Double electron excitation and the Glauber theory

W. Williamson, Jr., D. G. Ellis, and P. S. Ramanujam Department of Physics and Astronomy, University of Toledo, Toledo, Ohio 43606 (Received 8 March 1982)

The electron excitation cross sections for He $(1s^{21}S \rightarrow 2p^{23}P)$, Mg $(3s^{21}S \rightarrow 3p^{23}P)$, and Ca $(4s^{21}S \rightarrow 4p^{23}P)$ have been calculated with the use of the Ochkur, Glauber, and a simplified Glauber approximation. The results are compared with the Born-Oppenheimer approximation and, in the case of helium, with available experimental data. The Glauber and simplified Glauber approximations are found to differ significantly from the Born-Oppenheimer approximation, especially in the high-energy limit.

I. INTRODUCTION

The excitation of a single atomic electron by an incident electron has been a prodigious producer of experimental and theoretical physics publications for a number of years, but the study of double electron excitation in atoms is relatively recent. Becker and Dahler^{1,2} were the first to our knowledge to investigate the double electron excitation problem from a rigorous theoretical point of view. In their pioneering work on helium and beryllium they calculated differential and total cross sections through the use of the Born-Oppenheimer, and, for some excitations, the distorted-wave and two-state coupling approximations. They were specifically interested in doubly excited states which are stable against autoionization. They found that the differential cross sections vanished in the forward and backward scattering directions. Fano³ proved that if the spin-orbit interaction is negligible, then the differential cross sections for "parity unfavored" excitations must vanish in the forward and backward directions regardless of the approximation used in the calculation. Kulander and Dahler⁴ extended earlier calculations to study other doubly excited parity unfavored states including He $(1s^{21}S \rightarrow 2p^{23}P)$, Mg $(3s^{21}S \rightarrow 3p^{23}P)$, and Ca $(4s^{21}S \rightarrow 4p^{23}P)$. Roy and Sil⁵ calculated the He $({}^{1}S \rightarrow {}^{3}P)$ excitation cross section through the use of an integral form of the close-coupling approximation. They were primarily interested in the very low-energy regime and compared their theoretical results with the experimental data of Burrow.⁶ In 1979 Westerveld et al.⁷ published the first extensive experimental data for helium $({}^{1}S \rightarrow {}^{3}P)$ and normalized their data to the Born-Oppenheimer approximation at 120 eV.

In the case of some single-electron excitation it is known that the Born-Oppenheimer approximation gives spurious results.⁸ Hickerson *et al.* have investigated the excitation of ${}^{3}P_{g}$, and ${}^{1,3}D_{g}$ states of helium through the use of simple and configuration interaction wave functions in conjunction with the Born-Oppenheimer and Rudge approximations. Basically, they conclude that the Rudge approximation is more reliable than the Born-Oppenheimer because it is less sensitive to the choice of wave functions. They find that the two approximations appear to have different high-energy dependence but do not give cross sections for more than about twice threshold energy.⁸

There are additional reasons to believe⁸ that the Born-Oppenheimer total cross sections for parity unfavored excitations decrease much too rapidly for high impact energies. One may surmise that in double electron processes, higher-order effects may be important and in some manner they should be included in the approximation. The Glauber approximation includes some higher-order effects by way of an accumulated phase. In this paper we consider the double excitation of He $(1s^{2} S \rightarrow 2p^{2} P)$, Mg $(3s^{2} S \rightarrow 3p^{2} P)$, and Ca $(4s^{2} S \rightarrow 4p^{2} P)$ within the context of Glauber theory.

II. SCATTERING AMPLITUDES

The Glauber approximation was first applied to atomic collisions by Franco⁹ in 1968. Since the initial use by Franco, the theory has been utilized in a wide variety of atomic scattering processes, and several review articles have been written on the sub-

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ject, or have included discussions on Glauber theory.^{10,11} Rather than rederiving the Glauber amplitude, we refer the reader to one of the cited papers and merely give the extension of the formalism to double electron excitation. We will basically use the notation and units of Chan et al.¹¹ The subscripts zero, one, and two will refer to the incident and bound electrons, while i and f will refer to initial and final states. In the exchange amplitude we assume a $0 \leftrightarrow 2$ exchange process. The direct (f) and exchange $(g^{\pm}, plus and minus correspond to post$ and prior) amplitudes are given by

$$f = -(2\pi)^2 \frac{m}{\hbar^2} \langle \phi_f \mid V_+ \mid \psi_i^+ \rangle , \qquad (1a)$$

$$g^{+} = -(2\pi)^{2} \frac{m}{\hbar^{2}} \langle \phi_{P02} | V_{-} | \psi_{i}^{+} \rangle ,$$
 (1b)

$$g^{-} = -(2\pi)^{2} \frac{m}{\hbar^{2}} \langle \psi_{P02}^{-} | V_{+} | \phi_{i} \rangle . \qquad (1c)$$

In the above, the subscript P02 indicates that electron zero and two have been exchanged. In the coordinate representation these become

$$f = -\frac{1}{2\pi} \int d\vec{r}_0 d\vec{r}_1 d\vec{r}_2 \phi_f^{\dagger}(\vec{r}_1, \vec{r}_2) V_+ \phi_i(\vec{r}_1, \vec{r}_2) \\ \times \exp[i(\vec{k}_i - \vec{k}_f) \cdot \vec{r}_0 + i\chi_+], \quad (2a)$$

$$g^{\pm} = -\frac{1}{2\pi} \int d\vec{\mathbf{r}}_{0} d\vec{\mathbf{r}}_{1} d\vec{\mathbf{r}}_{2} \phi_{f}^{\dagger}(\vec{\mathbf{r}}_{1},\vec{\mathbf{r}}_{0}) V_{\mp} \phi_{i}(\vec{\mathbf{r}}_{1},\vec{\mathbf{r}}_{2}) \\ \times \exp(i\vec{\mathbf{k}}_{i}\cdot\vec{\mathbf{r}}_{0} - i\vec{\mathbf{k}}_{f}\cdot\vec{\mathbf{r}}_{2} + i\chi_{\pm}) ,$$
(2b)

$$V_{+} = -\frac{2}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}}$$
, (2c)

 $\phi_i(\vec{r}_1, \vec{r}_2) = \phi_{ns}(\vec{r}_1)\phi_{ns}(\vec{r}_2)\eta^{00}(12)$,

$$V_{-} = -\frac{2}{r_{2}} + \frac{1}{r_{12}} + \frac{1}{r_{20}} , \qquad (2d)$$

$$\begin{aligned} \chi_{+} &= \frac{1}{k_{i}} \int_{-\infty}^{z_{0}} dz'_{0} \left[\frac{2}{r_{0}} - \frac{1}{r_{01}} - \frac{1}{r_{02}} \right] \\ &= \frac{1}{k_{i}} \ln \left[\frac{(r_{01} - z_{01})(r_{02} - z_{02})}{(r_{0} - z_{0})^{2}} \right], \end{aligned} (2e) \\ \chi_{-} &= \frac{1}{k_{f}} \int_{z_{2}}^{-\infty} dz'_{2} \left[\frac{1}{r_{0}} - \frac{1}{r_{12}} - \frac{1}{r_{02}} \right] \\ &= \frac{1}{k_{f}} \ln \left[\frac{(r_{2} - z_{2})^{2}}{(r_{12} - z_{12})(r_{02} - z_{02})} \right], \end{aligned} (2f)$$

and

$$r_{ij} = |\vec{\mathbf{r}}_{ij}| = |\vec{\mathbf{r}}_i - \vec{\mathbf{r}}_j|$$

Note that the spin functions for the incident and exchange electrons have been supressed.

