Exchange amplitudes for electron-hydrogen scattering in the Glauber approximation*

George Khayrallah
Joint Institute for Laboratory Astrophysics, University of Colorado and National Bureau of Standards, Boulder, Colorado 80309
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An exact closed form expression for the Glauber-Bonham-Ochkur exchange amplitudes for electron-hydrogen scattering is derived. The results are applied to the elastic scattering from the ground state of the hydrogen atom, where a closed-form expression was also derived for the total exchange cross section. Investigation of the inclusion of exchange in the differential cross section for total electron scattering is also presented. It is shown that exchange effects are quite important and that their inclusion, rather than the inclusion of angle effect or the inclusion of the full eikonal effects, does tend to make the Glauber prediction in much better agreement with the experiment.

I. INTRODUCTION

During recent years, many calculations of the electron-hydrogen scattering cross sections have been performed in the different Glauber approximations.[1-6] However, the easiest of these approximations, and the one most commonly used for other scattering processes, is the "restricted Glauber" approximation (RG) where the electron trajectory during the collision is taken to be a straight-line path perpendicular to the final momentum-transfer vector. Few calculations in the restricted Glauber approximation considered the effect of exchange on the final results of the calculation. Byron and Joachain[4] have employed the Glauber approximation to calculate the exchange amplitude for the transtion $1\,{}^1S \rightarrow 2\,{}^3S$ of the helium atom. Although their results were an encouraging improvement over first-order exchange theories, they employed a time-consuming Monte Carlo integration technique to compute the six-dimensional integrals. Tenney and Yates[5] and Madan[6] approximated the exchange integral in the Bonham-Ochkur[7,8] approximation in which the amplitude is expanded in inverse powers of the initial or final velocity at fixed momentum transfer and only the first term is kept. For the $1s \rightarrow 1s$ and $1s \rightarrow 2s$ transitions of hydrogen, Madan[6] analytically reduced the resulting three-dimensional integral to one dimension and integrated the last form numerically. We concentrate in the present paper on the evaluation in closed form of the Glauber-Bonham-Ochkur exchange amplitude for all electron-hydrogen scattering processes.

Other than the inclusion of exchange, some attempts have been made within the Glauber eikonal approach to improve on the restricted straight-line approximation. The first attempt was to calculate the Glauber amplitude for a straight-line trajectory, but without the additional assumption that the momentum transfer was perpendicular to that trajectory.[1] This approach is called the "unrestricted Glauber" approximation. A second attempt at improvement was to consider a classical non-straight-line trajectory in the calculation of the Glauber amplitude.[2] This approach is called the "restricted Glauber angle" approximation. The term "restricted" is used since the momentum-transfer vector was still considered perpendicular to the final trajectory. A third attempt was to correct the Glauber-approximation treatment of small-angular-momentum contributions.[9] Another attempt was to include second-order potentials in the calculation of the Glauber phase.[10,11]

II. EXCHANGE AMPLITUDE

The Glauber-Bonham-Ochkur exchange amplitude for the rearrangement process

$$e_1^-(k_i) + e_2^-\, p(i) \rightarrow e_2^-(k_f) + e_1^-\, p(f)$$

is given by[6]

$$g_{if}^{\pm} \simeq -\frac{2}{k_i^2} \lim_{\epsilon\to 0} \exp(i\eta_\pm \ln\epsilon) \times \int d\vec{r}\, \phi_f^*(\vec{r}) \exp(i\vec{q}\cdot\vec{r}) \phi_i(\vec{r}) (\vec{r} \mp z)^{-i\eta_\pm}, \tag{1}$$

while the differential cross section for exchange is defined as

$$\frac{d\sigma^{ex}}{d\Omega} = |g_{if}|^2, \tag{2}$$

where $\vec{q} = \vec{k}_i - \vec{k}_f$ is the momentum transfer, k_i is the initial momentum, k_f is the final momentum, $\eta_+ = 1/k_i$, $\eta_- = 1/k_f$, and the +/− sign refers to the prior/post form.

