

Excitation cross sections of $e^- + \text{He} \rightarrow e^- + \text{He}(3^1P, 4^1P)$ and the polarization of the 5016-Å helium line resulting from e^- -He scattering in Glauber theory

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The recently derived generating function $I_p(\lambda_1, \lambda_2; q)$ in the Glauber amplitude for 2^1P excitation of He by electron impact is used to evaluate the cross sections for the 3^1P and 4^1P excitations of He by electron impact with incident energies from 50 to 1000 eV. Comparison is made with the Bethe approximation, the Born approximation, and the classical theory of Gryzinski. The theoretical results for the total excitation cross sections are in reasonable agreement with the experimental data. The positions of the peak values for the total cross section for both cases are found to be around 100 eV, which are consistent with the existing experimental findings. The n^{-3} rule is also briefly discussed. The polarization fraction of the 5016-Å helium line emitted in $e^- + \text{He}$ collisions is also calculated in the Glauber approximation. The theoretical results for the polarization fraction are in reasonable agreement with the existing experimental data in the energy range $50 < E_a < 1000$ eV.

I. INTRODUCTION

Recently, a large amount of experimental data¹⁻⁷ have become available on the total cross sections for the excitation of helium from its ground state to the 3^1P and 4^1P levels by electron impact. There appears to be good agreement between all the photon measurements so that the positions of the peak cross sections are around 100 eV, although there is considerable variation in peak height. On the theoretical side, calculations have been performed with the Born approximation,^{8,9} the Bethe approximation,¹⁰ and classical theory.¹¹ For energies greater than 200 eV, all these theoretical models produce results which are in reasonable agreement with the existing experimental data. However, the positions for the peak cross section predicted from these methods are in poor agreement with the experiments.

We want to do two things in this paper. First, we show that the generating function $I_p(\lambda_1, \lambda_2; q)$ recently derived¹² in the Glauber amplitude for the 2^1P excitation can be employed without much further effort to evaluate the cross sections for the 3^1P and 4^1P excitation of helium by electron impact. Second, we show that the properly computed polarization fraction $P(E_a)$ in Glauber theory does yield a reasonably good fit to the observed $P(E_a)$ in the range $50 < E_a < 1000$.

II. EXCITATION CROSS SECTIONS

The Glauber scattering amplitude $F_{fi}(\vec{q})$ describing the excitation of the He from the ground state $\Psi_{11S}(\vec{r}_1, \vec{r}_2)$ to the final state $\Psi_{n^1P}(\vec{r}_1, \vec{r}_2)$ by an incident charged particle $Z_i e$ with velocity v_i is given by

$$F_{fi}(\vec{q}) = (iK_i/2\pi) \int \Psi_{n^1P}^*(\vec{r}_1, \vec{r}_2) \Gamma(\vec{b}; \vec{r}_1, \vec{r}_2) \times \Psi_{11S}(\vec{r}_1, \vec{r}_2) e^{i\vec{q} \cdot \vec{b}} d^2b d\vec{r}_1 d\vec{r}_2, \quad (1)$$

where

$$\Gamma(\vec{b}; \vec{r}_1, \vec{r}_2) = 1 - (|\vec{b} - \vec{s}_1|/|\vec{b}|)^{2\eta} (|\vec{b} - \vec{s}_2|/|\vec{b}|)^{2\eta} \quad (2)$$

and

$$\eta \equiv -z_i/v_i \quad (\text{in atomic units}).$$

In Eqs. (1) and (2), \vec{b} , \vec{s}_1 , and \vec{s}_2 are the respective projections of the position vectors of the incident particle and the bound electrons (\vec{r}_1 and \vec{r}_2) onto the plane perpendicular to the direction of the Glauber path integration. The approximate ground-state wave function chosen (in atomic units) is the one described by Byron and Joachain,¹³

$$\Psi_{11S}(\vec{r}_1, \vec{r}_2) = (1.6966/\pi) (e^{-1.41r_1} + 0.799 e^{-2.61r_1}) \times (e^{-1.41r_2} + 0.799 e^{-2.61r_2}). \quad (3)$$