Mohan and Vidhani¹² have given an analytic expression for the double excitation of helium by electrons for the direct amplitude. Since we are concerned with states which may only be excited via the exchange amplitude, we now focus our attention upon it.

Kulander and Dahler⁴ give atomic wave functions which they generated using a pseudopotential formalism. They found good agreement in their helium calculations using the pseudopotential functions and comparing with answers obtained using Hartree-Fock wave functions. We use their pseudopotential wave functions and notation for the functions in this paper. The form of the wave functions is given by

$$\phi_{f}^{\dagger}(\vec{\mathbf{r}}_{1},\vec{\mathbf{r}}_{0}) = \phi_{1M_{L}}^{\dagger 1m}(\vec{\mathbf{r}}_{1},\vec{\mathbf{r}}_{0}) = \sum_{m_{1},m_{0}} C_{m_{1}m_{0}M_{L}}^{\dagger 111} \phi_{npm_{1}}^{\dagger}(\vec{\mathbf{r}}_{1}) \phi_{npm_{0}}^{\dagger}(\vec{\mathbf{r}}_{0}) \eta^{\dagger 1m}(10) , \qquad (3b)$$

where $\eta(ij)$'s are the two electron spin functions, the C's are Clebsch-Gordan coefficients, and the ϕ 's are single-particle wave functions, which will be given explicitly in the next section of this paper. Using these expressions for the atomic wave functions in the post exchange amplitude yields a sum of three terms $(g_1^+, g_2^+, g_2^+, g_1^+, g_2^+)$ and g_3^+) which come from V_- . The contribution from the nuclear term (g_1^+) is zero for ${}^1S \rightarrow {}^3P$ excitations in all of the approximations we consider. This null result arises from the coupling of the angular momenta. The surviving terms are

$$g^{+} = \sum_{m_{0},m_{1}} C^{\dagger 111}_{m_{1}m_{0}M_{L}} \eta^{\dagger 1m}(10) \eta^{00}(12) \eta^{\dagger m'_{s}}(2) \eta^{m_{s}}(0) [g_{2}^{+}(m_{0},m_{1}) + g_{3}^{+}(m_{0},m_{1})], \qquad (4a)$$

where

$$g_{2}^{+}(m_{0},m_{1}) = -\frac{1}{2\pi} \int d\vec{\mathbf{r}}_{0} d\vec{\mathbf{r}}_{1} d\vec{\mathbf{r}}_{2} \phi_{npm_{1}}^{\dagger}(\vec{\mathbf{r}}_{1}) \phi_{npm_{0}}^{\dagger}(\vec{\mathbf{r}}_{0}) \phi_{ns}(\vec{\mathbf{r}}_{1}) \phi_{ns}(\vec{\mathbf{r}}_{2}) \frac{\exp(i\vec{\mathbf{k}}_{i}\cdot\vec{\mathbf{r}}_{0}-i\vec{\mathbf{k}}_{f}\cdot\vec{\mathbf{r}}_{2}+i\chi_{+})}{r_{12}}, \quad (4b)$$

(2f)

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$$g_{3}^{+}(m_{0},m_{1}) = -\frac{1}{2\pi} \int d\vec{\mathbf{r}}_{0} d\vec{\mathbf{r}}_{1} d\vec{\mathbf{r}}_{2} \phi_{npm_{1}}^{\dagger}(\vec{\mathbf{r}}_{1}) \phi_{npm_{0}}^{\dagger}(\vec{\mathbf{r}}_{0}) \phi_{ns}(\vec{\mathbf{r}}_{1}) \phi_{ns}(\vec{\mathbf{r}}_{2}) \frac{\exp(i\vec{\mathbf{k}}_{i}\cdot\vec{\mathbf{r}}_{0}-i\vec{\mathbf{k}}_{f}\cdot\vec{\mathbf{r}}_{2}+i\chi_{+})}{r_{20}}, \quad (4c)$$

and $\eta^{m_s}(i)$ is a single-particle spin-wave function. The semiclassical interpretation of g_2^+ is that initially the two bound electrons interact with one another directly via the r_{12}^{-1} term, while only interacting with the incident particle through the accumulated phase (χ_+) . The ejected electron (2) then interacts with one of the bound electrons directly (r_{12}^{-1}) and also accumulates a phase. The g_3^+ term represents a direct interaction between a bound electron and the incoming and outgoing electron via r_{20}^{-1} , while the spectator electron (1) can only be excited via the accumulated phase. The high-energy dependence of g_2^+ and g_3^+ should be different providing the accumulated phase is nonzero.

III. BORN-OPPENHEIMER, OCHKUR, GLAUBER, AND SIMPLIFIED **GLAUBER AMPLITUDES**

The double electron excitation exchange amplitude given above is a nine-dimensional integral and its dimensionality must be reduced if numerical results are desired. We will reduce the amplitude to a tractable form for the Born-Oppenheimer (BO), Ochkur (OC), and Glauber (GA) approximations, as well as for a simplified Glauber (SG) approximation. In these cases the integrals can be considerably reduced and numerical evaluation is straightforward.

In each approximation we use the single-particle wave functions of Kulander and Dahler,⁴ but rewritten in the following form:

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$$\phi_{ns}(\vec{r}) = N_{ns} e^{-\alpha_{ns} r} Y_{00}(\Omega) , \qquad (5a)$$

$$\phi_{npm}^{\dagger}(r) = N_{np} r e^{-\alpha_{np} r} Y_{1m}^{\dagger}(\Omega) = \begin{cases} -i N_{np} \left[\frac{3}{4\pi} \right]^{1/2} \frac{\partial}{\partial \gamma_z} [\exp(-\alpha_{np} r + i \vec{\gamma} \cdot \vec{r})]_{\vec{\gamma}=0}, & m = 0 \\ \pm i N_{np} \left[\frac{3}{8\pi} \right]^{1/2} \left[\frac{\partial}{\partial \gamma_x} \mp i \frac{\partial}{\partial \gamma_y} \right] [\exp(-\alpha_{np} r + i \vec{\gamma} \cdot \vec{r})]_{\vec{\gamma}=0}, & m = \pm 1 \end{cases}$$
(5b)
(5c)

or, in general,

$$\phi(\vec{\mathbf{r}}) = [D(\mu\vec{\gamma})\exp(-\alpha r + i\vec{\gamma}\cdot\vec{\mathbf{r}})]_{\vec{\gamma}=0}.$$
 (5d)

This parametrization of the wave functions facilitates the analytic integrations because the operator on $\mu \vec{\gamma}$ may be pulled outside the integrals, the integrals evaluated in a general manner, and then the generating operator $[D(\mu \vec{\gamma})]$ applied, after which $\vec{\gamma}$ is set equal to zero. The numerical values of the α 's are given in Table I and the N's are determined from the normalization requirement.

