-Z^{J_2 - -}_{J_1 - -})] . \tag{30}$$

In Eqs. (28), (29), and (30), one can make the observation that the polarization of the scattered electron can be due to the polarization of the incoming electron and/or the orientation of the target nucleus.

III. RESULTS AND DISCUSSION

Using the expressions developed in Sec. II, one can study a number of different experiments that involve beam polarization and/or target orientation. The inclusion of the distortion effect distinguishes this work from the previous ones. Therefore, in what follows I will discuss this effect and its significance in an example and postpone an extensive study of the results of Sec. II to a future paper.

To study the distortion effect, consider the following process: An incoming partially polarized electron beam with polarization $P_x=0.2$, $P_y=0.3$, and $P_z=0.5$, and energy $E=20$ MeV interacts with an unoriented ^{238}U target. The outgoing electrons scatter through angle θ_e, while the nuclei undergo electric dipole transition. Using Eq. (26) in Eq. (27), I calculate σ_P/σ_0, where σ_P is elec-

TABLE I. σ_P/σ_0 calculated in DWBA for different values of excitation energy ω and scattering angle θ_e.

ω	θ_e (deg)							
(MeV)	20	40	60	80	100	120	140	160
8	0.973	0.984	0.988	0.992	0.994	0.997	1.000	1.000
11	0.940	0.963	0.972	0.978	0.982	0.987	0.991	0.995
14	0.885	0.922	0.940	0.952	0.961	0.970	0.979	0.989
18	0.786	0.798	0.831	0.866	0.898	0.925	0.951	0.976

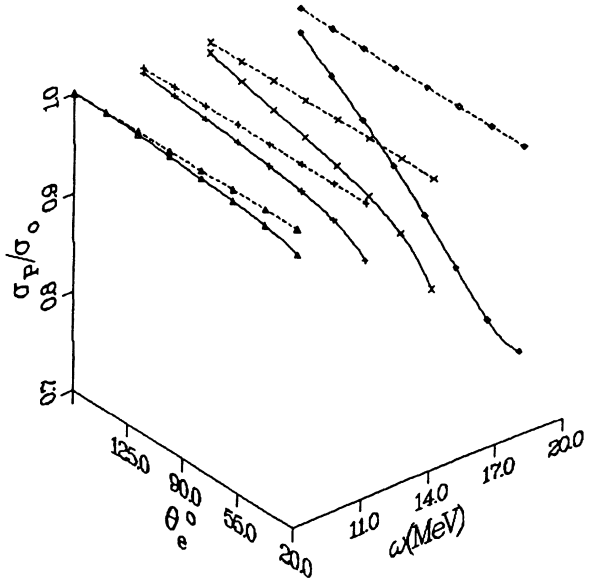

FIG. 1. σ_P/σ_0 vs the excitation energy ω and scattering angle θ_e. The marks are the calculated points, which have been connected by smooth lines to guide the eye. The dashed and solid lines represent plane- and distorted-wave results, respectively.

troexcitation cross section for polarized incoming electron beam and σ_0 is that for unpolarized incoming electron beam. One of the terms that has to be calculated is $R^{\lambda L}(\kappa_1,\kappa_2)$. This involves integration over an infinite range including inside the nucleus, which involves nuclear density functions (see Appendix B). For this I use here expressions derived from assuming irrotational incompressible flow in the nucleus:[8]

$$\begin{aligned} J_{L-1}(r)&=r^{L-1}\rho_0(r)\ , \\ J_L(r)&=d\rho_0(r)/dr\ , \\ J_{L+1}(r)&=0\ , \end{aligned} \tag{31}$$

where $\rho_0(r)$ is the ground-state charge distribution, which is taken to be the standard Fermi shape. In Table I, I show values of σ_p/σ_0 for different selections of transferred energy ω and scattering angle θ_e. In Fig. 1, I compare distorted-wave Born approximation (DWBA) results with the plane-wave Born Approximation (PWBA) results, which is equivalent to letting the charge of the nucleus go to zero. Numerically, we can achieve this in the distorted-wave calculation by letting Z (nuclear charge) become small (but not zero); for $Z=2$, for example, the results of the DWBA calculation agree with PWBA results to 3–4 digits.[14] As is well known, the polarization of the beam will have a null effect on the cross section in PWBA, as long as the target nucleus is unoriented. This effect is shown in Fig. 1 by dashed lines which are the PWBA results. However, in the distorted-wave method (solid lines in Fig. 1), the polarization of the incoming beam has significant effect on the cross section for high-excitation energies and forward-scattering angles. The observed significant effect of the Coulomb distortion in this example calls for a more detailed study of the expressions developed in this article, which, in turn, should lead to a better understanding of the nuclear structure.