In order to evaluate Eq. (2) for arbitrary hydrogenic states, we note that any product of two bound-state wave functions of hydrogen can be constructed from a linear combination of terms generated by differentiation of a generating function as follows:

$$\phi_f^* \phi_i = C_{if} D_{\mu\vec{\gamma}} [(1/r) e^{-\mu r - i\vec{\gamma}\cdot\vec{r}}] , \quad (3)$$

where C_{if} is the appropriate normalization constant, and $D_{\mu\vec{\gamma}}$ is a linear combination of the operators $\partial/\partial\beta$, $\partial/\partial\gamma_x$, $\partial/\partial\gamma_y$, and $\partial/\partial\gamma_z$. Note that this is a variation on the method of Gau and Macek.[1]

The undetermined phase factor $\lim_{\epsilon\to 0} \exp(i\eta \ln\epsilon)$ was evaluated by taking the limit of high energies where the present exchange amplitude should reduce to the Born-Bonham-Ochkur amplitude. The limiting values were found to be 1, which is the exact value of this factor at infinite velocities ($\eta = 0$). This value of 1 was used at all velocities; thus

$$g_{if}^{\pm} = -\frac{2}{k_i^2} C_{if} D_{\mu\vec{\gamma}} \int \exp(-\mu r - i\gamma\cdot\vec{r} + i\vec{q}\cdot\vec{r}) \times (r \mp z)^{i\eta_\pm} \frac{d\vec{r}}{r} . \quad (4)$$

We now use the method of Landau and Lifshitz[8] to evaluate this integral using parabolic coordinates defined as follows:

$$x = \sqrt{\xi\lambda}\cos\phi , \quad y = \sqrt{\xi\lambda}\sin\phi , \quad z = \tfrac{1}{2}(\xi - \lambda) ,$$
$$r = \tfrac{1}{2}(\xi + \lambda) , \quad d^3\vec{r} = \tfrac{1}{4}(\xi+\lambda)\, d\xi\, d\lambda\, d\phi . \quad (5)$$

Then

$$g_{if}^{\pm} = -\frac{1}{k_i^2} C_{if} D_{\mu\gamma} \int_0^\infty d\lambda \int_0^\infty d\xi \int_0^{2\pi} d\phi\, (\delta_- \lambda^{-i\eta_-} + \delta_+ \xi^{-i\eta_+}) \exp[\xi(\tfrac{1}{2} iq\cos\theta - \tfrac{1}{2}\mu - \tfrac{1}{2} ik)]$$
$$\times \exp[\lambda(-\tfrac{1}{2} iq\cos\theta - \tfrac{1}{2}\mu + \tfrac{1}{2} ik)] \exp[iq\sqrt{\lambda\xi}\sin\theta\cos\phi] , \quad (6)$$

where $\delta_+, \delta_- = 1, 0$ for the prior form, $\delta_+, \delta_- = 0, 1$ for the post form, where we chose the z axis parallel to the $\vec{\gamma}$ axis, and where ϕ is measured from the $\vec{\gamma}, \vec{q}$ plane. θ is the angle between $\vec{q}$ and $\vec{\gamma}$.

The prior form is evaluated by substituting $v = \sqrt{\lambda}\sin\phi$, $u = \sqrt{\lambda}\cos\phi$, and the post form is evaluated by exchanging λ and ξ, q and $-q$, k and $-k$. Thus

$$g_{if}^{\pm} = -\frac{2}{k_i^2} \pi C_{if} D_{\mu\vec{\gamma}} \{\Gamma(1 - i\eta_\pm)(-2)^{1\mp i\eta_\pm} \times [q^2\sin^2\gamma + \mu^2 + (k + q\cos\theta)^2]^{i\eta_\mp - 1} \times [\pm i(k - q\cos\theta) - \mu]^{-i\eta_\pm}\} , \quad (7)$$

where $\Gamma(1 - i\eta)$ is the gamma function. Alternatively

$$g_{if}^{\pm} = -\frac{\pi}{k_i^2} 2^{3 - i\eta_\pm} \Gamma(1 - i\eta_\pm) C_{if} D_{\mu\vec{\gamma}} \{[\mu^2 + |\vec{q} + \vec{\gamma}|^2]^{i\eta_\pm - 1} \times [\mu \mp i(q_z + \gamma_z)]^{-i\eta_\pm}\} . \quad (8)$$