A. Born-Oppenheimer amplitude

In order to compare the results of our calculations with those of Kulander and Dahler⁴ over a full range of energies we have recalculated their BO results. However, we used a different formulation of the amplitude. Our numerical results are in excellent agreement with theirs and we give a brief description of our BO amplitude.

The BO amplitude is retrieved from Eqs. (4) by setting the accumulated phase (χ_+) equal to zero. Since the \vec{r}_1 wave functions are orthogonal the only nonzero term is $g_2^+(m_0, m_1)$. This is

TABLE I. Values of wave-function parameters and threshold energies (eV).

Element	α_{ns}	α_{np}	Threshold energy (eV)
He	1.69	0.836	59.67
Mg	0.425	0.625	7.21
Ca	0.350	0.500	4.76

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$$g_{2}^{\text{BO}}(m_{0},m_{1}) = -\frac{1}{2\pi} \int d\vec{\mathbf{r}}_{0} d\vec{\mathbf{r}}_{1} d\vec{\mathbf{r}}_{2} \phi_{npm_{1}}^{\dagger}(\vec{\mathbf{r}}_{1}) \phi_{npm_{0}}^{\dagger}(\vec{\mathbf{r}}_{0}) \frac{\exp(i\vec{k}_{i}\cdot\vec{\mathbf{r}}_{0}-i\vec{k}_{f}\cdot\vec{\mathbf{r}}_{2})}{r_{12}} \phi_{ns}(\vec{\mathbf{r}}_{1}) \phi_{ns}(\vec{\mathbf{r}}_{2}) .$$
(6a)

First we concentrate on the integration over the \vec{r}_2 coordinate,

$$I_{2}^{BO} = \int d\vec{\mathbf{r}}_{2} \frac{\exp(-i\mathbf{k}_{f}\cdot\vec{\mathbf{r}}_{2})}{r_{12}} [\phi_{ns}(\vec{\mathbf{r}}_{2}) = D_{BO}(\mu_{2}\vec{\gamma}_{2})\exp(-\mu_{2}r_{2}+i\vec{\gamma}_{2}\cdot\vec{\mathbf{r}}_{2})] .$$
(6b)

By introducing the Fourier transform of the wave function and doing the \vec{r}_2 integral, we have

$$I_{2}^{BO} = \frac{1}{(2\pi)^{3}} D_{BO}(\mu_{2}\vec{\gamma}_{2}) \frac{\partial}{\partial\mu_{2}} \int d\vec{p}_{2} \frac{-4\pi \exp[-i(\vec{k}_{f} + \vec{p}_{2})\cdot\vec{r}_{1}]}{\mu_{2}^{2} + |\vec{p}_{2} + \vec{\gamma}_{2}|^{2}} \frac{4\pi}{|\vec{k}_{f} + \vec{p}_{2}|^{2}}$$
(7a)

$$= -\frac{2}{\pi} D_{\rm BO}(\mu_2 \vec{\gamma}_2) \frac{\partial}{\partial \mu_2} \int \frac{d\vec{q}_2}{q_2^2} \frac{\exp(-i\vec{q}_2 \cdot \vec{r}_1)}{\mu_2^2 + |\vec{q}_2 + \vec{\gamma}_2 - \vec{k}_f|^2} , \qquad (7b)$$

where $\vec{q}_2 = \vec{k}_f + \vec{p}_2$. Through the use of the Feynman parametrization,¹³ the denominator of the integral may be written

$$\frac{1}{q_2^2(\mu_2^2 + |\vec{q}_2 + \vec{\gamma}_2 - \vec{k}_f|^2)} = \int_0^1 \frac{d\chi}{\{[\vec{q}_2 + (1 - \chi)(\vec{\gamma}_2 - \vec{k}_f)]^2 + \chi(1 - \chi)(\vec{\gamma}_2 - \vec{k}_f)^2 + (1 - \chi)\mu_2^2\}^2}$$
(8a)

Introducing the variables

$$\vec{k}_2 = \vec{q}_2 + (1 - \chi)(\vec{\gamma}_2 - \vec{k}_f)$$
, (8b)

$$\Omega^{2} = (1 - \chi) [\mu_{2}^{2} + \chi (\vec{\gamma}_{2} - \vec{k}_{f})^{2}], \qquad (8c)$$

we have

$$I_{2}^{BO} = -\frac{2}{\pi} D_{BO}(\mu_{2}\vec{\gamma}_{2}) \frac{\partial}{\partial\mu_{2}} \int_{0}^{1} d\mathcal{X} \exp[i(1-\mathcal{X})(\vec{\gamma}_{2}-\vec{k}_{f})\cdot\vec{r}_{1}] \int d\vec{k}_{2} \frac{\exp(-i\vec{k}_{2}\cdot\vec{r}_{1})}{(k_{2}^{2}+\Omega^{2})^{2}}$$
(9a)

$$= -\frac{2}{\pi} D_{\rm BO}(\mu_2 \vec{\gamma}_2) \frac{\partial}{\partial \mu_2} \int_0^1 d\chi \exp[-\Omega r_1 + i(1-\chi)(\vec{\gamma}_2 - \vec{k}_f) \cdot \vec{r}_1] .$$
^(9b)

The integral over the \vec{r}_0 coordinate is straightforward:

$$I_{0}^{BO} = \int d\vec{r}_{0} \phi_{npm_{0}}^{\dagger}(\vec{r}_{0}) e^{i\vec{k}_{i}\cdot\vec{r}_{0}} = D_{BO}(\mu_{0}\vec{\gamma}_{0}) \int d\vec{r}_{0} \exp[-\mu_{0}r_{0} + i(\vec{\gamma}_{0} + \vec{k}_{i})\cdot\vec{r}_{0}]$$
(10a)

$$= \boldsymbol{D}_{\rm BO}(\mu_0 \vec{\gamma}_0) \frac{\partial}{\partial \mu_0} \left[\frac{-4\pi}{\mu_0^2 - (\vec{\gamma}_0 + \vec{k}_i)^2} \right].$$
(10b)

Finally, the integral over \vec{r}_1 may be done by writing

$$\phi_{npm_1}^{\dagger}(\vec{\mathbf{r}}_1)\phi_{ns}(\vec{\mathbf{r}}_1) = D(\mu_1\vec{\gamma}_1)\exp(-\mu_1r_1 + i\vec{\gamma}_1\cdot\vec{\mathbf{r}}_1) .$$
(11)