A. 1^1S - 3^1P excitation

For the 3^1P state of He, we use the variationally determined wave function given by Goldberg and Clogston,¹⁴ namely,

$$\Psi_{3^1P}(\vec{r}_1, \vec{r}_2) = (N_{3P}/\sqrt{3\pi}) [e^{-2r_1}(c-r_2)r_2 e^{-\mu r_2} \times Y_{1m}(\theta_2, \phi_2) + e^{-2r_2}(c-r_1) \times r_1 e^{-\mu r_1} Y_{1m}(\theta_1, \phi_1)], \quad (4)$$

with

$$\mu = 0.325, \quad c = 5A/\mu, \quad A = (1 + 0.97/2\mu)^{-1},$$

$$N_{3P}^2 = \mu^7 / (25A^2 - 25A + 7.5).$$

In the case of excitation to the $m=0$ state, one sees that by introducing the cylindrical coordinates for \vec{r}_1 and \vec{r}_2 , $F(\vec{q})$ vanishes from Eq. (1) since the integrand under the integral is an odd function of z .¹²

For excitation to either $m=+1$ or $m=-1$, the values of $|F_{fi}(\vec{q})|^2$ are equal. Let us calculate the excitation to $m=-1$ only. Substituting expressions (3) and (4) for $m=-1$ into Eq. (1), we find the amplitude $F(\vec{q})$ in terms of the generating function $I_p(\lambda_1, \lambda_2; q)$,

$$I_p(\lambda_1, \lambda_2; q) = \frac{i}{\pi} \int e^{-\lambda_1 r_1 - \lambda_2 r_2} \frac{1}{r_1 r_2} \left(\frac{|\vec{b} - \vec{s}_1|}{b} \right)^{2i\eta} \left(\frac{|\vec{b} - \vec{s}_2|}{b} \right)^{2i\eta} e^{i\varphi_{s_1}} e^{i\vec{q} \cdot \vec{r}} r_1 \sin\theta_1 d^2b d\vec{r}_1 d\vec{r}_2$$

$$= i128\eta e^{i\phi_q} \left(\Gamma(1+i\eta)\Gamma(2-i\eta)q^{2i\eta-3} [-(1+i\eta)\lambda_2^{-2}\lambda_1^{-2i\eta-2} {}_2F_1(2-i\eta, 1-i\eta; 2; -\lambda_1^2/q^2) \right.$$

$$\quad \left. + \lambda_2^{-2}\lambda_1^{-2i\eta-2} {}_2F_1(2-i\eta, 1-i\eta; 1; -\lambda_1^2/q^2) \right]$$

$$- (2i\eta)^2 \int_0^\infty b^6 db J_1(qb) [(1+i\eta)(i\lambda_1 b)^{-2i\eta-3} \mathcal{L}_{2i\eta,1}(i\lambda_1 b) - i\eta(i\lambda_1 b)^{-2i\eta-2} \mathcal{L}_{2i\eta-1,0}(i\lambda_1 b)]$$

$$\times (i\lambda_2 b)^{-2i\eta-2} \mathcal{L}_{2i\eta-1,0}(i\lambda_2 b) \Big), \quad (6)$$

where Γ , J_1 , ${}_2F_1$, and $\mathcal{L}_{\mu\nu}$ are the usual gamma, Bessel, hypergeometric, and modified Lommel functions,¹⁵ respectively.

B. 1^1S-4^1P excitation

For the highly excited state 4^1P , we adopt Heisenberg's choice,¹⁶ i.e., we consider the screening of the inner on the outer electron as "complete," so we have

$$\Psi_{4^1P}(\vec{r}_1, \vec{r}_2) = \frac{1}{8} (5/3\pi)^{1/2} [e^{-2r_1} e^{-r_2/4} (r_2 - \frac{1}{4}r_2^2 + \frac{1}{80}r_2^3)$$

$$\times Y_{1m}(\theta_2, \phi_2) + e^{-2r_2} e^{-r_1/4}$$

$$\times (r_1 - \frac{1}{4}r_1^2 + \frac{1}{80}r_1^3) Y_{1m}(\theta_1, \phi_1)]. \quad (7)$$

