Polarization fractions of Lyman- α radiation in e^- -H(1s) collision

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The Lyman- α polarization fractions resulting from e^- -H(1s) collision are calculated within the conventional Glauber and modified Glauber methods, in which the Glauber exchange effects are no longer neglected. It is found that in the conventional Glauber case, the inclusion of exchange effect completely changes the shape of the theoretical result curve at energies below 30 eV in comparison to the one obtained in the previous calculation without exchange and, furthermore, worsens somewhat the agreement with experimental data at energies between 30 and 60 eV. The new theoretical values obtained with the modified Glauber method with exchange are found to improve significantly the agreement with experimental data at intermediate scattering energies. However, the modified method still fails to account for experimental data below 30 eV, as expected.

I. INTRODUCTION

In the recent years,1 the Glauber and Glauberrelated methods have been considered in the analysis of various atomic and molecular collision processes at intermediate energies with a reasonable degree of success. The polarization fractions of the Lyman- α radiation in e^- -H(1s) collision were calculated with the conventional Glauber method by Gerjuoy et al.2 and the results were found to be in satisfactory agreement with experimental data³ at energies as low as 30 eV. The new calculation by Gerjuoy et al. resolved a mystery existing in a previous calculation,4 namely, the Glauber method seemed to yield the theoretical values in contradiction to what had been achieved with the differential cross sections in the 1-2 excitation processes. However, the deviation of the Glauber results of polarization fraction from experimental data at energies E > 30 eV in the new calculation by Gerjuoy et al. was still clearly noticeable, while the values at E < 30 eV were in a serious disagreement with experimental data. It was speculated by Gerjuoy et al.2 that the neglect of the Glauber exchange effect in the calculation might be one of the factors which is responsible for the disagreement, since the exchange effect is expected to be quite significant at energies lower than 30 eV. The exchange effect was neglected in the calculation because a simple method of calculation of the Glauber exchange amplitude had not been available at that time. This paper is, therefore, intended to serve two purposes. On the one hand, the polarization fractions of the Lyman- α radiation resulting from e^- -H(1s) collision will be recalculated with the conventional Glauber method, but with the Glauber exchange effect no longer neglected, to find out how the Glauber results at intermediate energies (30 \leq $E \leq$ 300 eV) would vary in the case of inclusion of exchange. I am also

interested in finding whether the disagreement with experimental data at E < 30 eV indeed originates from the neglect of exchange as was speculated by Gerjuoy et al. On the other hand, the polarization fractions of Lyman- α radiation will also be calculated with the modified Glauber method proposed recently.5 Since some serious deficiencies of the conventional Glauber amplitude are adequately corrected in the modified method, it is hoped that the method would also provide improved values for the polarization fractions as it did in the calculation of differential cross sections of e-H1-2 excitation.6 In Sec. II, the formalism of polarization fraction in the case of inclusion of exchange will be derived for both conventional and modified Glauber methods. The results of the calculation will be presented with the discussion and compared to experimental data in Sec. III.

II. THEORY

As was pointed out by Gerjuoy et al., the integrated cross sections Q_0 and Q_1 appearing in the equation of polarization fraction for Lyman- α radiation are calculated from the scattering amplitudes $F_{2p,1s}^{(a)}(\bar{\mathbf{q}},m_L)$ quantized along the direction of the momentum $\bar{\mathbf{K}}_i$ of incident electron. However, in the conventional and modified Glauber methods, both direct and exchange scattering amplitudes are calculated by quantizing along the direction of \hat{z} perpendicular to the momentum transfer of. Therefore, in order to apply the equation of polarization fraction for Lyman- α radiation,

$$P(E) = 3(Q_0 - Q_1)/(7Q_0 + 11Q_1), \qquad (1)$$

the expressions for the amplitudes are first required to transform into those quantized along K_i by a rotation.

