First-order correction to Glauber approximation for electron-hydrogen and positron-hydrogen scattering

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The first realistic systematic correction to the Glauber approximation for scattering of charged particles by atoms is made, and it leads to substantial improvements for electron-hydrogen $(e^{-}-H)$ elastic scattering at all energies equal to or greater than 30 eV and angles $(10^{\circ}-140^{\circ})$ for which data exist. At the lower energies and larger angles disagreement with the data persists because of limitations in the approximation. The calculations also yield e^{+} -H and e^{-} -H cross sections which differ from each other even when exchange is neglected.

The Glauber approximation (GA) has been one of the most widely used and successful methods for analyzing both atomic^{1,2} and nuclear³ collisions. Its first application to atomic physics was made to scattering of charged particles by hydrogen atoms,⁴ with detailed calculations for electronhydrogen (e^{-} -H) elastic scattering. Since then many applications to e^{-} -H collisions, as well as to a wide variety of other atomic collisions, have been made.^{1,2}

Although relative e^{-} -H elastic scattering differential cross-section measurements⁵ indicated that the GA gave excellent results, more recent absolute measurements^{6,7} have revealed that the calculated values lie significantly below the data at energies as high as 400 eV. Using the eikonal exchange amplitude⁸ we find that even with the inclusion of exchange effects the calculated values still lie significantly below the data. In addition, apart from exchange effects, the GA does not distinguish between e^{-} -H and e^{+} -H scattering.

It has been known for some time^{9,10} that there exist systematic corrections to the GA for potential scattering and that, in principle, they may be applied to the Glauber multiple scattering theory for collisions with nuclei or multielectron atoms. We have generalized those results to include the nuclear contribution in atomic collisions and have thereby obtained a first-order correction for scattering by H atoms (i.e., monoelectron atoms). We describe the first calculation of the first-order correction to the GA, with application to e^{\pm} -H scattering. As we shall see, this correction yields substantial improvements in the calculated elastic scattering differential cross sections at all energies considered (30-680 eV) at all angles $(10^\circ-140^\circ)$ for which data exist. Furthermore, it leads to differences between the e^- -H and e^+ -H cross sections which do not arise from exchange effects, thereby rectifying a long-standing shortcoming of the GA.

Let b denote the impact-parameter vector of an incident projectile (of charge Ze and momentum $\hbar k$) relative to the target proton (taken to be infinitely massive and at the origin) and let $\vec{r} = \vec{s} + \vec{z}$ denote the position vector of the target electron, with \vec{s} and \vec{b} perpendicular to the direction of \vec{z} along which the eikonal integration is performed. In the GA the amplitude $F_{fi}(\vec{q})$ for collisions in which the H atom undergoes a transition from state *i* with wave function ψ_i to state *f* with wave function ψ_f and the projectile imparts momentum $\hbar \vec{q}$ to the target is given by⁴

$$F_{fi}(\vec{q}) = \frac{1}{2}ik\pi^{-1}\int \psi_f^*(\vec{r})[1-e^{i\chi}] \\ \times \psi_i(\vec{r})e^{i\vec{q}\cdot\vec{b}}d^2b\,d\vec{r}, \qquad (1)$$

where the phase-shift function χ is simply⁴

$$2\eta \ln(|\mathbf{b} - \vec{\mathbf{s}}|/b) \equiv \chi_0$$

$$\eta = -Ze^2/\hbar v ,$$

and v is the velocity of the incident particle relative to the target. The leading correction to the GA for scattering by multielectron atoms (neglecting the effects of the atomic nucleus) may be expressed¹⁰ as an additive correction χ_1 to the phase-shift function χ_{0} , so that

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$$\chi \approx \chi_0 + \chi_1 . \tag{2}$$