Then,

$$I_{1}^{\text{BO}} = \int d\vec{r}_{1} \phi_{npm_{1}}^{\dagger}(\vec{r}_{1}) \phi_{ns}(\vec{r}_{1}) \exp[-\Omega r_{1} + i(1-\chi)(\vec{\gamma}_{2} - \vec{k}_{f}) \cdot \vec{r}_{1}]$$
(12a)

$$= \mathcal{D}_{\rm BO}(\mu_1 \vec{\gamma}_1) \left[\frac{8\pi(\mu_1 + \Omega)}{\{(\mu_1 + \Omega)^2 + [\vec{\gamma}_1 + (1 - \chi)(\vec{\gamma}_2 - \vec{k}_f)]^2\}^2} \right].$$
(12b)

The BO amplitude may now be written as

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$$g_{2}^{BO}(m_{0},m_{1}) = D_{BO}(\mu_{0}\vec{\gamma}_{0})\frac{\partial}{\partial\mu_{0}}\left[\frac{1}{\mu_{0}^{2} + |\vec{\gamma}_{0} - \vec{k}_{i}|^{2}}\right] D_{BO}(\mu_{1}\vec{\gamma}_{1})D_{BO}(\mu_{2}\vec{\gamma}_{2})\frac{\partial}{\partial\mu_{2}} \\ \times \left[\int_{0}^{1}\frac{d\chi}{\Omega}\frac{8\pi(\mu_{1}+\Omega)}{[(\mu_{1}+\Omega)^{2} + |\vec{\gamma}_{1}+(1-\chi)(\vec{\gamma}_{1}-\vec{k}_{f})|^{2}]^{2}}\right].$$
(12c)

The advantage of using this form of the BO amplitude is that after the generators have been applied, and the Racah algebra done, only one term survives and it may be evaluated by doing a very simple and well-behaved one-dimensional integral.

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B. Ochkur amplitude

The OC approximation is a simplification of the BO approximation. Let us consider Eq. (7a) for high energies, i.e., $k_f \sim k_i \gg \epsilon$, where ϵ is the threshold excitation energy. It is argued that the major contribution to the momentum phase space of the bound electron (\vec{p}_2) comes from low values of $|\vec{p}_2|$ because electron two is a bound electron, i.e., for large values of $|\vec{p}_2|$ the exponential term of the Fourier transform is rapidly oscillating and the denominator terms in $|\vec{p}_2|$ cut off significant contributions for large momenta. The $|\mathbf{k}_f + \vec{\mathbf{p}}_2|$ term is expanded and as a function of k_f and only the leading term is retained. Thus,

$$I_{2}^{\rm oc} = \frac{1}{(2\pi)^{3}} \frac{4\pi}{k_{f}^{2}} D_{\rm oc}(\mu_{2}\vec{\gamma}_{2}) \frac{\partial}{\partial\mu_{2}} \\ \times \int d\vec{p}_{2} \frac{(-4\pi)\exp[-i(\vec{k}_{f}+\vec{p}_{2})\cdot\vec{r}_{1}]}{\mu_{2}^{2}+|\vec{p}_{2}+\vec{\gamma}_{2}|^{2}}.$$
(13a)

This is equivalent to the traditional replacement,

$$\int d\vec{r}_{2}\phi_{ns}(\vec{r}_{2}) \frac{\exp(-i\,\mathbf{k}_{f}\cdot\vec{r}_{2})}{r_{12}} = \frac{4\pi}{k_{f}^{2}} \exp(-i\,\vec{k}_{f}\cdot\vec{r}_{1})\phi_{ns}(\vec{r}_{1}) . \quad (13b)$$

All of the integrations for the OC approximation may be done analytically. The result is

$$g_{2}^{0}(m_{0},m_{1}) = -\frac{2}{k_{f}^{2}} D_{0}(\mu_{0}\vec{\gamma}_{0}) \frac{\partial}{\partial\mu_{0}} \left[\frac{-4\pi}{\mu_{0}^{2} + |\vec{\gamma}_{0} + \vec{k}_{i}|^{2}} \right] D_{0}(\mu_{1}\vec{\gamma}_{1}) \left[\frac{-4\pi}{\mu_{1} + |\vec{\gamma}_{1} + \vec{k}_{f}|^{2}} \right],$$
(14)

where the generators are defined by the following relationships:

$$\phi_{npm_0}^{\dagger}(\vec{r}_0) = D_0(\mu_0 \vec{\gamma}_0) \exp(-\mu_0 r_0 + i \vec{\gamma}_0 \cdot \vec{r}_0) , \qquad (15a)$$

$$\phi_{npm_1}^{\dagger}(\vec{r}_1)\phi_{ns}^2(\vec{r}_1) = D_0(\mu_1\vec{\gamma}_1)\exp(-\mu_1r_1 + i\vec{\gamma}_1\cdot\vec{r}_1) .$$
(15b)

C. Glauber amplitude

In the GA, $g_2^+(m_0,m_1)$ and $g_3^+(m_0,m_1)$ both contribute. If the accumulated phase is explicitly included they become

$$g_{2}^{G}(m_{0},m_{1}) = -\frac{1}{2\pi} \int d\vec{r}_{0} d\vec{r}_{1} d\vec{r}_{2} \phi_{npm_{1}}^{\dagger}(\vec{r}_{1}) \phi_{npm_{0}}^{\dagger}(\vec{r}_{0}) \phi_{ns}(\vec{r}_{1}) \phi_{ns}(\vec{r}_{2}) \frac{\exp(i\,\mathbf{k}_{i}\cdot\vec{r}_{0}-i\,\mathbf{k}_{f}\cdot\vec{r}_{2})}{r_{12}} \\ \times \left[\frac{(r_{01}-z_{01})(r_{02}-z_{02})}{(r_{0}-z_{0})^{2}} \right]^{i\eta_{+}},$$
(16a)
$$g_{3}^{G}(m_{0},m_{1}) = -\frac{1}{2\pi} \int d\vec{r}_{0} d\vec{r}_{1} d\vec{r}_{2} \phi_{npm_{1}}^{\dagger}(\vec{r}_{1}) \phi_{npm_{0}}^{\dagger}(\vec{r}_{0}) \phi_{ns}(\vec{r}_{1}) \phi_{ns}(\vec{r}_{2}) \frac{\exp(i\,\vec{k}_{i}\cdot\vec{r}_{0}-i\,\vec{k}_{f}\cdot\vec{r}_{2})}{r_{02}} \\ \times \left[\frac{(r_{01}-z_{01})(r_{02}-z_{02})}{(r_{0}-z_{0})^{2}} \right]^{i\eta_{+}},$$
(16b)