Again, $F(\vec{q})=0$ for excitation to $m=0$, and the values of $|F_{fi}(\vec{q})|^2$ are equal for excitation to either $m=-1$ or $m=+1$. For excitation to $m=-1$, substituting expressions (3) and (7) for $m=-1$ into Eq. (1), we obtain

$$F(1^1S-4^1P; \vec{q}) = (2.605/64)\sqrt{\frac{5}{2}} K_i \sum_{n=1}^4 c(n)$$

$$\times \left(\frac{\partial^2 I_p}{\partial \lambda_1 \partial \lambda_2} + 0.25 \frac{\partial^3 I_p}{\partial \lambda_1^2 \partial \lambda_2} \right.$$

$$\left. + 0.0125 \frac{\partial^4 I_p}{\partial \lambda_1^3 \partial \lambda_2} \right) \Big|_{\lambda_1=\lambda_1(n), \lambda_2=\lambda_2(n)} \quad (8)$$

$$F(1^1S-3^1P; \vec{q}) = (1.3025N_{3P}/\sqrt{2}) K_i \sum_{n=1}^4 c(n)$$

$$\times \left(c \frac{\partial^2 I_p}{\partial \lambda_1 \partial \lambda_2} + \frac{\partial^3 I_p}{\partial \lambda_1^2 \partial \lambda_2} \right) \Big|_{\lambda_1=\lambda_1(n), \lambda_2=\lambda_2(n)} \quad (5)$$

with

$$c(n) = 1, \quad 0.799, \quad 0.799, \quad (0.799)^2;$$

$$\lambda_1(n) = 1.735, \quad 2.935, \quad 1.735, \quad 2.935;$$

$$\lambda_2(n) = 3.41, \quad 3.41, \quad 4.61, \quad 4.61.$$

In Eq. (5), $I_p(\lambda_1, \lambda_2; q)$ is as defined and given in Eqs. (6) and (20) of Ref. 12:

where

$$\lambda_1(n) = 1.66, \quad 2.86, \quad 1.66, \quad 2.86;$$

$$\lambda_2(n) = 3.41, \quad 3.41, \quad 4.41, \quad 4.41.$$

From Eq. (A10) of Ref. 15,

$$(d/dx) \mathcal{L}_{\mu,\nu}(ix) = i(\mu + \nu - 1) \mathcal{L}_{\mu-1,\nu-1}(ix)$$

$$- (\nu/x) \mathcal{L}_{\mu,\nu}(ix) \quad (9)$$

and¹⁷

$$\frac{d}{dx} {}_2F_1(a, b, c; x) = \frac{ab}{c} {}_2F_1(a+1, b+1, c+1; x), \quad (10)$$

one can easily obtain the expressions $\partial^2 I_p / \partial \lambda_1 \partial \lambda_2$, $\partial^3 I_p / \partial \lambda_1^2 \partial \lambda_2$, and $\partial^4 I_p / \partial \lambda_1^3 \partial \lambda_2$ and hence the Glauber amplitudes $F(1^1S-3^1P; \vec{q})$ and $F(1^1S-4^1P; \vec{q})$. The procedures for numerical computation of $\partial^2 I_p / \partial \lambda_1 \partial \lambda_2$, $\partial^3 I_p / \partial \lambda_1^2 \partial \lambda_2$, and $\partial^4 I_p / \partial \lambda_1^3 \partial \lambda_2$ are the same as those of $I_p(\lambda_1, \lambda_2; q)$, and are described in detail in Refs. 15 and 12.

C. Results and discussion on the cross sections

We have calculated the differential cross sections $d\sigma/d\Omega$ for excitation to 3^1P and 4^1P by means of Eqs. (5) and (8) and the expressions for $\partial^2 I_p / \partial \lambda_1 \partial \lambda_2$, $\partial^3 I_p / \partial \lambda_1^2 \partial \lambda_2$, and $\partial^4 I_p / \partial \lambda_1^3 \partial \lambda_2$ for various incident electron energies, as a function of the scattering angle. The differential cross sections for the 3^1P