We have made a simple generalization to include

the nuclear contribution and, as a result, we find a first-order correction χ_1 for scattering by H atoms. For e^{\pm} -H collisions we obtain

$$\chi_{1} = \eta^{2} k^{-1} \int_{-\infty}^{\infty} d\zeta \left[\left\{ (b^{2} + \zeta^{2}) \left[|\vec{b} - \vec{s}|^{2} + (\zeta - z)^{2} \right] \right\}^{-1/2} - \left[\vec{b} \cdot (\vec{b} - \vec{s}) / b^{2} |\vec{b} - \vec{s}|^{2} \right] \\ \times (1 - \zeta(\zeta - z) / \left\{ (b^{2} + \zeta^{2}) \left[|\vec{b} - \vec{s}|^{2} + (\zeta - z)^{2} \right] \right\}^{-1/2} \right]$$
(3)

which we see depends on z, as well as on \vec{b} and \vec{s} . We have evaluated χ_1 , obtaining

$$\chi_{1} = \frac{\sqrt{8}\eta^{2} [1 + (1 - x^{2})^{1/2}]^{1/2}}{kxR} \left[\frac{1 + x + (1 - x^{2})^{1/2}}{1 + (1 - x^{2})^{1/2}} E\left[\frac{1 - x}{1 + x} \right] - \left[1 + \frac{\vec{b} \cdot (\vec{b} - \vec{s})}{b \mid \vec{b} - \vec{s} \mid} \right] E\left[\frac{2(1 - x^{2})^{1/2}}{1 + (1 - x^{2})^{1/2}} \right] \right], \quad (4)$$

where

$$R^{2} = b^{2} + |\vec{b} - \vec{s}|^{2} + z^{2}, \quad x = 2b |\vec{b} - \vec{s}| / R^{2},$$
(5)

and E denotes the complete elliptic integral of the second kind.¹¹ For elastic scattering

 $\psi_i = \psi_f = \exp(-r/a_0)/(\pi a_0^3)^{1/2}$.

Upon making the change of variable $\vec{s} = \vec{b} + \vec{b}$, integrating over the azimuth of \vec{b} , introducing spherical polar coordinates

 $z = r \sin\theta \sin\varphi, \ \delta = r \sin\theta \cos\varphi, \ b = r \cos\theta$

and performing the r integration, we obtain

$$F_{ii}(q) = (4ika_0^2/\pi) \int_0^{\pi/2} d\omega \int_0^{\pi/2} d\theta \int_0^{\pi/2} d\varphi x \sin\theta [3(\beta^2 + \gamma^2)^{-9/2}(8\beta^4 - 24\beta^2\gamma^2 + 3\gamma^4) + 2\exp[2i\eta \ln(\tan\theta\cos\varphi)](d^5/d\beta^5) \times (J_0\{(2\alpha)^{1/2}[(\beta^2 + \gamma^2)^{1/2} - \beta]^{1/2}\} \times K_0\{(2\alpha)^{1/2}[(\beta^2 + \gamma^2)^{1/2} + \beta]^{1/2}\})], \qquad (6)$$

where

$$x = \sin 2\theta \cos \varphi, \ \gamma = a_0 q \cos \theta, \ \beta = 2(1 + x \cos 2\omega)^{1/2},$$

and

$$d = -\frac{\sqrt{8}i\eta^2}{kxa_0} \left[1 + (1-x^2)^{1/2}\right] \left[\frac{1+x+(1-x^2)^{1/2}}{1+(1-x^2)^{1/2}} E\left(\frac{1-x}{1+x}\right) - (1-\cos 2\omega) E\left(\frac{2(1-x^2)^{1/2}}{1+(1-x^2)^{1/2}}\right)\right].$$
 (7)

This volume integral over a cube may be computed by means of standard numerical methods.

Since χ_1 is proportional to η^2 (i.e., to Z^2) and χ_0 is proportional to η (i.e., to Z), the moduli of the e^{-} -H and e^{+} -H scattering amplitudes will no longer be equal, and hence the corresponding cross sections will differ, as they should.

We have applied Eq. (6) to e^{\pm} -H elastic scattering, and in Figs. 1–3 we present $d\sigma/d\Omega$ as a

function of q^2 and compare the results with absolute measurements. In Fig. 1 we see that the results are in excellent agreement with the data (which range from scattering angles of 20 to 140°) at 680 and 400 eV. The e^+ -H cross section is always lower than the e^- -H cross section. For e^- -H collisions, exchange effects are included by numerically calculating the "exact" eikonal exchange amplitude⁸ corresponding to the choice $\vec{q} \cdot \vec{z} = 0$.



FIG. 1. Electron-hydrogen and positron-hydrogen elastic scattering differential cross sections at 680 and 400 eV incident energies as functions of the squared momentum transfer. The solid curves (FE) are the present first-order calculations including exchange. The long-dashed curve (GA) is the Glauber approximation without exchange. The short-dashed-dotted curves (P) are the present calculations for positron-hydrogen scattering. The data are from Ref. 7.