It should be noted that in the conventional Glau-

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ber method, the direct scattering amplitude quantized along \hat{z} for the process $1s-2p_0$ is identically equal to zero, but the exchange amplitude is not. After the performance of rotation, one obtains for the direct amplitudes,

$$F_{2h,1}^{(a)}(\bar{q},m_{L}=0) = \sqrt{2} \cos\theta_{a} h_{2h,1}^{(g)}(q)$$
, (2a)

$$F_{2b,1s}^{(a)}(\bar{q}, m_L = \pm 1) = \sin\theta_a e^{\mp i\phi_a} h_{2b,1s}^{(e)}(q) , \qquad (2b)$$

where $e^{i\phi}dh_{2\rho,1s}^{(g)}(q)$ are the conventional Glauber

amplitudes of the process $1s-2p_{\star}$ quantized along the direction of \hat{z} perpendicular to \bar{q} . Other notations have their usual meanings. Equations (2a) and (2b) are slightly different from the expressions given by Gerjuoy et al. by the phase and sign, since the spherical harmonics used here are defined as Schiff rather than as Newton. The phases of the elements of the rotation matrix were modified accordingly. The expression of the rotation matrix in this case is found to be

$$D = \begin{bmatrix} \frac{1}{2}(1 + \sin\theta_{q}) & -(1/\sqrt{2})\cos\theta_{q}e^{-i\phi_{q}} & \frac{1}{2}(\sin\theta_{q} - 1)e^{-2i\phi_{q}} \\ (1/\sqrt{2})\cos\theta_{q}e^{i\phi_{q}} & \sin\theta_{q} & (1/\sqrt{2})\cos\theta_{q}e^{-i\phi_{q}} \\ \frac{1}{2}(\sin\theta_{q} - 1)e^{2i\phi_{q}} & -(1/\sqrt{2})\cos\theta_{q}e^{i\phi_{q}} & \frac{1}{2}(1 + \sin\theta_{q}) \end{bmatrix}.$$
(3)

The Glauber exchange amplitudes quantized along \vec{K}_i are related to those quantized along \hat{z} according to,

$$G_{2b,1s}^{(a)}(\bar{q}, m_L = 0) = \sqrt{2} \cos\theta_a g_1 + \sin\theta_a g_0,$$
 (4a)

$$G_{2h,1s}^{(a)}(\vec{q},m_L=\pm 1)=e^{\mp i\,\phi_q}[\sin\!\theta_q g_1-(\cos\!\theta_q/\!\sqrt{2})g_0]\,,\ (4b)$$

where $e^{\mp i\phi_0}g_1$ and g_0 are the Glauber exchange amplitudes quantized along z for the processes $1s-2p_\pm$ and $1s-2p_0$, respectively. The integrated cross sections Q_0 and Q_1 with exchange are then found to be

$$Q_{0} = 2\pi \frac{k_{f}}{k_{4}} \int_{0}^{\pi} d\theta \sin\theta \left[\frac{3}{4} \left| \sqrt{2} \cos\theta_{q} (h_{2p,1s}^{(g)}(q) - g_{1}) - \sin\theta_{q} g_{0} \right|^{2} + \frac{1}{4} \left| \sqrt{2} \cos\theta_{q} (h_{2p,1s}^{(g)}(q) + g_{1}) + \sin\theta_{q} g_{0} \right|^{2} \right], \tag{5a}$$

$$Q_{1} = 2\pi \frac{k_{f}}{k_{4}} \int_{0}^{\pi} d\theta \sin\theta \left(\frac{3}{4} \left| \sin\theta_{q}(h_{2p,1s}^{(g)}(q) - g_{1}) + \frac{\cos\theta_{q}}{\sqrt{2}} g_{0} \right|^{2} + \frac{1}{4} \left| \sin\theta_{q}(h_{2p,1s}^{(g)}(q) + g_{1}) - \frac{\cos\theta_{q}}{\sqrt{2}} g_{0} \right|^{2} \right), \tag{5b}$$

or equivalently.