(16b)

where the notation $\eta_{+} = 1/k_i$ is used to keep the phase terms separate from other terms which depend on the incident momentum. Direct reduction of each of these two terms to four-dimensional integrals is possible. However, they may be reduced to two-dimensional integrals by making an approximation similar to that established by Franco and Halpern.¹⁴ We give the results here and refer to the references cited for complete details of the method. We wish to stress that if the standard Ochkur-type reduction of the amplitude is attempted, then an indeterminate phase factor is introduced into the amplitude. The Franco-Halpern technique yields the following. For $g_2^{C}(m_0, m_1)$

$$\int d\vec{r}_{2}\phi_{ns}(\vec{r}_{2}) \frac{\exp(-i\vec{k}_{f}\cdot\vec{r}_{2})}{r_{12}} (r_{02}-z_{02})^{i\eta} \rightarrow \frac{4\pi}{k_{f}^{2}}\phi_{ns}(\vec{r}_{1})e^{-i\vec{k}_{f}\cdot\vec{r}_{1}} (r_{01}-z_{01})^{i\eta} \qquad (17a)$$

and for $g_3^G(m_0, m_1)$

$$\int d\vec{r}_{0} \frac{e^{i\vec{k}_{i}\cdot\vec{r}_{0}}}{r_{02}} \phi^{\dagger}_{npm_{0}}(\vec{r}_{0}) \left[\frac{(r_{01}-z_{01})(r_{02}-z_{02})}{(r_{0}-z_{0})^{2}} \right]^{i\eta} + \\ \rightarrow e^{i\vec{k}_{i}\cdot\vec{r}_{2}} \phi^{\dagger}_{npm_{0}}(\vec{r}_{2}) \left[\frac{r_{21}-z_{21}}{(r_{2}-z_{2})^{2}} \right]^{i\eta} + \int \frac{d\vec{r}e^{i\vec{k}_{i}\cdot\vec{r}}}{r} (r-z)^{i\eta} + . \quad (17b)$$

Substituting these expressions into Eqs. (16) we have the following:

$$g_{2}^{G}(m_{0},m_{1}) = -\frac{2}{k_{f}^{2}} \int d\vec{r}_{0}d\vec{r}_{1}\phi_{npm_{1}}^{\dagger}(\vec{r}_{1})\phi_{npm_{0}}^{\dagger}(\vec{r}_{0})\phi_{ns}^{2}(\vec{r}_{1})\exp(i\vec{k}_{i}\cdot\vec{r}_{0}-i\vec{k}_{f}\cdot\vec{r}_{1}) \left[\frac{r_{01}-z_{01}}{r_{0}-z_{0}}\right]^{2i\eta_{+}}, \quad (18a)$$

$$g_{3}^{G}(m_{0},m_{1}) = -\frac{1}{2\pi} \int d\vec{r} \frac{e^{i\vec{k}_{1}\cdot\vec{r}}}{r} (r-z)^{i\eta} + \int d\vec{r}_{1}\phi_{npm_{1}}^{\dagger}(\vec{r}_{1})\phi_{ns}(\vec{r}_{1}) \\ \times \int d\vec{r}_{2}e^{i\vec{q}\cdot\vec{r}_{2}}\phi_{npm_{0}}^{\dagger}(\vec{r}_{2})\phi_{ns}(\vec{r}_{2}) \left[\frac{r_{21}-z_{21}}{(r_{2}-z_{2})^{2}}\right]^{i\eta} + , \quad (18b)$$

where $\vec{q} = \vec{k}_i - \vec{k}_f$. The reduction of these rather formidable looking six-dimensional integrals to twodimensional integrals may be done by following the Gau-Macek procedure.¹⁵ This yields

$$g_{2}^{G}(m_{0},m_{1}) = \frac{8(2\pi)^{2}}{2^{2i\eta}+k_{f}^{2}} \frac{\Gamma(1-2i\eta_{+})}{\Gamma(-2i\eta_{+})} D_{G2}(\mu_{1}\vec{\gamma}_{1}) D_{G2}(\mu_{0}\vec{\gamma}_{0}) \frac{\partial}{\partial\mu_{1}^{2}} \int_{0}^{\infty} \frac{d\lambda}{\lambda^{2i\eta_{+}}} I_{2\chi} , \qquad (19a)$$

$$g_{3}^{G}(m_{0},m_{1}) = \frac{8\pi}{2^{2i\eta_{+}}} \frac{\Gamma(1-2i\eta_{+})}{\Gamma(-i\eta_{+})} \int \frac{d\vec{r}}{r} e^{i\vec{k}_{i}\cdot\vec{\tau}} (r-z)^{i\eta_{+}} D_{G3}(\mu_{1}\vec{\gamma}_{1}) D_{G3}(\mu_{2}\vec{\gamma}_{2}) \frac{\partial}{\partial\mu_{1}^{2}} \int_{0}^{\infty} \frac{d\lambda}{\lambda^{i\eta_{+}}} I_{3\chi} .$$
(19b)

In the above, $I_{j\chi}$ indicates an integral over the parameter χ where

$$\vec{a}_3 = (1 - \chi)\vec{\gamma}_1 + (\vec{\gamma}_2 + \vec{q}) - i\lambda\chi\hat{z} .$$
 (20f)

$$I_{j\chi} = \int_{0}^{1} \frac{d\chi \chi}{(1-\chi)\Lambda_{j}} \frac{(\alpha_{j} - ia_{jz})^{-2i\eta}}{(\alpha_{j}^{2} + a_{j}^{2})^{1-2i\eta}}$$
(20a)

The generators $[D(\mu \vec{\gamma})]$ are defined as

$$\phi_{npm_{1}}^{\dagger}(\vec{r}_{1})\phi_{ns}^{2}(\vec{r}_{1})$$

$$= D_{G2}(\mu_{1}\vec{\gamma}_{1}) \left[\frac{\exp(-\mu_{1}r_{1} + i\vec{\gamma}_{1}\cdot\vec{r}_{1})}{r_{1}} \right], \quad (21a)$$

$$\phi_{npm_0}^{\dagger}(\vec{\mathbf{r}}_0) = D_{G2}(\mu_0 \vec{\gamma}_0) \left(\frac{\exp(-\mu_0 r_0 + i \vec{\gamma}_0 \cdot \vec{\mathbf{r}}_0)}{r_0} \right),$$
(21b)

1

$$\alpha_2 = \mu_0 + \Lambda_2, \quad \alpha_3 = \mu_2 + \Lambda_3 , \qquad (20b)$$

$$\Lambda_{2}^{2} = \lambda^{2} \chi^{2} + (1 - \chi) [\mu_{1}^{2} + \chi(\vec{\gamma}_{1} - \vec{k}_{f})^{2} + 2i\lambda\chi(\vec{\gamma}_{1} - \vec{k}_{f})\cdot\hat{z}], \qquad (20c)$$

$$\Lambda_3^2 = \lambda^2 \chi^2 + (1 - \chi)(\mu_1^2 + \chi \gamma_1^2 + 2i\lambda \chi \vec{\gamma}_1 \cdot \hat{z}) , \qquad (20d)$$

$$\vec{a}_2 = (1 - \chi)(\vec{\gamma}_1 - \vec{k}_f) + (\vec{\gamma}_0 + \vec{k}_i) - i\lambda\chi\hat{z}$$
, (20e)

(24)

$$\begin{split} \phi^{\dagger}_{npm_1}(\vec{\mathbf{r}}_1)\phi_{ns}(\vec{\mathbf{r}}_1) \\ = D_{G3}(\mu_1\vec{\gamma}_1) \Biggl[\frac{\exp(-\mu_1r_1 + i\vec{\gamma}_1\cdot\vec{\mathbf{r}}_1)}{r_1} \Biggr], \end{split} \tag{21c}$$

$$= D_{G3}(\mu_2 \vec{\gamma}_2) \left\{ \frac{\exp(-\mu_2 r_2 + i \vec{\gamma}_2 \cdot \vec{r}_2)}{r_2} \right\}.$$
(21d)

The differential operators generate a multitude of terms but fortunately the angular momentum algebra only requires that $g_2^G(0, +1)$ and $g_3^G(+1,0)$ be evaluated.