Note that for elastic scattering $\eta_+ = \eta_- = 1/k$, but one still has a post-prior discrepancy in Eq. (8). This results from the particular choice of the $\vec{z}$ axis. A more complete analysis of the choice of the z axis, i.e., the trajectory, has been given by Gerjuoy and Thomas.[3] For scattering from s states, $\gamma_z = 0$, and the operator $D_{\mu\vec{\gamma}}$ contains no reference to $\vec{\gamma}$. Hence for this case only, one can choose the z axis along $\vec{k}_i + \vec{k}_f$, and q_z will be zero, thus

$$g_{ns,ns}^{\pm} = -\frac{\pi}{k^2} 2^{3 - i\eta} C_{if} \Gamma(1 - i\eta) D_\mu \{(\mu^2 + q^2)^{i\eta - 1} (\mu)^{-i\eta}\} \quad (9)$$

and consequently there is no post-prior discrepancy for elastic scattering from s states.

III. 1s-1s EXCHANGE CROSS SECTION

For the 1s-1s transition, $\vec{\gamma} = \vec{0}$, $D_{\mu\gamma} = -\partial/\partial\mu$, $C_{if} = +1/\pi a_0^3$, and $\mu = 2/a_0$ ($a_0 = 1$ in a.u.). Thus

$$g_{1s,1s} = +\frac{2^{2-2i\eta}}{k^2} \Gamma(1 - i\eta) \frac{-8 + i\eta(4 - q^2)}{(4 + q^2)^{2 - i\eta}} \quad (10)$$

and

$$\frac{d\sigma^{ex}}{d\Omega} = |g|^2 = \frac{2^4}{k^4} \frac{\pi\eta}{\sinh\pi\eta} \left(\frac{64 + \eta^2(4 - q^2)^2}{(4 + q^2)^4}\right) . \quad (11)$$

At high energies ($\eta \to 0$) this reduces to

$$\frac{d\sigma^{ex}}{d\Omega} = \frac{2^{10}}{k^4} \frac{1}{(4 + q^2)^4} , \quad (12)$$

while at small angles it tends to a finite limit

$$\frac{d\sigma^{ex}}{d\Omega} = \frac{4 + \eta^2}{k^4} \frac{\pi\eta}{\sinh\pi\eta} . \quad (13)$$

The total exchange cross section is given by

$$\sigma^{ex} = \int_0^{2k} \frac{d\sigma}{d\Omega}\left(\frac{2\pi}{k^2} q\, dq\right) \quad (14)$$

$$= \frac{4}{3} \frac{\pi^2}{k^7} \frac{1}{\sinh(\pi/k)} \frac{3 + 3k^2 + 4k^4 + k^6}{[1 + k^2]^3} . \quad (15)$$

At high energies ($k \to \infty$), the exchange cross section is reduced to

$$\sigma^{ex} \simeq \frac{4\pi}{3}\left(\frac{3}{k^{12}} + \frac{3}{k^{10}} + \frac{4}{k^8} + \frac{1}{k^6}\right) \simeq \frac{4\pi}{3k^6} . \quad (16)$$

Compare this to the high-energy asymptotic value

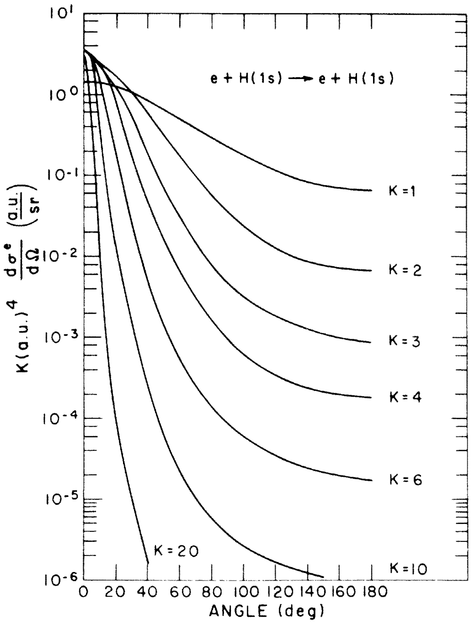

FIG. 1. "Scaled" differential exchange cross sections for elastic scattering of electrons by ground-state hydrogen atoms. The incident momentum k is given in a.u. The differential cross section is in a.u./sr.