$$Q_{0} = \frac{2\pi}{k_{\perp}^{2}} \int_{h_{1}-h_{2}}^{k_{i}+k_{f}} dq \, q\left[\frac{3}{4} \left| \sqrt{2} \cos \theta_{q}(h_{2p,1s}^{(g)} - g_{1}) - \sin \theta_{q} g_{0} \right|^{2} + \frac{1}{4} \left| \sqrt{2} \cos \theta_{q}(h_{2p,1s}^{(g)} + g_{1}) + \sin \theta_{q} g_{0} \right|^{2} \right], \tag{6a}$$

$$Q_{1} = \frac{2\pi}{k_{i}^{2}} \int_{k_{i}-k_{f}}^{k_{i}+k_{f}} dq \, q\left[\frac{3}{4} \left| \sqrt{2} \cos\theta_{q}(h_{2p,1s}^{(g)} - g_{1}) - \sin\theta_{q}g_{0} \right|^{2} + \frac{1}{4} \left| \sqrt{2} \cos\theta_{q}(h_{2p,1s}^{(g)} + g_{1}) + \sin\theta_{q}g_{0} \right|^{2} \right]. \tag{6b}$$

In the modified Glauber method,⁵ the direct scattering amplitude $h_{2p,1s}^{(0)}(q)$ of the process $1s-2p_0$ is also not identically equal to zero. The integrated cross sections Q_0 and Q_1 are, therefore, given by

$$Q_{0} = 2\pi \frac{k_{f}}{k_{i}} \int_{0}^{\pi} d\theta \sin\theta \left[\frac{3}{4} \left| \sqrt{2} \cos\theta_{q}(h_{2p,1s}^{(g)} - g_{1}) + \sin\theta_{q}(h_{2p,1s}^{(0)} - g_{0}) \right|^{2} + \frac{1}{4} \left| \sqrt{2} \cos\theta_{q}(h_{2p,1s}^{(g)} + g_{1}) + \sin\theta_{q}(h_{2p,1s}^{(0)} + g_{0}) \right|^{2} \right], \tag{7a}$$

$$Q_1 = 2\pi \frac{k_f}{k_*} \int_0^{\tau} d\theta \sin\theta \left(\frac{3}{4} \left| \sin\theta_q(h_{2p,1s}^{(g)}(q) - g_1) - \frac{\cos\theta_q}{\sqrt{2}} (h_{2p,1s}^{(0)} - g_0) \right|^2$$

$$+\frac{1}{4}\left|\sin\theta_{q}(h_{2\,b,1\,s}^{(g)}(q)+g_{1})-\frac{\cos\theta_{q}}{\sqrt{2}}(h_{2\,b,1\,s}^{(0)}+g_{0})\right|^{2}\right). \tag{7b}$$

The calculations of the direct and exchange Glauber amplitudes¹⁰ for the processes $1s-2p_{\pm}$ and $1s-2p_0$ in both conventional and modified methods were discussed in detail in my previous publication.⁶

