PHYSICAL REVIEW A VOLUME 16, NUMBER 1 JULY 1977

Elastic electron-hydrogen scattering in a modified Glauber method with the inclusion of Glauber exchange*

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(Received 9 February 1977)

Elastic electron-hydrogen scattering at intermediate energies is analyzed with a modified Glauber amplitude proposed earlier by this author and the Glauber exchange effect included through a recent eikonal formula by Foster and Williamson. The results of the calculation are found to be in very good agreement with experimental data. This work, therefore, confirms rather clearly that the deficiency of the Glauber amplitude, when applied to these atomic processes, stems mainly from the inadequacy of the second-order term of its eikonal expansion in representing the second-Born term and that the Glauber exchange effect is of a considerable magnitude and, hence, cannot be neglected in these processes, especially at very large scattering angles.

I. INTRODUCTION

In a recent paper[1] a new and rather simple amplitude (called the modified Glauber amplitude) was proposed for the study of electron-atom scattering at intermediate energies and was applied with some degree of success to the calculations of elastic scatterings of electrons by hydrogen and helium atoms. In this amplitude, the second-order term of the Glauber eikonal expansion has been singled out and treated in a substantially different fashion than the remaining terms of the expansion. The choice of this amplitude for atomic scatterings was based on the following reasoning. In view of the fair success that the Glauber amplitude[2] has enjoyed earlier[3] since it was first applied to the domain of atomic and molecular collision by Franco in his pioneering work,[4] we believe that its failure to reproduce differential cross sections agreeing well with experimental data may have originated from the defects of some term of the amplitude. These defects are caused by the approximations considered in the derivation of this amplitude. Thus, the Glauber amplitude could be retained as a good approximation for atomic and molecular scatterings at intermediate energies if these defects were to be identified and adequately corrected.

We have, therefore, made a careful review on the derivation of the Glauber amplitude in order to find out which term of the amplitude needs to be rectified the most.[1] We have found that the so-called straight-line approximation considered along with the setting to zero of all the excited energies of the target intermediate states affects seriously the second-order term of the Glauber eikonal expansion. It is this approximation which makes the real part of the second-order Born term (which is of considerable magnitude) disappear from the Glauber amplitude on the one hand and, its imaginary part becomes singular in the forward direction on the other hand. Thus, the second-order term of the Glauber eikonal expansion obviously fails to represent adequately the second-order Born term which is its counterpart prior to eikonization. The simplest way to improve the Glauber method is, therefore, to replace the second-order eikonal term by the second-order Born term. With the Glauber amplitude so modified, a serious defect of this amplitude is removed, while the characteristics of the eikonal method contained in the rest of the amplitude still can be preserved. The reasonable success of our previous calculations with this modified Glauber amplitude for electron-hydrogen and electron-helium scattering confirms clearly that the failure of the conventional Glauber amplitude in atomic scatterings stems mainly from this second-order eikonal term.

Our calculations were done with the neglect of exchange effect, since at that time no simple expressions for the Glauber exchange amplitude were available, while the so-called Glauber-Ochkur exchange amplitude was shown unacceptable to represent correctly the exchange effect in an eikonal theory.[5] Recently, through an ingenious application of a similar method used by Gau and Macek[6] for the direct amplitude, Foster and Williamson[7] have been successful in transforming the eikonal exchange amplitude into a two-dimensional integral which can easily be evaluated by numerical computation. With this simplified expression for the eikonal exchange amplitude at hand, a much improved analysis within the modified Glauber method is carried out for elastic scattering of electrons by a hydrogen atom in its ground state. The results of the analysis will be reported in this paper. In Sec. II, a brief review on the expressions of the amplitudes needed for our subsequent computations will be made. Results of our calculations will be shown in Sec. III together with discussion and comparison to those obtained in other theoretical models, as well as to experimental data.

II. FORMALISM

As was discussed above for atomic scatterings at intermediate energies, the Glauber amplitude should be modified as follows:

$$f_{GM}=f_G+f_{B2}-f_{G2}\ , \tag{1}$$

where f_G is the conventional Glauber amplitude, f_{G2} the second-order eikonal term, and f_{B2} the second-order Born term. For elastic electron-hydrogen scattering in the 1s state, f_G can be calculated in closed form[8] or by using the well-known formula obtained by Franco,[4]

$$f_G=2ik_\mu\int_0^{\pi/2}d\alpha\,\sin^3\alpha\cos\alpha[\sin^2\alpha-\tfrac{1}{2}q^2\cos^2\alpha][\sin^2\alpha+\tfrac{1}{4}q^2\cos^2\alpha]^{-4}$$
$$\times[1-(|\cos 2\alpha|/\cos\alpha)^{2i/k_\mu}|\cos 2\alpha|F(1/2|+i/2k_\mu;1+i/2k_\mu;1;\ \sin^2 2\alpha)]. \tag{2}$$