of the direct Glauber cross section[12]:

$$\sigma^{\rm dir} \simeq \pi\left(\frac{7}{3k^2} - \frac{1}{k^4} + \frac{306}{k^6}\right) \simeq \frac{7}{3}\frac{\pi}{k^2}\,. \qquad (17)$$

However, while the direct Glauber cross section reduces to the direct first Born cross section at large impact energies, the present exchange cross section tends to a value one third as large as the Bonham-Ochkur cross section at large energies.

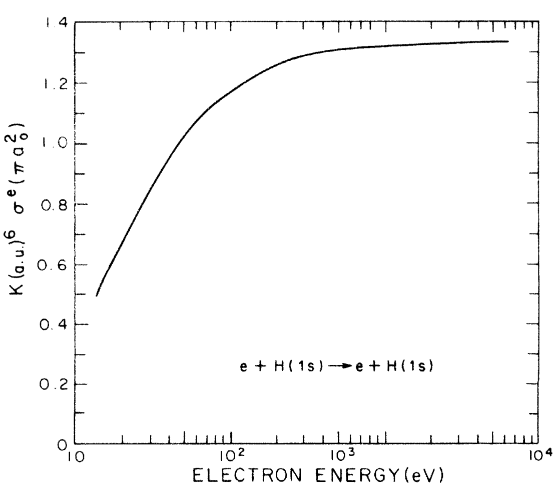

FIG. 2. "Scaled" total cross section for elastic exchange scattering in collisions of electrons by ground-state hydrogen atoms.

Also, in contrast with the Bonham-Ochkur approximation for the exchange amplitudes in the Born approximation, where the exchange amplitude is related simply to the first Born amplitude

$$g^{\rm Ochkur} = (q^2/k^2) f^{B1}\,, \qquad (18)$$

the present Ochkur-like approximation to the Glauber exchange amplitude is not simply related to the direct Glauber amplitude. The main reason for this difference is the dependence of the angular part of the present exchange amplitude on the incident energy, in contrast with the Bonham-Ochkur approximation to the Born amplitude.

The result of the evaluation of Eq. (11) for the differential cross section is plotted in Fig. 1 for different incident momenta k (a.u.), where the quantity $k^4 |g|^2$ is plotted. One notices three things: (i) for $k = 2$ ($E = 54.4$ eV) the results agree with those evaluated by Madan[6] numerically; (ii) in contrast with the Bonham-Ochkur differential cross section, the present shape of the differential cross section depends on the incident energy; (iii) at higher and higher energies the differential cross section becomes more peaked in the forward direction. The total Glauber-Bonham-Ochkur cross section for exchange scattering is plotted in Fig. 2, where the cross section was scaled by k^6. It is seen that the exchange cross section reaches its high-energy asymptotic limit at 200 eV.

IV. 1s-1s DIFFERENTIAL ELASTIC CROSS SECTION

For the calculation of the differential cross section for elastic scattering from the ground state of atomic hydrogen it is necessary to know both the direct and the exchange amplitudes. If one assumes that the polarization and the identity of the two participating electrons are unspecified, or unmeasurable, then the elastic differential cross section (called total in the following) is given by

$$d\sigma/d\Omega = \tfrac{1}{4}\,|f + g|^2 + \tfrac{3}{4}\,|f - g|^2\,, \qquad (19)$$

where f is the amplitude for direct scattering, and g is the amplitude for electron exchange scattering. Thus

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma^{\rm direct}}{d\Omega} + \frac{d\sigma^{\rm ex}}{d\Omega} - {\rm Re}(fg^*)\,. \qquad (20)$$

When f is given by the first Born approximation, many approximations have been performed for the exchange amplitudes for elastic, and inelastic, scattering of electrons from the ground state of atomic hydrogen.[13] However, in the present paper no comparison with such calculations is presented, except in a few places. The interested reader is referred to the excellent review of all such calculations of Truhlar *et al.*[13]

Instead since the restricted-Glauber straight-line calculation (RG) is a special case of the Eikonal calculations[1] where $\vec{q}\cdot\vec{z}=0$, a comparison will be made with such calculations of the unrestricted-Glauber straight-line approximation (URG), the difference being that $\vec{q}\cdot\vec{z}=0$ in the RG calculation.