D. Simplified Glauber amplitude

In the GA, the amplitudes may be reduced to an expression which necessitates the numerical evalua-

$$I_{30} = \int d\vec{r}_{2} e^{i\vec{q}\cdot\vec{r}_{2}} \phi^{\dagger}_{npm_{0}}(\vec{r}_{2}) \phi_{ns}(\vec{r}_{2}) \left[\frac{r_{21} - z_{21}}{(r_{2} - z_{2})^{2}} \right]^{i\eta_{+}}$$

$$\rightarrow (r_{1} + z_{1})^{i\eta_{+}} \int d\vec{r}_{2} e^{i\vec{q}\cdot\vec{r}_{2}} \phi^{\dagger}_{npm_{0}}(\vec{r}_{2}) \phi_{ns}(\vec{r}_{2})(r_{2} - z_{2})^{-2i\eta_{+}}.$$

We now have the amplitudes

$$g_{2}^{S}(m_{0},m_{1}) = -\frac{2}{k_{f}^{2}} \int d\vec{\mathbf{r}}_{1} \exp(-i\vec{\mathbf{k}}_{f}\cdot\vec{\mathbf{r}}_{1})\phi_{npm_{1}}^{\dagger}(\vec{\mathbf{r}}_{1})\phi_{ns}^{2}(\vec{\mathbf{r}}_{1})(r_{1}+z_{1})^{2i\eta} + \\ \times \int d\vec{\mathbf{r}}_{0}e^{i\vec{\mathbf{k}}_{i}\cdot\vec{\mathbf{r}}_{0}}\phi_{npm_{0}}^{\dagger}(\vec{\mathbf{r}}_{0})(r_{0}-z_{0})^{-2i\eta} + , \qquad (25a)$$

$$g_{3}^{S}(m_{0},m_{1}) = -\frac{1}{2\pi} \int d\vec{r} \frac{e^{i\vec{k}_{i}\cdot\vec{r}}}{r} (r-z)^{i\eta} \int d\vec{r}_{1}\phi_{npm_{1}}^{\dagger}(\vec{r}_{1})\phi_{ns}(\vec{r}_{1})(r_{1}+z_{1})^{i\eta} + \\ \times \int d\vec{r}_{2}e^{i\vec{q}\cdot\vec{r}_{2}}\phi_{npm_{0}}^{\dagger}(\vec{r}_{2})\phi_{ns}(\vec{r}_{2})(r_{2}-z_{2})^{-2i\eta} + .$$
(25b)

The generators are defined as

$$\phi_{npm_{1}}^{\dagger}(\vec{r}_{1})\phi_{ns}^{2}(\vec{r}_{1}) = D_{S2}(\mu_{1}\vec{\gamma}_{1})\exp(-\mu_{1}r_{1} + i\vec{\gamma}_{1}\cdot\vec{r}_{1}), \qquad (26a)$$

$$\phi_{npm_0}^{\dagger}(\vec{r}_0) = D_{S2}(\mu_0 \vec{\gamma}_0) \exp(-\mu_0 r_0 + i \vec{\gamma}_0 \cdot \vec{r}_0) , \qquad (26b)$$

$$\phi_{npm_1}^{\dagger}(\vec{r}_1)\phi_{ns}(\vec{r}_1) = D_{S3}(\mu_1\vec{\gamma}_1)\exp(-\mu_1r_1 + i\vec{\gamma}_1\cdot\vec{r}_1), \qquad (26c)$$

$$\phi_{npm_0}^{\dagger}(\vec{r}_0)\phi_{ns}(\vec{r}_0) = D_{S3}(\mu_0\vec{\gamma}_0)\exp(-\mu_0r_0 + i\vec{\gamma}_0\cdot\vec{r}_0) .$$
(26d)

The amplitudes $g_2^S(m_0, m_1)$ and $g_3^S(m_0, m_1)$ reduce to analytic form,

tion of two-dimensional integrals. It is always tempting to try to reduce an expression to analytic form and we find this may be done for the GA, providing one additional approximation is made.

Consider the integral (second term, integral over electron zero)

$$I_{20} = \int d\vec{r}_{0} e^{i\vec{k}_{i}\cdot\vec{r}_{0}} \phi^{\dagger}_{npm_{0}}(\vec{r}_{0}) \left[\frac{r_{01}-z_{01}}{r_{0}-z_{0}}\right]^{2i\eta_{+}}.$$
(22)

By changing coordinates to $\vec{r}_{01} = \vec{r}_0 - \vec{r}_1$, introducing the Fourier transforms, and splitting off the singular function $(r_{01} - z_{01})^{2i\eta}$, the Franco-Halpern approximation may be used. We then find that

A.

$$I_{20} \rightarrow (r_1 + z_1)^{2i\eta} + \\ \times \int d\vec{r}_0 e^{i\vec{k}_1 \cdot \vec{r}_0} \phi^{\dagger}_{npm_0}(\vec{r}_0)(r_0 - z_0)^{-2i\eta} + .$$
(23)

Similarly we find that

$$g_{2}^{S}(m_{0},m_{1}) = -\frac{2}{k_{f}^{2}} D_{S2}(\mu_{0}\vec{\gamma}_{0}) \frac{\partial}{\partial\mu_{0}} \left[\frac{-\pi 2^{2-2i\eta} + \Gamma(1-2i\eta_{+})}{[\mu_{0}-i(\vec{\gamma}_{0}+\vec{k}_{i})\cdot\hat{z}]^{2i\eta} + (\mu_{0}^{2}+|\vec{\gamma}_{0}+\vec{k}_{i}|^{2})^{1-2i\eta_{+}}} \right] \\ \times D_{S2}(\mu_{1}\vec{\gamma}_{1}) \frac{\partial}{\partial\mu_{1}} \left[\frac{-\pi 2^{2+2i\eta} + \Gamma(1+2i\eta_{+})}{[\mu_{1}+i(\vec{\gamma}_{1}-\vec{k}_{f})\cdot\hat{z}]^{-2i\eta} + (\mu_{1}^{2}+|\vec{\gamma}_{1}-\vec{k}_{f}|^{2})^{1+2i\eta_{+}}} \right]$$
(27a)