Here, $\vec{q}$ is the momentum transfer and F is a hypergeometric function. Other notations are as usual. f_{G2} for 1s elastic e-H scattering is given by[1]

$$f_{G2}=\frac{k_\mu i}{2!}\int db_2 b_2 J_0(qb_2)\langle\nu|\chi_G|\mu\rangle\ , \tag{3}$$

where both $|\mu\rangle$ and $|\nu\rangle$ are given by

$$\phi_{1s}=(1/\sqrt{\pi})e^{-r_1} \tag{4}$$

and

$$\chi_G=(1/k_\mu)\ln[1-(2b_1/b_2)\cos\varphi+b_1^2/b_2^2]\ . \tag{5}$$

b_1 is the impact parameter corresponding to the coordinate of the bound electron. In order to calculate the second-Born term, one starts with the exact formula[9]

$$f_{B2}=8\pi^2\int d^3k\sum_n\frac{\langle\phi_\nu|V|n,\vec{k}\rangle\langle n,\vec{k}|V|\phi_\mu\rangle}{k^2-k_\mu^2-2(\omega_n-\omega_\mu)-i\epsilon}\ , \tag{6}$$

where

$$\phi_\nu=(2\pi)^{-3/2}e^{i\vec{k}_\nu\cdot\vec{r}_1}|\nu\rangle \tag{7}$$

and

$$V=1/r_{12}-1/r_2\ . \tag{8}$$

The integration over the plane-wave parts of the matrix elements in Eq. (6) can be done easily and one obtains

$$f_{B2}=\frac{2}{\pi^2}\int d^3k\sum_n\frac{1}{K_\mu^2K_\nu^2}\ \frac{\langle\nu|e^{-i\vec{K}_\nu\cdot\vec{r}}-1|n\rangle\langle n|e^{i\vec{K}_\mu\cdot\vec{r}}-1]|\mu\rangle}{k^2-k_\mu^2-2(\omega_n-\omega_\mu)-i\epsilon}\ . \tag{9}$$

Finally, the average closure summation method as usually used in the second-Born scattering theory[1,9] yields

$$\bar{f}_{B2}=\frac{2}{\pi^2}\int d^3k\ \frac{1}{K_\mu^2K_\nu^2}\ \frac{\langle\nu|[e^{-i\vec{K}_\nu\cdot\vec{r}}-1][e^{i\vec{K}_\mu\cdot\vec{r}}-1]|\mu\rangle}{k^2-p_\mu^2-i\epsilon}\ . \tag{10}$$

For elastic scattering of electrons by a hydrogen atom in its ground state, one obtains

$$\bar{f}_{B2}=\frac{2}{\pi^2}\int d^3k\ \frac{1}{K_\mu^2K_\nu^2}\ \frac{1}{k^2-p_\mu^2-i\epsilon}\langle\phi_{1s}|e^{i\vec{q}\cdot\vec{r}}-e^{i\vec{K}_\mu\cdot\vec{r}}-e^{-i\vec{K}_\nu\cdot\vec{r}}+1|\phi_{1s}\rangle\ . \tag{11}$$

The integration over $\vec{k}$ can be reduced to a single-order integral over a parameter t by the well-known Feynman technique.[10] This integral can then be evaluated numerically with ease. Other notations used in these formulas have the usual meanings.[1]

As for the eikonal exchange amplitude the reduced formula obtained by Foster and Williamson[7] is used,

$$f_{\rm ex}=-\pi 2^{4-i\eta_\mu}\frac{\Gamma(1-i\eta_\mu)}{\Gamma(-i\eta_\mu)}C_\nu^*C_\mu D_\mu(m,\vec{\gamma})D_\nu(m,\vec{\Gamma})$$
$$\times\int_0^{+\infty}d\lambda\,\lambda^{-i\eta_\mu-1}\int_0^1 dx\ \frac{1}{x}\left[m\left(\frac{d}{dm^2}\right)^2\mathfrak{F}(1,0,0,0,0)-x^{-1}\left(\frac{d}{dm^2}\right)^2\mathfrak{F}(1,0,0,1,0)\right]_{\vec{\gamma}=\vec{\Gamma}=0}\ , \tag{12}$$

where

$$\mathfrak{F}(n,p,r,s,t)=\lambda^s(1-x)^s\Lambda^{-p}(\beta^2+Q^2)^{i\eta_\mu-\eta}(\beta-iQ_z)^{-i\eta_\mu-r}\beta^t\ . \tag{13}$$