For evaluating Eq. (19) in the RG approximation, the expression of Thomas and Gerjuoy[12] has been used for the calculation of f, while Eq. (10) has been used for the calculation of g. For the URG approximation, the expression of Gau and Macek[1] have been used to calculate f while the expressions of Foster and Williamson[14] have been used for the calculation of g. The URG result for the "total" differential cross sections were taken from the work of Foster and Williamson.[14]

Figure 3 shows a comparison of the present calculation of the RG differential cross section at 200 eV with the URG calculation,[14] as well as a comparison with the experimental data.[15,16] It is seen that exchange contributes very little to the experimentally measured total differential cross section. The figure also shows that for angles smaller than 25° the URG results are closer to the experimental results than the RG results. At larger angles, especially beyond 60°, the RG results are in more satisfactory agreement with the present experimental data. What is not shown

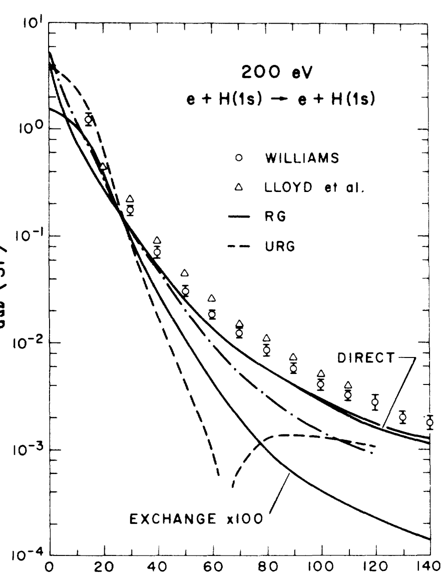

FIG. 3. Differential cross section for elastic scattering of electrons by H(1*s*) at 200 eV. (——), present calculations of the RG cross sections; (----), URG results for the exchange cross sections with prior form (Ref. 14); (— • —), URG results for the total cross section also in the prior form (Ref. 14); ☿ experimental data of Williams (Ref. 16); △, experimental data of Lloyd *et al.* (Ref. 15).

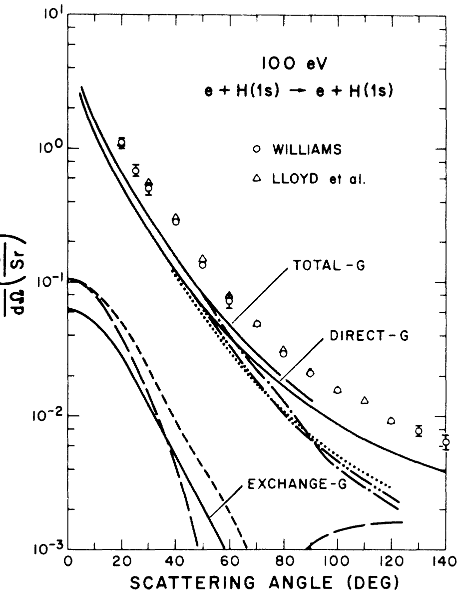

FIG. 4. Differential cross section for elastic scattering of electron by H(1*s*) at 100 eV. (——), present calculation; (— —), prior-exchange URG results (Ref. 14); (– – –), post-exchange URG results (Ref. 14); (• • • •), direct URG results (Ref. 17); (— • —), prior corrected total URG (Ref. 14); (— • • —), post corrected total URG (Ref. 14); △ experimental results of Lloyd *et al.* (Ref. 15); ☿, experimental results of Williams (Ref. 16).