III. RESULTS

The scattering amplitudes (direct and exchange) of the modified and conventional Glauber amplitudes are calculated for scattering energies ranging from 15 to 300 eV (with the method already described in Ref. 6). The value of 15 eV is in the vicinity of the threshold energy of the modified Glauber method and thereby, chosen to be the lower limit of the energy range in my analysis. At energies higher than 200 eV, while the exchange effects are negligible, the values of polarization fraction in the conventional and modified Glauber methods are expected to be different insignificantly from each other (see the results shown below). Since the conventional Glauber values were already available elsewhere² for energies higher than 300 eV, I shall concentrate my attention only on the range of intermediate energies where the comparison between the results of the two methods of approximation (modified and conventional Glauber) is of greatest interest. The integrated cross sections Q_0 and Q_1 are obtained by using either Eqs. (5a) and (5b) in the conventional Glauber case or Eqs. (7a) and (7b) in the modified Glauber case. The calculations are carried out with or without the inclusion of exchange effects. The polarization fractions of the Lyman- α radiation are finally deduced, using Eq. (1). The results are shown in Fig. 1, together with the experimental data by Ott et al.3 for comparison. Also shown are the values recalculated in the first Born approximation. It is found that at energies lower than about 30 eV, the inclusion of the Glauber exchange effect drastically modifies the polarization fractions of the Lyman- α radiation obtained in the conventional Glauber method. As the energy decreases to threshold, while the results of the conventional Glauber calculation without exchange increase toward the Percival and Seaton limit of P $=\frac{3}{7}$, the values with exchange fall off sharply to almost zero. The falloff is much sharper than what was found in experimental data which reach a value near 0.14. The exchange effects influence the cross sections Q_1 much more drastically than the cross sections Q_0 and thereby, reverse the direction of variation of the polarization fractions as the energy decreases. It is therefore concluded that the failure of the Glauber results in providing an agreement with experimental data at energy E < 30 eV does not originate from the neglect of exchange effect. The disagreement can, however, be understood, since the Glauber theory is not expected to work very well at these very low energies. The asymmetric influence of the exchange effects on Q_1 and Q_0 also reduces the values of polarization fraction at energies between 30 and

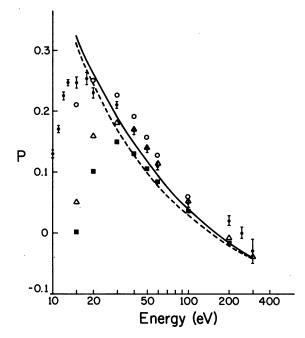


FIG. 1. Polarization fractions of Lyman- α radiation in e^- – H(1s) collision: -----, first Born approximation; -----, Glauber without exchange; , conventional Glauber with exchange; \bigcirc , modified Glauber without exchange; \triangle , modified Glauber with exchange; , experimental data of Ref. 3.

60 eV and thereby, worsens somewhat the agreement with experimental data. Thus, the discrepancy between the conventional Glauber values calculated previously² and experimental data at the intermediate energy range is also not due to the neglect of exchange effect in the calculation. At energies higher than 200 eV, the exchange effect becomes neglibible.

At lower energies, only the shape of the theoretical results of polarization fraction given by the modified Glauber method is in agreement with experimental data, namely, as the energy decreases, the polarization fraction curve reverses its direction of variation rather than continues to go up as in the conventional Glauber method. At energies higher than 30 eV, the modified Glauber values are somewhat higher than experimental data, while the values given by the conventional method are somewhat lower. The inclusion of exchange effects decreases the modified Glauber values at intermediate energies somewhat and thereby, provides a very good agreement with experimental data in this range of energy. The inclusion of exchange, however, makes the theoretical values at lower energies fall off much faster than what would be expected from experimental data as the energy decreases to threshold. The

disagreement with experimental data at energies lower than 30 eV is as expected for a Glauber-related method. The theoretical values at energies below 15 eV in a Glauber-related method are expected to disagree with experimental data as well and thereby, are not calculated here. At energies higher than 200 eV, the various sets of theoretical values obtained approach those of the conventional Glauber method which were already available in the previous calculation by Gerjuoy et al.2 The slight discrepancy with experimental data at high energies may be explained by the neglect of the cascade effects in the calculation. As was discussed previously,6 in the modified Glauber method, some deficiencies experienced in the conventional method are corrected. Especially, the longranged polarization effect is represented more adequately in the modified method through the real part of the second Born term. Since the longranged polarization effect is closely related to the distortion of the atomic charge distribution which should correlate with the asymmetry in the decay of photons of the atomic excited states, while the polarization fractions, to some extent, measure the degree of asymmetry in the decay radiation, these polarization fractions should, therefore, be given more correctly by the modified Glauber method than by the conventional one. In conclusion, the modified Glauber method which already yielded a good agreement with experimental data of differential cross section in the 1-2 excitation process, again provides a set of theoretical values of polarization fraction in satisfactory agreement with experimental data in the intermediate scattering-energy range.

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