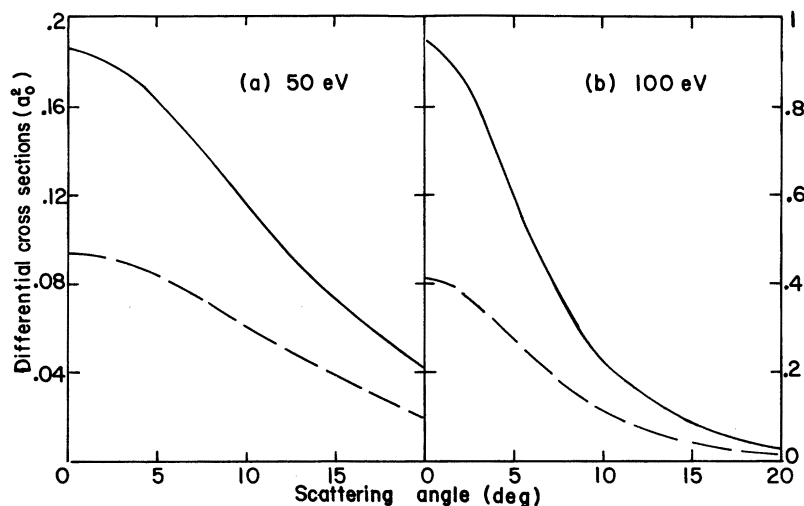


FIG. 1. Differential cross sections for 3^1P and 4^1P excitation of helium by electrons at (a) 50 eV, (b) 100 eV. Solid curve, 3^1P (this work); dashed curve, 4^1P (this work).

and 4^1P excitations are shown in Figs. 1 and 2 and need not be discussed in detail; the patterns follow that of the 2^1P case.¹² For comparison, we also present in Fig. 2 the results from the Born approximation⁸ for the 3^1P excitation. For scattering angles smaller than 20° , we find that differential-cross-section ratios for the 3^1P and 4^1P levels are in the range from 1.5 to 2.8. Since the most important contribution to the total cross section comes from the region from 0° to 20° , the n^{-3} rule for the total cross section, which is equal to $4^3/3^3 \sim 2.4$ for the present case, is approximately valid only in the average sense. We have also integrated the differential cross sections and therefore obtained the total excitation cross sections as a function of the incident electron energy. The results are shown in Figs. 3 and 4. We note from

Fig. 3 that the Glauber theory predicts a peak value for the total 3^1P excitation cross section around 100 eV, which is consistent with the experimental findings,²⁻⁷ whereas the Born approximation (BA) gives a peak value around 55 eV.⁹ However, the Glauber approximation (GA) seems to underestimate the experimental results. Perhaps an even better wave function than Eq. (4) is required in order to obtain better agreement with experiment for the 3^1P excitation. From Fig. 4, we note that the Glauber results for the 4^1P excitation are in good agreement with the existing experimental data.²⁻⁷ The predictions on the peak value for the total 4^1P excitation cross section from the Born approximation⁷ and the classical theory¹¹ gives values around 55 and 75 eV, respectively, which are again too low in comparison with experiments.

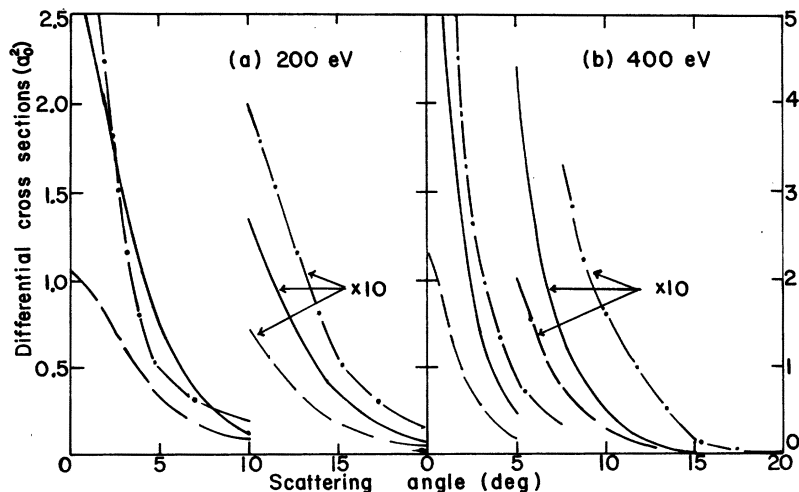


FIG. 2. Differential cross sections for 3^1P and 4^1P excitation of helium by electrons at (a) 200 eV, (b) 400 eV. Solid curve 3^1P (this work); dashed curve 4^1P (this work); dot-dashed curve, Born approximation for 3^1P (Altshler).