and

$$g_{3}^{S}(m_{0},m_{1}) = -\frac{1}{2\pi} \left[\pi 2^{2+i\eta} \Gamma(1+i\eta_{+}) \frac{(-ik_{iz})^{i\eta_{+}}}{k_{i}^{2+2i\eta_{+}}} \right] \\ \times D_{S3}(\mu_{0}\vec{\gamma}_{0}) \frac{\partial}{\partial\mu_{0}} \left[\frac{-\pi 2^{2-2i\eta_{+}}}{\left[\mu_{0}-i(\vec{\gamma}_{0}+\vec{q})\cdot\hat{z}\right]^{2i\eta_{+}}} \frac{\Gamma(1-2i\eta_{+})}{(\mu_{0}^{2}+|\vec{\gamma}_{0}+\vec{q}|^{2})^{1-2i\eta_{+}}} \right] \\ \times D_{S3}(\mu_{1}\vec{\gamma}_{1}) \frac{\partial}{\partial\mu_{1}} \left[\frac{-\pi 2^{2+i\eta_{+}}}{(\mu_{1}+i\gamma_{1z})^{-i\eta_{+}}} \frac{\Gamma(1+i\eta_{+})}{(\mu_{1}^{2}+\gamma_{1}^{2})^{1+i\eta_{+}}} \right].$$
(27b)

The differential and total scattering cross section have also been evaluated through the use of this approximation.

IV. DIFFERENTIAL AND TOTAL CROSS SECTIONS

The unpolarized differential and total cross sections are found in the usual manner,

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i} \frac{1}{2} \sum_{m_s, m'_s, m} |2g^+|^2, \qquad (28)$$

where g^+ is given by Eq. (4a). The factor of one half is from the average over the incident electron's spin, and the factor of two arises from the symmetrization of the amplitude. By choosing \vec{k}_i along the z-axis and only considering ${}^{1}S \rightarrow {}^{3}P$ excitations, all but two of the terms vanish when the Racah algebra is done. The differential cross section becomes

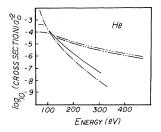


FIG. 1. \log_{10} of the total excitation cross section in units of a_0^2 vs incident electron energy in eV for He (${}^{1}S \rightarrow {}^{3}P$). Legend: Born-Oppenheimer —, Ochkur ----, Glauber —, Simplified Glauber

$$\frac{d\sigma}{d\Omega}({}^{1}S \rightarrow {}^{3}P) = 3\frac{k_{f}}{k_{i}} |g_{2}(0,+1) - g_{3}(+1,0)|^{2}.$$
(29)

We have made use of the following symmetry:

$$|g_{2}(0,+1)-g_{3}(+1,0)|^{2} = |g_{2}(0,-1)-g_{3}(-1,0)|^{2}.$$
 (30)

The total cross section is found by integrating the above,

$$\sigma({}^{1}S \rightarrow {}^{3}P) = 3\frac{k_{f}}{k_{i}} \int d\Omega |g_{2}(0,+1) - g_{3}(+1,0)|^{2}.$$
(31)

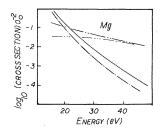


FIG. 2. \log_{10} of the total excitation cross section in units of a_0^2 vs incident electron energy in eV for Mg (${}^{1}S \rightarrow {}^{3}P$). Legend: Born-Oppenheimer —, Ochkur ----, Glauber —, Simplified Glauber

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A. Specific amplitudes

If the generators are applied to the various amplitudes, we then find the following:

$$g_{\rm BO}(0,+1) = \frac{3(2^{11/2})(N_s N_p)^2}{(\alpha_p^2 + k_i^2)^3} \alpha_s \alpha_p k_i I(\chi) \sin\theta = g_{\rm BO} \sin\theta , \qquad (32a)$$

$$I(\chi) = \int_0^1 \frac{d\chi (1-\chi)^{1/2}}{(\alpha_s^2 + \chi k_f^2)^{3/2}} \frac{(\mu_1 + 6\Omega)(\mu_1 + \Omega)^2 + \mu_1 (1-\chi)^2 k_f^2}{[(\mu_1 + \Omega)^2 + (1-\chi)^2 k_f^2]^4} ,$$
(32b)

$$g^{O}(0,+1) = -\frac{3(2^{13/2})(N_{s}N_{p})^{2}\alpha_{p}(2\alpha_{s}+\alpha_{p})}{(\alpha_{p}^{2}+k_{i}^{2})^{3}[(2\alpha_{s}+\alpha_{p})^{2}+k_{f}^{2}]^{3}}\frac{k_{i}}{k_{f}}\sin\theta = g^{O}\sin\theta .$$
(33)

The full GA results must be obtained by numerically performing the integrals in Eqs. (19). For energies above two times threshold we find that g_2^G may be neglected compared with g_3^G . Ellis⁸ describes our numerical procedures and GA results.

From the SG approximation we find

$$g_{2}^{S}(0,+1) - g_{3}^{S}(+1,0) = -3\sqrt{2} \left[\frac{N_{np}N_{ns}}{4\pi k_{f}} \right]^{2} \left\{ Z(-2\eta_{+},\alpha_{np},\vec{k}_{i})X(2\eta_{+},2\alpha_{ns}+\alpha_{np},\vec{k}_{f}) + \left[\frac{k_{f}}{k_{i}} \right]^{2} \Gamma(1+i\eta_{+}) \right\}$$

$$\times \exp\left[\eta_{+} \left[\frac{\pi}{2} + i\ln 2/k_{i} \right] X(-2\eta_{+},\alpha_{ns}+\alpha_{np},\vec{q})Z(\eta_{+},\alpha_{np}+\alpha_{ns},\vec{0}) \right]. \quad (34a)$$

In the above,

$$X(b,\mu,\vec{a}) = -a_x \pi 2^{4+ib} (1+ib) \Gamma(1+ib) \left[\frac{ib}{2} \frac{(\mu - ia_z)^{-1+ib}}{(\mu^2 + \vec{a}^2)^{2+ib}} -\mu(2+ib) \frac{(\mu - ia_z)^{ib}}{(\mu^2 + a^2)^{3+ib}} \right],$$
(34b)

$$Z(b,\mu,\vec{\mathbf{a}}) = \pi 2^{3+ib} \Gamma(1+ib) \begin{pmatrix} \frac{b}{2}(1-ib)\frac{(\mu-ia_z)^{-2+ib}}{(\mu^2+\vec{\mathbf{a}}^2)^{1+ib}} \\ +b(1+ib)(\mu+ia_z)\frac{(\mu-ia_z)^{-1+ib}}{(\mu^2+\vec{\mathbf{a}}^2)^{2+ib}} \\ -2\mu a_z(1+ib)(2+ib)\frac{(\mu-ia_z)^{ib}}{(\mu^2+\vec{\mathbf{a}}^2)^{3+ib}} \end{pmatrix}.$$
(34c)

The differential and total cross sections were numerically evaluated through the use of these amplitudes in Eqs. (32), (33), (19), and (34). This evaluation is very straightforward and efficient for the BO, OC, and SG approximations. These programs were written in Speakeasy and run on an IBM 4341 at The University of Toledo Computing Center.