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APPENDIX A

The time-independent Dirac equation with a central potential in standard notation is

$$[\boldsymbol{\alpha}\cdot\mathbf{k}+\beta m_e+V(r)]\psi=E\psi\ . \tag{A1}$$

The solution when separated in polar coordinates is written as

$$\psi_\kappa^\mu=\begin{bmatrix} g_\kappa(r)\chi_\kappa^\mu \\ if_\kappa(r)\chi_{-\kappa}^\mu \end{bmatrix}\ , \tag{A2}$$

where χ_κ^μ are the two-spinor angular momentum eigenfunctions:

$$\chi_\kappa^\mu=\sum_{\tau=\pm1/2} C(l,\tfrac{1}{2},j;\mu-\tau,\tau)Y_l^{\mu-\tau}(\theta,\phi)\chi^\tau\ . \tag{A3}$$

In Eq. (A3) the subsidiary angular momentum eigenvalues j and l are regarded as functions of the Dirac angular momentum eigenvalue which specifies both:

$$\begin{aligned} j&=|\kappa|-\tfrac{1}{2}\ , \\ l&=\kappa \text{ for } \kappa>0\ , \\ l&=-\kappa-1 \text{ for } \kappa<0\ . \end{aligned} \tag{A4}$$

For a Coulomb potential having charge Ze as its source, one gets

$$\begin{aligned} f_\kappa^{C,R,I}(r)&=-\sqrt{E-m_e}\,\mathrm{Im}[V_{\pm\gamma}(kr)]\ , \\ g_\kappa^{C,R,I}(r)&=\sqrt{E+m_e}\,\mathrm{Re}[V_{\pm\gamma}(kr)]\ , \end{aligned} \tag{A5}$$

where V_γ can be written as a combination of Whittaker functions of the second kind, $W_{\kappa,\mu}$, as follows:

$$\begin{aligned} V_\gamma(kr)=&2(2kr)^{-3/2}\Gamma(\gamma+i\eta)(\gamma+i\eta)\exp\left[-\pi\frac{\eta}{2}+i\left[\phi-\gamma\frac{\pi}{2}-\frac{\pi}{4}\right]\right] \\ &\times\left[\exp\left[i\frac{\pi}{2}\right]\frac{W_{i\eta+1/2,\gamma}(-2ikr)}{\Gamma(\gamma+1+i\eta)}+\exp[i\pi(\gamma+1)]\frac{W_{-i\eta-1/2,\gamma}(2ikr)}{\Gamma(\gamma-i\eta)}\right]\ , \end{aligned} \tag{A6}$$

with

$$\gamma=(\kappa^2-\alpha^2Z^2)^{1/2}\ ,$$
$$\eta=\alpha ZE/k\ , \tag{A7}$$
$$\exp(2i\phi)=\exp(-i\pi)\left[\frac{\kappa-i\alpha Zm_e/P}{\gamma+i\eta}\right]\ .$$

The superscript C in Eq. (A5) denotes a point Coulomb solution, while R and I refer to regular and irregular solutions, respectively. The choice of the sign of γ in Eq. (A5) is (+) for the regular function and (−) for the irregular function. The asymptotic forms of $f_\kappa^{C,R,I}$ and $g_\kappa^{C,R,I}$ are

$$f_\kappa^{C,R,I}(kr)\rightarrow-\left[\frac{(E-m_e)}{\pi k}\right]^{1/2}\frac{\sin[kr+\eta\ln(2kr)-\frac{1}{2}(l+1)\pi+\delta_\kappa^{R,I}]}{r}\ ,$$
$$g_\kappa^{C,R,I}(kr)\rightarrow\left[\frac{(E+m_e)}{\pi k}\right]^{1/2}\frac{\cos[kr+\eta\ln(2kr)-\frac{1}{2}(l+1)\pi+\delta_\kappa^{R,I}]}{r}\ , \tag{A8}$$

where

$$\delta_\kappa^R(\gamma)=\phi-\frac{1}{2}\pi\gamma-\arg\Gamma(\gamma+i\eta)+\frac{l+1}{2}\pi \tag{A9}$$

and

$$\delta_\kappa^I(\gamma)=\delta_\kappa^R(-\gamma) \tag{A10}$$

are point Coulomb phase shifts.