Their inclusion (corresponding curves not shown) increases the calculated e^{-} -H cross section above the conventional GA results without exchange, but at 680 eV these effects are negligible, and at 400 eV they are quite small and the improvement is not sufficient to yield satisfactory results. However, the addition of our correction term χ_1 leads to yet further improvement and to excellent agreement. At 680 eV, the chi square (χ^2) per degree of freedom is 0.69 and at 400 eV it is 0.79. Even at the very large angles $120^{\circ}-140^{\circ}$, at 680 eV ($a_0^2q^2 \ge 150$) we have a chi square per degree of freedom equal to 0.71, and at 400 eV ($a_0^2q^2 \ge 80$) it is equal to 0.97.

Although the GA is a high-energy and smallangle approximation, the correction term Eq. (4) should extend the regions of validity to lower ener-



FIG. 2. Same as Fig. 1, for 200 and 100 eV. In addition, the long-dashed dotted curve (FO) is the present first-order calculation without exchange, and the shortdashed curves (GE) are the Glauber approximation including exchange. The triangle data point is from Ref. 6.

gies and larger angles. In Fig. 2 we compare the calculations with the data⁷ (which range from 10 to 140°) at 200 and 100 eV. At these energies we see the differences between the e^+ -H and e^- -H cross sections are quite large, ranging from factors of ~ 1.3 to 2.2. Exchange effects generally improve the e^- -H results, and the correction term consistently improves the results even further. At 200 eV, before the correction term is included the Glauber approximation (even including exchange) is not in agreement with the data. When the correction term is added, the agreement becomes excellent for angles $\leq 70^{\circ}$ and the larger angle results are somewhat improved. At the lower energy (100 eV), the improvement obtained is quite substantial and the agreement in shape is good although the calculated values are about 25 to 30% lower than the measured values. (We have included the measurement of Ref. 6 at $q^2 \approx 0.5$ for which



FIG. 3. Same as Fig. 2, for 50 and 30 eV.

no datum appears in Ref. 7. The data of Ref. 6 are $\sim 5\%$ higher on average than those of Ref. 7 at 100 eV and $\sim 16\%$ higher at 200 eV.)

In Fig. 3 we compare our results with the data' (which range from 10° to 140°) at the rather low energies of 50 and 30 eV. At 50 eV the correction term produces a very substantial improvement over the Glauber approximation (with or without exchange), particularly for $q^2 \leq 4$ where the present calculation agrees reasonably well in shape with the data. At 30 eV the correction term again yields a substantial improvement in the results which, perhaps fortuitously, are in agreement with the data for $q^2 \leq 0.35(\theta \leq 23^\circ)$. Our calculation reveals structure at 30 eV at large q^2 . This structure, however, is due to the exchange effects, not to

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the first-order correction. Although the improvement at 50 and 30 eV resulting from the first-order correction is quite large, at these low energies disagreement with the data persists. It would be interesting to see the effects of a second-order correction.

In conclusion, for the first time a systematic correction has been applied to the Glauber approximation phase-shift function χ for atomic scattering involving a composite target. The results indicate that the first-order correction to the GA produces a substantial improvement at all energies (30-680 eV) and angles $(10^{\circ}-140^{\circ})$ for e^{-} -H elastic scattering. Our calculations are in excellent agreement with the data at 680 eV, at 400 eV, and for $\theta \leq 65^{\circ}$ $(q^2 < 17)$ at 200 eV. This completely removes the disagreement with the data which had heretofore characterized the GA at 400 eV and $\theta < 55^{\circ}$ $(q^2 < 25)$ and at 200 eV and $\theta \le 65^\circ$. We also obtain agreement with the data at 30 eV and $\theta < 23^{\circ}$ $(q^2 < 0.35)$. Furthermore our calculations produce different cross sections for corresponding e^+ -H scattering.

The same techniques may be used to calculate first-order corrections for other transitions and projectiles. Since χ_1 is $O(k^{-1})$ and χ_0 is O(1), the correction will be negligible for proton-hydrogen collisions and the excellent agreement¹² between the GA and proton-hydrogen measurements will not be affected. Detailed calculations will be presented elsewhere, and will include comparisons with other methods for the correction of the Glauber approximation, such as those based on the principle of least action or the two-potential correction, for example.¹³

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