Here,

$$\Lambda=[\lambda^2(1-x)^2+m^2x+(\vec{k}_\nu-\vec{\gamma})^2x(1-x) - 2i\lambda x(1-x)(k_{\nu z}-\gamma_z)]^{1/2}, \quad (14a)$$

$$\beta=\Lambda+M, \quad (14b)$$

$$\vec{Q}=\vec{k}_\mu-x\vec{k}_\nu-i\lambda(1-x)\hat{z}+x\vec{\gamma}-\vec{\Gamma}. \quad (14c)$$

For elastic scattering of electrons by a hydrogen atom in its ground state, and with the choice of the z direction similar to the one used in the Glauber amplitude, one has,

$$\Lambda=[\lambda^2(1-x)^2+m^2x+k_\mu^2x(1-x) - 2i\lambda x(1-x)k_\mu\cos(\tfrac{1}{2}\Theta)]^{1/2}, \quad (15a)$$

$$\beta=\Lambda+1, \quad (15b)$$

$$\vec{Q}=\vec{k}_\mu-x\vec{k}_\nu-i\lambda(1-x)\hat{z}, \quad (15c)$$

where Θ is the scattering angle. The differential cross sections for e-H scattering is calculated with

$$\frac{d\sigma}{d\Omega}=\tfrac{3}{4}|f_{GM}-f_{ex}|^2+\tfrac{1}{4}|f_{GM}+f_{ex}|^2. \quad (16)$$

III. RESULTS AND DISCUSSION

We have numerically integrated the differential cross sections for $1s$ elastic scattering e-H with the Glauber exchange effect included via Eq. (16) above. These calculations[11] were done for incident electron energies of 50, 100, and 200 eV and scattering angles from 0.5° to 180°. We also find that to facilitate the numerical convergence of f_{ex}, it is preferable to perform an integration by parts for this amplitude first.

In Table I, the differential cross sections computed within the modified Glauber method at incident energy equal to 50 eV are presented. In Figs. 1–3, results of the modified Glauber method with and without Glauber exchange are plotted versus scattering angles, along with experimental data and results of theoretical calculations in the first Born approximation, the conventional Glauber approximation and the conventional Glauber approximation remedied with Glauber exchange (all recalculated by us) for incident electron energies of 50, 100, and 200 eV. The results of the modified Glauber method with exchange are found in excellent agreement with experimental data acquired by absolute measurements.[12] For incident electron of 50 eV, the agreement is almost perfect at intermediate scattering angles. At larger angles, our theoretical values seem to lie somewhat lower than the experimental points, but due to a considerable uncertainty of experimental data, the agreement still can be regarded as very good. For

TABLE I. Differential cross sections of $1s$ elastic e-H scattering in a modified Glauber theory in $a_0^2\,\text{sr}^{-1}$ units.

Angles (deg)	Modified Glauber without exchange	Modified Glauber with exchange	Experimental data Williams	Experimental data Teubner *et al.*
0.5	10.07	11.53	···	···
1	9.76	11.19	···	···
3	8.49	9.81	···	···
5	7.27	8.47	···	···
10	4.67	5.60	5.04	3.7
15	2.91	3.63	3.18	2.9
20	1.83	2.38	2.17	2.1
25	1.19	1.60	···	···
30	8.10×10^{-1}	1.11	1.12	1.1
40	4.26×10^{-1}	5.74×10^{-1}	5.51×10^{-1}	5.9×10^{-1}
50	2.54×10^{-1}	3.22×10^{-1}	3.08×10^{-1}	3.5×10^{-1}
60	1.65×10^{-1}	1.95×10^{-1}	2.05×10^{-1}	2.2×10^{-1}
70	1.13×10^{-1}	1.26×10^{-1}	1.46×10^{-1}	1.6×10^{-1}
80	8.04×10^{-2}	8.77×10^{-2}	9.93×10^{-2}	1.1×10^{-1}
90	5.97×10^{-2}	6.44×10^{-2}	7.16×10^{-2}	8.0×10^{-2}
100	4.60×10^{-2}	4.92×10^{-2}	5.58×10^{-2}	5.8×10^{-2}
110	3.66×10^{-2}	3.84×10^{-2}	4.21×10^{-2}	5.2×10^{-2}
120	3.02×10^{-2}	3.04×10^{-2}	3.49×10^{-2}	4.1×10^{-2}
130	2.57×10^{-2}	2.44×10^{-2}	2.88×10^{-2}	···
140	2.25×10^{-2}	2.07×10^{-2}	2.73×10^{-2}	···
150	2.03×10^{-2}	2.01×10^{-2}	···	···
160	1.89×10^{-2}	2.42×10^{-2}	···	···
170	1.81×10^{-2}	3.45×10^{-2}	···	···
180	1.79×10^{-2}	5.17×10^{-2}	···	···