For an electron of energy E_1, momentum $\mathbf{k}_1$, and polarization m_1, the appropriate combination of the functions ψ_κ^μ describing an incident distorted plane wave and outgoing Coulomb scattered waves normalized in energy scale is

$$\psi_1^{m_1}(\mathbf{k}_1,\mathbf{r})=4\pi\left[\frac{\pi}{2E_1k_1}\right]\sum_{\kappa_1,\mu_1}e^{i\delta_{\kappa_1}}i^{l_1}C(l_1,\tfrac{1}{2},j_1;\mu_1-m_1,m_1)Y_{l_1}^{\mu_1-m_1}(\hat{k}_1)\psi_{\kappa_1}^{\mu_1}(k_1\mathbf{r})\ . \tag{A11}$$

The final-state wave function must be taken to be outgoing distorted plane waves plus incoming Coulomb scattered waves:[15]

$$\psi_2^{m_2}(\mathbf{k}_2,\mathbf{r})=4\pi\left[\frac{\pi}{2E_2k_2}\right]\sum_{\kappa_2,\mu_2}e^{-i\delta_{\kappa_2}}i^{l_2}C(l_2,\tfrac{1}{2},j_2;\mu_2-m_2,m_2)Y_{l_2}^{\mu_2-m_2*}(\hat{k}_2)\psi_{\kappa_2}^{\mu_2}(k_2\mathbf{r})\ , \tag{A12}$$

which describes an electron of energy E_2, momentum $\mathbf{k}_2$, and polarization m_2, which has been scattered by the Coulomb interaction of the nucleus. A general spin state can be represented by superposition of two possible spin states; hence

$$\psi_{e_1}(\mathbf{k}_1,\mathbf{r})=\sum_{m_1=\pm1/2}c_{m_1}\psi_{e_1}^{m_1}\ , \tag{A13}$$

where $c_{-1/2}$ and $c_{1/2}$ are arbitrary constants.

For the case that the source is an extended nucleus, the radial wave functions outside the nucleus can be written as[16]

$$f_\kappa(kr)=A_\kappa f_\kappa^{C,R}(kr)+B_\kappa f_\kappa^{C,I}(kr)\ ,$$
$$g_\kappa(kr)=A_\kappa g_\kappa^{C,R}(kr)+B_\kappa g_\kappa^{C,I}(kr)\ , \tag{A14}$$

with the following asymptotic form:

$$f_\kappa(kr)\rightarrow-\left[\frac{(E-m_e)}{\pi k}\right]^{1/2}\frac{\sin[kr+\eta\ln(2kr)-\frac{1}{2}(l+1)\pi+\delta_\kappa^R+\bar{\delta}_\kappa]}{r}\ ,$$
$$g_\kappa(kr)\rightarrow\left[\frac{(E+m_e)}{\pi k}\right]^{1/2}\frac{\cos[kr+\eta\ln(2kr)-\frac{1}{2}(l+1)\pi+\delta_\kappa^R+\bar{\delta}_\kappa]}{r}\ , \tag{A15}$$

where $\bar{\delta}_\kappa$ is the additional phase shift arising from the finite extent of the nuclear charge distribution. Using Eqs. (A8) and (A14), one finds

$$\bar{\delta}_\kappa=\arctan\left[\frac{\sin(\theta_\kappa)}{A_\kappa/B_\kappa+\cos(\theta_\kappa)}\right], \tag{A16}$$

where

$$\theta_\kappa=\delta_\kappa^I-\delta_\kappa^R . \tag{A17}$$

APPENDIX B: RADIAL INTEGRALS

In the following I briefly discuss the radial integrals (details are available in Refs. 6–8). The interaction between the appropriate components of the electron current and charge densities $J^{\lambda L},\rho^{\lambda L}$ and those of the nuclear vector and scalar potentials $A^{\lambda L},\phi^{\lambda L}$ is written as

$$R_I^{\lambda L}(\kappa_1,\kappa_2)=\int_0^\infty(\mathbf{A}^{\lambda L}\cdot\mathbf{J}^{\lambda L}-\phi^{\lambda L}\rho^{\lambda L})r^2dr , \tag{B1}$$

where the quantity $R_I^{\lambda L}$ is, aside from normalization, the same as the radial integral $R^{\lambda L}$ introduced in the text [see Eq. (19)]. The charge and current transition charge densities are written in terms of f_κ,g_κ, the two radial components of the Dirac wave function for the electron moving in the Coulomb field of the nucleus:

$$J^{EL}=i[L(L+1)]^{-1/2}[L(f_{\kappa_1}g_{\kappa_2}-g_{\kappa_1}f_{\kappa_2})+(\kappa_1-\kappa_2)(f_{\kappa_1}g_{\kappa_2}+g_{\kappa_1}f_{\kappa_2})] , \tag{B2}$$

$$J^{ML}=-i[L(L+1)]^{-1/2}(\kappa_1+\kappa_2)(f_{\kappa_1}g_{\kappa_2}+g_{\kappa_1}f_{\kappa_2}) , \tag{B3}$$

$$\rho^{EL}=f_{\kappa_1}f_{\kappa_2}+g_{\kappa_1}g_{\kappa_2} . \tag{B4}$$

The nuclear current density is also broken down into a multipole:

$$\mathbf{J}_{\rm nuc}(\mathbf{r})=\sum_{M,L,L'}J_{L'}(r)\mathbf{Y}_{LL'}^M(\hat{\mathbf{r}}) , \tag{B5}$$

and the corresponding potentials (in the least singular gauge[10]) are then

$$\begin{aligned}A^{EL}(r)=&h_{L-1}^{(1)}(\omega r)\int_0^r\{-j_{L+1}(\omega r')[L/(L+1)]^{1/2}J_{L+1}(r')+j_{L-1}(\omega r')J_{L-1}(r')\}r'^2dr'\\&+j_{L-1}(\omega r)\int_r^\infty\{-h_{L+1}^{(1)}(\omega r')[L/(L+1)]^{1/2}J_{L+1}(r')+h_{L-1}^{(1)}(\omega r')J_{L-1}(r')\}r'^2dr'\\&-[L/(L+1)]^{1/2}(2L+1)\omega^{-3}r^{L-1}\int_r^\infty J_{L+1}(r')r'^{-L}dr' ,\end{aligned} \tag{B6}$$

$$A^{ML}(r)=h_L^{(1)}(\omega r)\int_0^r j_L(\omega r')J_L(r')r'^2dr'+j_L(\omega r)\int_r^\infty h_L^{(1)}(\omega r')J_L(r')r'^2dr' , \tag{B7}$$

$$\begin{aligned}\phi^{EL}(r)=&[L/(L+1)]^{1/2}h_L^{(1)}(\omega r)\int_0^r\{-j_{L+1}(\omega r')[L/(L+1)]^{1/2}J_{L+1}(r')+j_{L-1}(\omega r')J_{L-1}(r')\}r'^2dr'\\&+[L/(L+1)]^{1/2}j_L(\omega r)\int_r^\infty\{-h_{L+1}^{(1)}(\omega r')[L/(L+1)]^{1/2}J_{L+1}(r')+h_{L-1}^{(1)}(\omega r')J_{L-1}(r')\}r'^2dr'\\&-[(L+1)/(2L+1)]^{1/2}\omega^{-2}r^2\int_r^\infty J_{L+1}(r')r'^2dr' .\end{aligned} \tag{B8}$$

The complicated forms given in Eqs. (B6)–(B8) apply only where the range of integration extends throughout the nucleus. Once outside the nucleus (i.e., for $r>R_{\rm nuc}$ where all $J_{L'}=0$), they take on the the simple forms

$$A^{EL}(r)=h_{L-1}^{(1)}(\omega r)R_N^{EL} , \tag{B9}$$

$$A^{ML}(r)=h_L^{(1)}(\omega r)R_N^{ML} , \tag{B10}$$

$$\phi^{EL}(r)=[L/(L+1)]^{1/2}h_L^{(1)}(\omega r)R_N^{EL} , \tag{B11}$$

where R_N^{EL},R_N^{ML} are the radial parts of the nuclear transition matrix elements:

$$R_N^{EL}=\int_0^{R_{\rm nuc}}\{-j_{L+1}(\omega r')[L/(L+1)]^{1/2}J_{L+1}(r')+j_{L-1}(\omega r')J_{L-1}(r')\}r'^2dr' , \tag{B12}$$

$$R_N^{ML}=\int_0^{R_{\rm nuc}}j_L(\omega r')J_L(r')r'^2dr' . \tag{B13}$$

If we extract the factor $R_N^{\lambda L}$ from the transition integral $R_I^{\lambda L}$, we get the normalized radial integral

$$R^{\lambda L}(\kappa_1,\kappa_2)=R_I^{\lambda L}(\kappa_1,\kappa_2)/R_N^{\lambda L} . \tag{B14}$$

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