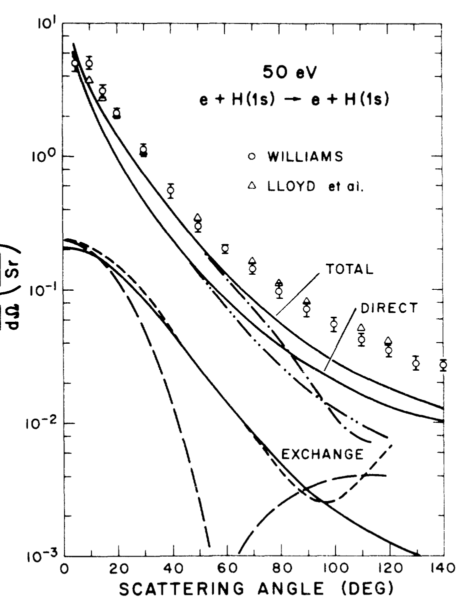

FIG. 5. Differential cross section for elastic scattering of electrons by H(1*s*) at 50 eV. (——), present calculation; (— —) prior exchange URG results (Ref. 14); (– – –), post-exchange URG results (Ref. 14); (----), direct URG results (Ref. 17); (— • —), prior corrected total URG (Ref. 14); (— • • —), post corrected total URG (Ref. 14); △, experimental results of Lloyd *et al.* (Ref. 15); ☿, experimental results of Williams (Ref. 16).

in the figure is the first Born results. These first Born results seem to be in better agreement with the data for angles greater than 20°. One also notices that the RG results are very close in shape to the experimental results, and if the experimental data were renormalized to the RG result they would agree at all angles equal to or greater than 20°.

Figures 4 and 5 compare the present results for RG with those of Ref. 14 for URG, as well as with the experimental results of Lloyd *et al.*[15] and of Williams,[16] at 100 and 50 eV respectively. It is seen that in both the RG and URG approximations, the differential cross section for electron exchange is significant, relative to the direct differential cross section, the total differential cross section being larger than the direct different cross section by about 8% at 100 eV and 27% at 50 eV. However, it is obvious that the direct RG results[12] are larger than the direct URG cross section[1] at large angles, being closer to the experimental results, in contrast with the claimed improvement[1] of the URG over the RG at large angles. A very similar behavior is seen in the total differential cross section. Another feature of Fig. 3 worthy of notice is the "prior-post" discrepancy of the URG exchange cross section. Such a discrepancy is unphysical.

At this point it should be mentioned that the other attempts at improving on the straight-line restricted-Glauber approximation (other than the inclusion of exchange, or the inclusion of the full eikonal) has been carried out by Chen *et al.*[2] and Ishihara and Chen.[9] The first[2] was called the restricted-Glauber angle approximation in the Introduction. The path integral was taken over two straight-line trajectories intersecting at the target atom. It is seen that the inclusion of exchange has at least as large an effect on improving on the RG straight-line direct cross sections as the inclusion of the angle effects. Thus it is quite interesting to find whether the results of Ref. 2 reproduce the elastic scattering amplitude correctly when the effects of exchange are also included. In the second attempt Ishihara and Chen[9] corrected for the inadequate semiclassical treatment of close-coupling encounter collisions in the Glauber approximation. In their attempt they included the effect of exchange using an optical static-exchange potential. A remarkable agreement with the experiment was found at 20 eV. At 100 eV, although their calculation was more in agreement with the experiment than with the restricted-Glauber calculation, their result was equal to the first Born results at all angles greater than 20°. Hence it is difficult to assess what caused the improvement—the inclusion of exchange, or the correction in the inadequacy of the Glauber approximation in treating close-coupling encounters.