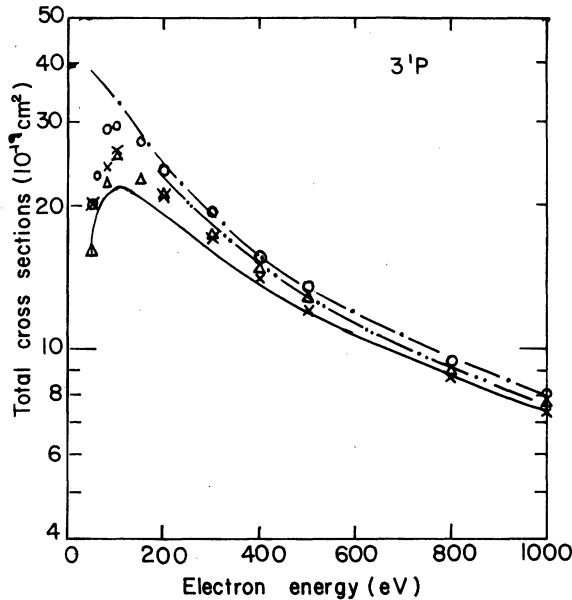


FIG. 3. Total cross sections for $1^1S \rightarrow 3^1P$ excitation of helium by electron impact. Solid curve, this work; single-dot-dashed curve, Born approximation (Bell *et al.*); double-dot-dashed curve, Bethe approximation (Kim and Inokuti); circles, Donaldson *et al.*; triangles, De Jongh and Van Eck; crosses, Moustafa *et al.*

We also find that

$$\frac{\sigma_T(2^1P)}{\sigma_T(4^1P)} \sim 7.8,$$

$$\frac{\sigma_T(2^1P)}{\sigma_T(3^1P)} \sim 4.1,$$

$$\frac{\sigma_T(3^1P)}{\sigma_T(4^1P)} \sim 1.9.$$

These values are close to the n^{-3} rule, which predicts the values of 8, 3.38, and 2.37, respectively. The discrepancy again indicates the underestimation from the 3^1P calculation.

III. POLARIZATION OF 5016-Å HELIUM LINE

For the 5016-Å line emitted by the helium atom following electron excitation to the 3^1P state, the polarization fraction

$$P = \frac{(I_{\parallel} - I_{\perp})}{(I_{\parallel} + I_{\perp})}, \quad (11)$$

according to the theory of Percival and Seaton,¹⁸ is given by

$$P(E_a) = (Q_0 - Q_1)/(Q_0 + Q_1). \quad (12)$$

In Eq. (11), I_{\parallel} and I_{\perp} are the intensities, observed at 90° to the incident electron beam direction, of the respective 5016-Å line having electric vectors parallel and perpendicular to the incident electron

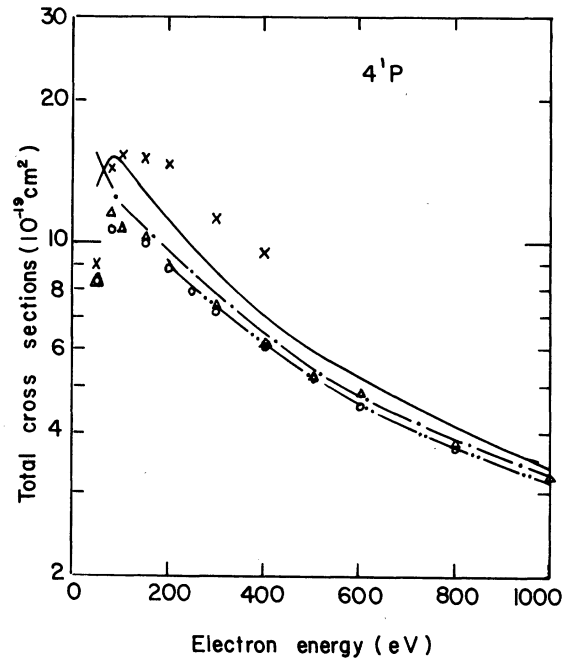


FIG. 4. Total cross sections for $1^1S \rightarrow 4^1P$ excitation of helium by electron impact. Solid curve, this work; single-dot-dashed curve, Born approximation (Bell *et al.*); double-dot-dashed curve, Bethe approximation (Kim and Inokuti); circles, Donaldson *et al.*; triangles, De Jongh and Van Eck; crosses, St. John *et al.*