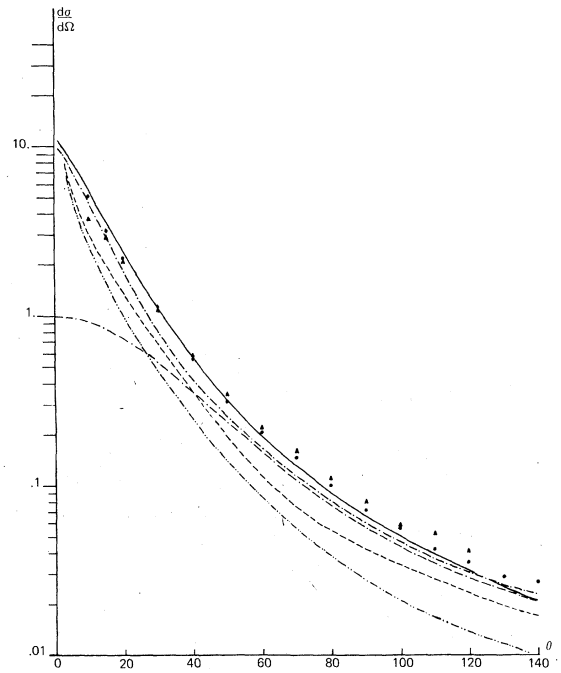

FIG. 1. Differential cross sections of e-H 1s elastic scattering at $E = 50$ eV. Solid line: modified Glauber with Glauber exchange; –.–.–.: modified Glauber without exchange; –..–..–..: conventional Glauber without exchange; ------: conventional Glauber with Glauber exchange; ––.––.––.: first-Born without exchange; ●: data by Williams; ▲: data by Teubner *et al*.

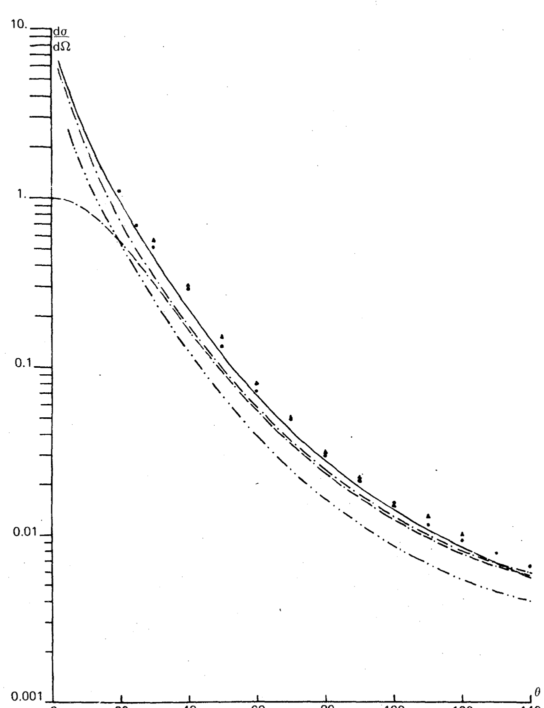

FIG. 2. Same as in Fig. 1, but at 100 eV.

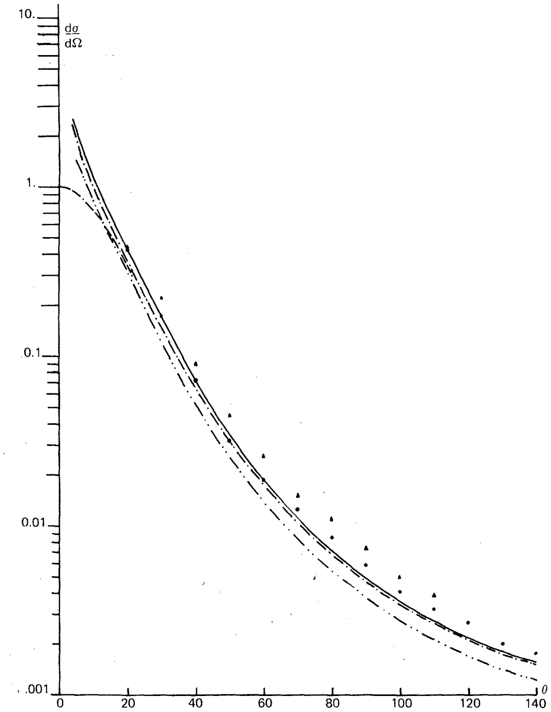

FIG. 3. Same as in Fig. 1, but at 200 eV.