Below 50 eV no calculation of the cross section for elastic electron scattering from H(1*s*) in the URG approximation exists. However, a comparison with the available experimental data can be

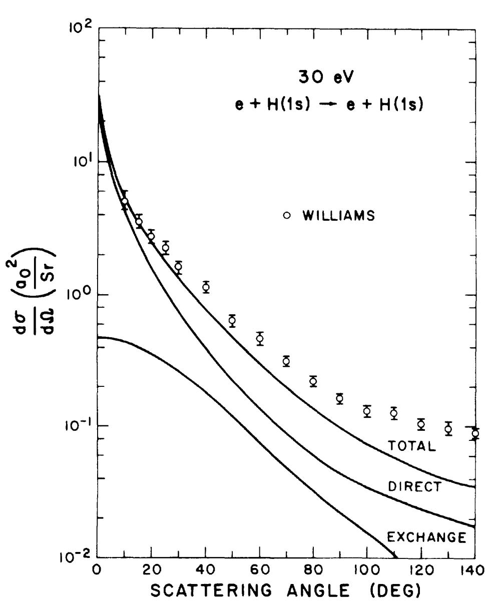

FIG. 6. Differential cross section for elastic scattering of electrons by H(1*s*) at 30 eV. The ⧲ are the experimental results of Williams (Ref. 16).

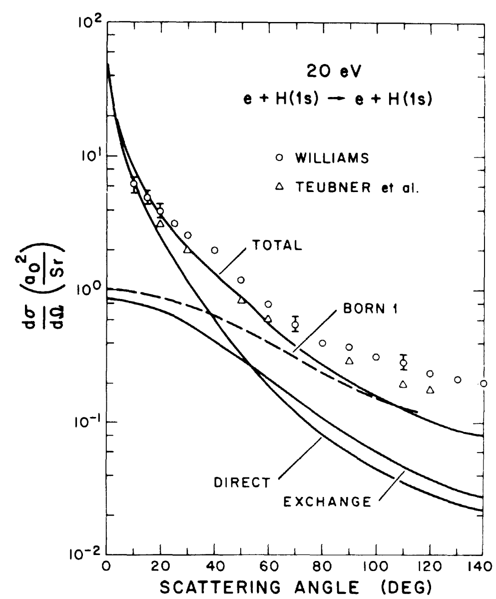

FIG. 7. Differential cross section for elastic scattering of electrons by H(1*s*) at 20 eV. Also shown: (----), results of the first Born calculation; ⧲, the experimental results of Williams (Ref. 16).

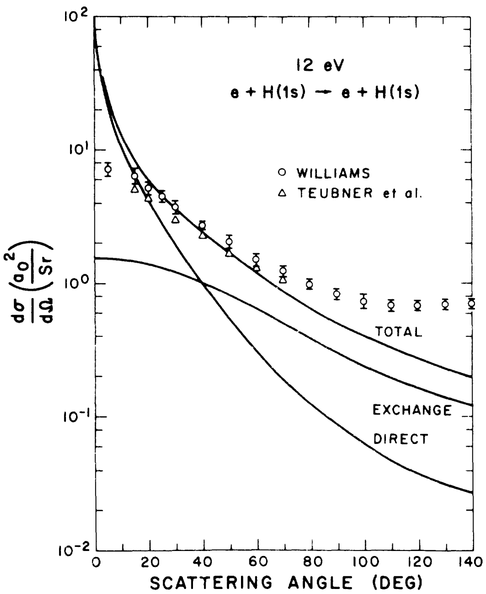

FIG. 8. Differential cross section for elastic scattering of electrons by H(1*s*) at 12 eV, ☉, experimental results of Williams (Ref. 16); △, experimental results of Teubner *et al.* (Ref, 18).

made. In Fig. 6 comparison with the data[15,16] at 30 eV is made. It is seen that the probability for exchange becomes larger at lower energies, and that the total cross section becomes modified especially at the large angles, the modification tending to improve the agreement with the experimental data.

At 20 eV (Fig. 7) the exchange cross section becomes larger than the direct cross section for angles greater than 54°. The modification of the total cross section is now drastic, and the modified differential cross section agrees quite well