beam direction. In Eq. (12), E_a is the incident electron energy, the quantities Q_m , $m = 0$ and ± 1 , are the total cross section for exciting the helium atom from ground state to the $3p_m$ sublevels. Since $Q_0 = 0$ in the GA, the theory predicts $P(E_a) = -1$ at all incident energies. However, the observed $P(E_a)$ gives monotonically decreasing values¹⁹⁻²² from about +0.4 to -0.15 as E_a increases from 50 to 1000 eV. A similar situation appears in the polarization of Lyman- α radiation resulting from e^- -H(1S) collisions.^{23,24} This puzzle was solved by Gerjuoy, Thomas, and Sheorey (GTS),²⁴ who demonstrated that the properly computed Glauber-predicted $P(E_a)$ —using the direction perpendicular to \vec{q} (momentum transfer of the incident electron) as the z axis (and quantum axis) at each \vec{q} for which the Glauber amplitude is evaluated—does yield a reasonably good fit to the observed $P(E_a)$ in the range $30 < E_a < 700$ eV. In what follows, we will use the results of GTS to remove the inconsistency of simultaneous comparisons with observation of the Glauber-predicted 5016-Å line polarization and the 3^1P excitation cross sections.

Let $C^{\xi}(\vec{\xi})$ denote the \vec{q} -dependent coordinate system, whose z axis lies along $\vec{\xi}$ and is perpendicular to \vec{q} , in which the Glauber amplitudes $F_{3^1P,1S}^{(\xi)}(\vec{q}, m_2)$

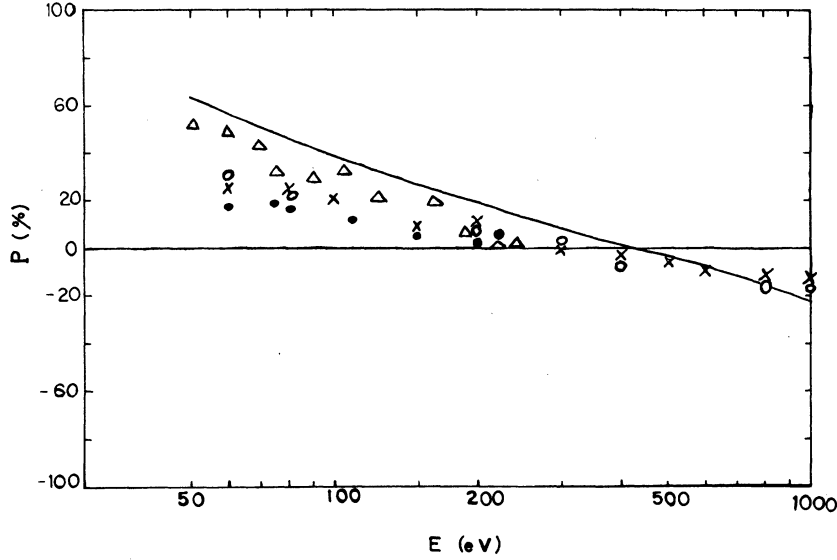


FIG. 5. Polarization fraction of the 5016-Å helium line excited by electron impact. Solid curve, Glauber; triangles, Heddle and Lucas; crosses, Moussa *et al.*; open circles, Van Raan; closed circles, McFarland and Soltysik.

are readily computable. The $1^1S-3^1P_m$ Glauber amplitudes are given by Eqs. (5) and (6) of Sec. II:

$$F_{3P,1S}^{(\zeta)}(\vec{q}, m_2 = 0) = 0 \quad (13a)$$

and

$$F_{3P,1S}^{(\zeta)}(\vec{q}, m_2 = \pm 1) = \pm e^{\mp i \phi_q} h_{3P,1S}^{\zeta}(q), \quad (13b)$$