Energy (eV)	Born-Oppenheimer	Ochkur	Glauber	S. Glauber	Expt. ^a
65	3.67(-4)	9.16(-3)		1.32(-5)	
80	4.59(-4)	1.21(-3)		3.41(-5)	2.9(-4)
100	1.76(-4)	1.85(-4)	6.36(-5)	5.05(-5)	1.36(-4)
120	6.03(-5)	4.01(-5)	4.50(-5)	4.41(-5)	6.4(-5)
150	1.32(-5)	5.93(-6)	2.54(-5)	2.93(-5)	4.8(-5)
200	1.47(-6)	4.61(-7)	1.04(-5)	1.40(-5)	
300	4.80(-8)	1.03(-8)	2.62(-6)	3.93(-6)	
500	4.30(-10)	6.12(-11)	4.00(-7)	6.45(-7)	
1000	4.53(-13)	3.60(-14)	2.60(-8)	4.63(-8)	
2000	3.73(-16)	1.44(-17)	1.65(-9)	3.01(-9)	

TABLE II. Total cross sections for He $(1s^{2}S_{g} \rightarrow 2p^{2}P_{g})$ in units of a_{0}^{2} .

^aInterpolated from the figures given in Westerveld et al. (Ref. 7).

B. Results and discussion

We have calculated the differential and total cross sections for the following excitations: He $(1s^{21}S \rightarrow 2p^{23}P)$, Mg $(3s^{21}S \rightarrow 3p^{23}P)$, and Ca $(4s^{21}S \rightarrow 4p^{23}P)$. The incident electron energies, which we have chosen for each excitation, range from about twice threshold energy to ten times threshold energy.

As may be seen from Eqs. (32) and (33), the BO and OC differential cross sections have a $\sin^2\theta$ behavior as expected. The GA and SG approximations do not have this functional dependence on the scattering angle, but shift the peak of the differential cross section towards smaller angles at higher energies. This is not unexpected, because the accumulated phase in the Glauber theory essentially includes higher-order perturbation terms, which are not present in the first-order BO and OC approximations and, at high energies, there should be more forward scattering.

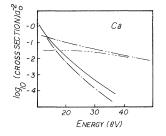


FIG. 3. Log_{10} of the total excitation cross section in units of a_0^2 vs incident electron energy in eV for Ca (${}^{1}S \rightarrow {}^{3}P$). Legend: Born-Oppenheimer —, Ochkur ----, Glauber —, Simplified Glauber

The total cross sections are shown in Figs. 1-3. Tables II-IV display numerical values (GA results are from Ellis et al.⁸). Although we have calculated the excitation cross sections at low energies (about twice threshold), not much credence should be placed in these values. All of the approximations are intermediate to high-energy approximations, and the results are intended only for comparison purposes. At intermediate energies (about five times threshold), the GA and SG approximations are larger than the BO and OC approximations. This is because $g_3^+(0, +1)$ becomes the dominant term and, as we mentioned earlier, it is identically zero in the BO and OC approximations. In this energy range the numerical agreement between GA and SG is much better for Mg and Ca than it is for He. This is primarily due to the fact that the principal quantum number changes for the He excitation but not for Mg or Ca. At high energies (about ten times threshold), the GA and SG approximations are several orders of magnitude larger than the BO and OC approximations.

The asymptotic energy dependence of the total cross sections may be determined by analytical and numerical methods. They are

TABLE III. Total cross sections for Mg $(3s^{2} {}^{1}S_{g} \rightarrow 3p^{2} {}^{3}P_{g})$ in units of a_{0}^{2} .

Energy (eV)	Born- Oppenheimer	Ochkur	Glauber	S. Glauber
15	9.20(-1)	6.96(-1)	1.75(-1)	3.46(-2)
20	1.46(-1)	7.89(-2)	1.13(-1)	3.99(-2)
- 30	6.97(-3)	2.75(-3)	4.43(-2)	2.75(-2)
40	6.26(-4)	2.08(-4)	1.95(-2)	1.61(-2)
50	8.59(-5)	2.52(-5)	9.70(-3)	9.43(3)

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TABLE IV. Total cross sections for Ca $(4s^{2} {}^{1}S_{g} \rightarrow 4p^{2} {}^{3}P_{g})$ in units of a_{0}^{2} .

Energy (eV)	Born- Oppenheimer	Ochkur	Glauber	S. Glauber
10	1.87	1.39	3.14(-1)	3.04(-2)
20	1.37(-2)	5.33(-3)	1.05(-1)	4.35(-2)
25	2.14(-3)	7.24(-4)	5.60(-2)	3.36(-2)
35	1.07(-4)	2.99(-5)	2.29(-2)	1.81(-2)
50	3.65(-6)	8.33(-7)	7.30(-3)	7.43(-3)

$$\sigma_{\rm BO}({}^1S \longrightarrow {}^3P) \sim E^{-10} , \qquad (35a)$$

$$\sigma_0({}^1S \to {}^3P) \sim E^{-12} , \qquad (35b)$$

$$\sigma_G({}^1S \to {}^3P) \sim E^{-4} , \qquad (35c)$$

$$\sigma_S({}^1S \to {}^3P) \sim E^{-4} . \tag{35d}$$

Thus, a crucial test of the validity of the approximations is to compare them with experimental data at high energies. Unfortunately, there is a limited amount of experimental data available. In Table II we show the He data of Westerveld *et al.*, which they normalized to the BO at 120 eV. The only data point above 120 eV is at 150 eV and no definitive conclusions about the asymptotic energy dependence of the experimental cross section may be drawn.

V. CONCLUSIONS

Double electron excitation cross sections have been calculated for He $(1s^{2}S \rightarrow 2p^{2}P)$, Mg $(3s^{2}S \rightarrow 3p^{2}P)$, and Ca $(4s^{2}S \rightarrow 4p^{2}P)$ with the

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use of several different approximations. At high energies we find that the BO and OC approximations fall rapidly as a function of the incident energy. The GA and SG approximations do not have this strong energy dependence, but vary as E^{-4} . Our SG approximation includes both of the contributing terms in the amplitude, while the GA only includes the dominant high-energy term. The agreement between the latter two approximations for Mg and Ca demonstrate that the SG approximation serves a useful purpose because it is easier to evaluate than the BO approximation and gives the same asymptotic energy dependence as the GA. However, none of the calculations agree with the experimental helium data of Westerveld. Additional experimental data for these elements is necessary before any definite conclusions about the validity of the theories can be made. It is hoped that these would be absolute cross sections and include several high-energy measurements.

In our GA and SG calculations we have chosen \vec{k}_i as the z axis and have not set $q_z=0$. We are currently investigating the wide angle Glauber approximation $(\vec{k}_i \text{ not along } z, \text{ but } q_z=0)$, the inclusion of $g_2^+(0,+1)$ in the GA, and a Born-Eikonal series type of approximation. It would also be interesting to examine the feasibility of doing a higher-order BO approximation.

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