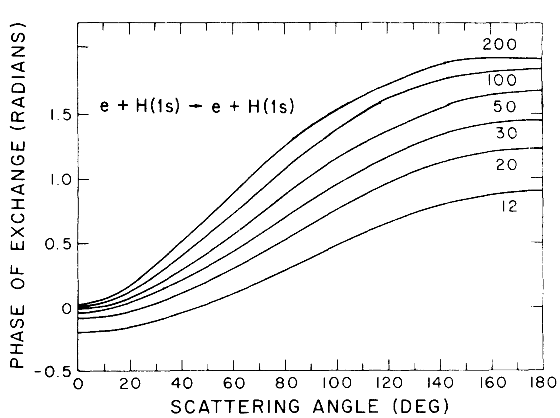

FIG. 9. Phase of the exchange amplitude for $e+\mathrm{H}(1s)$ elastic scattering, plotted as a function of the scattering angle. The different curves are labeled with their respective energies in eV.

with the experimental differential cross sections.[16,18] We note that the Born cross section is quite bad, as expected, and that the exchange effect, even if included, does not tend to correct the Born results at these energies.

Figures 8 shows the results at 12 eV as well as it shows the results of the experiments of Ref. 2 and Ref. 16. One notes that the inclusion of exchange does improve the RG differential cross section considerably at all angles, especially for angles greater than 10°. It is seen that agreement with the experimental measurements[2,16] is much better than had the exchange being neglected. However, small differences still exist at angles greater than 70° where the straight line assumed in the RG and URG calculation is not a good approximation to the true path. Unfortunately Chen *et al.*[2] did not extend their angle approximation to these lower energies, so an estimate of the effect is not possible.

Finally, the phase of the electron exchange amplitude used in the present calculation is plotted in Fig. 9 as a function of both the electron scattering angle and the electron incident energy. Also tabulated in Table I are the total cross sections for elastic scattering from ground-state atomic hydrogen where a comparison, when possible, is made with the URG results of Ref. 14.

V. CONCLUSION

The paper presents a calculation of a closed-form expression of the Glauber amplitude in the Ochkur approximation, where it is found that for elastic scattering from hydrogenic *ns* states, no prior-post discrepancy exists. In the limit of high energies the 1*s*-1*s* Glauber exchange amplitude reduces to the Bonham-Ochkur amplitude, while for $k=2$ the differential cross section reduces to the numerical results of Madan[6] at all angles. It is found that the inclusion of electron-exchange in the calculation of the total electron differential elastic cross section is certainly necessary for angles greater than 50°, and for energies below 50 eV. It is also noted that in the present case exchange effects tend to increase the differential cross section since the exchange terms tend to add up constructively to the direct differential cross section at all investigated angles and energies. Finally, exchange effect were found to be most important at low energies, where the electrons have time to correlate and to exchange while they are insignificant at large energies and small angles where the incident electrons tends its scatter directly.

The present results are not in disagreement with

TABLE I. The total elastic scattering cross section for e-H(1s) collisions in units of πa_0^2. The numbers in parentheses are the powers of 10 by which the number should be multiplied.

Energy	Restricted-Glauber			Unrestricted-Glauber[16]		
(eV)	Exchange	Direct	Total	Direct	Total (prior)	Total (post)
12	1.82	2.54	5.048			
20	0.668	1.50	2.695			
30	0.393	0.994	1.594			
50	7.325 (−2)	0.598	0.832	0.72	0.94	0.84
100	1.108 (−2)	0.304	0.365	0.39	0.44	0.43
200	1.525 (−3)	0.155	0.170	0.22	...	0.24

the observations of Byron and Joachain[19] and Ishihara and Chen[9] that the inclusion of exchange, among other things, is a necessary improvement over the restricted Glauber approximation. Other improvements may include (i) the angle approximation[2] which includes correction to the straight-line trajectory, (ii) the eikonal-optical model,[10,11] which includes the second-order optical potential in the evaluation of the Glauber phase, (iii) the addition of Ref_{B2}[19] that is missing from the Glauber amplitude, (iv) the removal of the frozen core approximation,[9] and the correction of the treatment of the small-angular-momentum contributions in the Glauber approximation.[9]

Note added in proof. (i) Dr. G. Foster has brought to my attention the Comment of R. N. Madan [Phys. Rev. A 12, 2631 (1975)] who did a reduction of the exchange amplitude using a different technique; (ii) D. P. Dewangan [Phys. Lett. 56A, 279 (1976)] has published the same reduction technique. The present results for the exchange amplitude formula agree with both of these results.

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