where

$$h_{3P,1S}^{\zeta}(q) = \frac{i1.3025 \times 1.28 N_{3P} K_i}{\sqrt{2}} \sum_{n=1}^4 c(n) \times \left[\left(c \frac{\partial^2}{\partial \lambda_1 \partial \lambda_2} + \frac{\partial^3}{\partial \lambda_1^2 \partial \lambda_2} \right) \left(\Gamma(1+i\eta) \Gamma(2-i\eta) q^{2i\eta-3} \lambda_2^{-2} \lambda_1^{-2i\eta-2} \left[-(1+i\eta) {}_2F_1(2-i\eta, 1-i\eta; 2; -\lambda_1^2/q^2) + {}_2F_1(2-i\eta, 1-i\eta; 1; -\lambda_1^2/q^2) \right] - (2i\eta)^2 \int_0^{\infty} b^6 db J_1(qb) [(1+i\eta)(i\lambda_1 b)^{-2i\eta-3} \mathcal{E}_{2i\eta,1}(i\lambda_1 b) - i\eta(i\lambda_1 b)^{-2i\eta-2} \mathcal{E}_{2i\eta-1,0}(i\lambda_1 b)] \times (i\lambda_2 b)^{-2i\eta-2} \mathcal{E}_{2i\eta-1,0}(i\lambda_2 b) \right] \right]_{\lambda_1 = \lambda_1(n), \lambda_2 = \lambda_2(n)} \quad (13c)$$

Equations (13a)–(13c) differ from expressions (5) and (6) by the phase $\pm i$ (when $m_L = \pm 1$) since we here use the same convention as those of GTS.

The Glauber amplitudes $F_{3P,1S}^{(a)}(\vec{q}, m_2)$, quantized along \vec{K}_a , have been obtained by GTS and are given by

$$F_{3P,1S}^{(a)}(\vec{q}, m_L = 0) = -i\sqrt{2} \cos \theta_q h_{3P,1S}^{\zeta}(q), \quad (14a)$$

$$F_{3P,1S}^{(a)}(\vec{q}, m_L = \pm 1) = \pm i e^{\mp i \phi_q} \sin \theta_q h_{3P,1S}^{\zeta}(q), \quad (14b)$$

where θ_q and ϕ_q are the angular coordinates of \vec{q} in $C(\vec{K}_a)$ with the z axis along \vec{K}_a .

The cross sections Q_0 and Q_1 in Eq. (12) are found from Eqs. (14) by

$$Q_{m_L}(E_a) = (K_f/K_i) \int d\hat{n}_b |F_{3P,1S}^{(a)}(\vec{q}, m_L)|^2. \quad (15)$$

We have calculated the polarization fraction $P(E_a)$ at incident energies from 50 to 1000 eV for the 5016-Å helium line via Eqs. (12)–(15). The

results are shown in Fig. 5. The Glauber $P(E_a)$ decreases monotonically from about 0.64 to -0.22 as E_a increases from 50 to 1000 eV. For $E_a \leq 150$ eV, the Glauber results are close to experimental values of Heddle and Lucas and are larger than those of Moussa *et al.*, van Raan *et al.*, and McFarland *et al.* by a factor of 2. For $E_a \geq 500$ eV, the Glauber results are close to the experimental data. Therefore the Glauber theory does give a reasonably good fit to the observed $P(E_a)$ in the range $50 < E_a < 1000$ eV.

Finally, we would like to mention the experimental results²⁵ of Eminyany *et al.* Using the coincidence techniques, these investigators were able to measure the ratio of $(d\sigma/d\Omega)_{m_2=0,\pm 1}$ and the phase between the corresponding excitation amplitudes in the e^- -He collisions. The experimental results and the Glauber predictions are presented in Table I. From Table I, we notice the Glauber

TABLE I. Experimental results and comparison with the GA and BA, where all the quantities are defined in Ref. 25.

Excited state	E (eV)	θ_e (deg)	Expt	λ		Expt	$ \chi $ (deg)	
				BA	GA		BA	GA
3^1P	77.7	30	0.45 ± 0.01	0.299	0.2993	53 ± 2	0	0
2^1P	80.0	16	0.39 ± 0.02	0.357	0.3569	53 ± 2	0	0

predictions for the λ are identical with the Born results which are in reasonable agreement with the experimental data. However, both the GA and BA predict the zero phase difference between $F_{nP,1S}^{(0)}(q, m_2=0)$ and $F_{nP,1S}^{(q)}(q, m_2=1)$ for all angles and energies, which is incorrect in light of the measurement.

In conclusion, it should also be mentioned that the method used in this paper applies equally well to higher n^1P excitation ($n=5, 6, \dots$); that is, one generating function $I_p(\lambda_1, \lambda_2; q)$ and the recur-

rence relations (9) and (10) would be enough to carry out the calculation. The Glauber theory is reliable in predicting the magnitudes but is incapable of finding the relative phase for the e^- -He excitation amplitude in the intermediate- and high-energy ranges.

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