higher energies of 100 and 200 eV, again the agreement still can be considered as quite good, in view of the error in the experimental data. The Born approximation gives a very poor result at small scattering angles, while the conventional Glauber method without exchange yields results lying much lower than experimental points at all angles (except, of course, at very small angles where the conventional Glauber results become divergent). With the Glauber exchange effect included, the conventional Glauber results do show an improvement, but are still far from being regardable as in good agreement with data at all angles, especially at lower scattering energies. We also find that the exchange effect becomes less significant as the scattering energy becomes greater.

An interesting feature of the modified Glauber (as well as conventional Glauber) calculations with the Glauber exchange effect considered via Foster and Williamson's formula is that at very large scattering angles (about 145° up), the differential cross sections seem to rise a little bit, but very slowly. This characteristic behavior is due to the fact that at these very large angles, the Glauber exchange effect begins to overtake the contribution from direct scattering and then becomes dominant in this range of angles. We therefore call for an accurate measurement of differential cross sections at these very large scattering angles to determine

TABLE II. Integrated cross sections of 1s e-H elastic scattering in πa_0^2 units.

Energy (eV)	Glauber [a]	Glauber with exchange	Born [a]	Full eikonal [a]	Full eikonal with post exchange [a]	Full eikonal with prior exchange [a]	Modified Glauber	Modified Glauber with exchange	Data [b]
50	0.64	0.79	0.51	0.72	0.84	0.94	1.05	1.26	1.20
100	0.29	0.38	0.29	0.39	0.43	0.44	0.43	0.53	···
200	0.15	0.18	0.15	0.22	0.24	···	0.19	0.21	···

[a]Values quoted from Ref. 7.
[b]See Refs. 3 and 12.

whether this feature would exist in experimental data as was predicted theoretically. However, it should be cautioned ahead that should experimental data fail to reproduce this characteristic feature at very large scattering angles for differential cross sections, this would likely mean a failure on the part of the eikonal exchange amplitude at these very large angles, rather than of our modified Glauber method as a whole.

Finally, the differential cross sections are integrated over scattering angles to obtain the 1s elastic e-H integrated cross sections at 50, 100, and 200 eV. The results are shown in Table II together with those predicted in some other theoretical models as well as those estimated from data of Teubner *et al.*[12] at 50 eV. At 50 eV, our values of 1.26 πa_0^2 and 1.05 πa_0^2 for the modified Glauber amplitude with and without Glauber exchange can both be considered as in excellent agreement with the value of 1.20 πa_0^2 estimated from data of Teubner *et al.*,[3,12] in view of the great uncertainty of the latter (±50%).

IV. CONCLUSION

A few conclusions can be drawn from our work presented here. First, the success of our Glauber method seems to indicate reasonably clearly that the failure of the conventional Glauber amplitude in representing atomic scatterings at intermediate energies arises mainly from the inadequacy of its second-order eikonal term. This term has been so drastically modified by approximations considered in the derivation of the Glauber amplitude that it can no longer represent adequately its counterpart prior to eikonization, i.e., the second-Born term. Thus, the rather simple but quite effective remedy as proposed by us for the Glauber method does seem to point to a right direction. Second, the exchange effect represented by the Glauber exchange amplitude is of a considerable magnitude at intermediate energies, especially at the lower end of this energy range, and cannot, thereby, be neglected in the calculation of cross sections. At very large angles, this effect may even overtake the contribution of the direct amplitude. An accurate measurement at these very large angles to verify this specific feature of the differential cross sections would be very much desirable. Finally, the success of our Glauber model shown here may suggest the need for deriving a new scattering amplitude for e-atom scatterings at intermediate energies, in which the recovery of a loss due to the second-order eikonal term can be incorporated directly during the process of its derivation.

ACKNOWLEDGMENT

I wish to thank the National Research Council of Canada for its financial support of this work.

*Work supported by the National Research Council of Canada (Operating Grant No. A-3962).
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