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Eikonal exchange amplitudes

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The exchange scattering of electrons by atomic hydrogen is considered in the eikonal approximation. The six-dimensional integrals for the "post" and "prior" forms of the eikonal exchange amplitudes are reduced to two-dimensional integral expressions. A comparison of the eikonal-exchange cross section, nonexchange Glauber, and experimental results for 50-, 100-, and 200-eV electron-hydrogen elastic scattering is given. Numerical convergence problems were not encountered in the evaluation of the scattering amplitudes and the procedure demonstrates that eikonal exchange calculations are almost as easily done as Glauber calculations in the single active electron approximation.

In recent years there has been much emphasis on the use of Glauber and eikonal-type approximations in calculating electron-atom scattering cross sections. In particular, the Glauber approximation has been extensively used to study electron-atom scattering problems.[1] The Glauber method generally gives good results for cross-section calculations at intermediate energies; however, it has a number of shortcomings. The Glauber assumption $q_z = 0$ is in principle valid only for small-angle elastic scattering and high-energy intermediate-angle inelastic scattering[2]; furthermore, the Glauber approximation predicts identical cross sections for both electron and positron scattering,[3] and predicts linear polarization of the Ly-α radiation resulting from excitation of the $2p$ states of atomic hydrogen unless the axis of quantization is redefined.[4] There have thus been recent efforts to utilize the full eikonal approximation in the investigation of atomic scattering problems.[5] Gau and Macek recently showed that the six-dimensional integral expression for the full eikonal direct scattering amplitude for electron-hydrogen scattering can be reduced to a two-dimensional expression suitable for numerical calculations.[6] This reduced eikonal amplitude has been utilized to study the elastic scattering of electrons[7] and positrons[8] from atomic hydrogen. However, at the intermediate energies of interest in these calculations, the corrections to the cross sections due to electron exchange effects may be important. Hence, it would be quite useful to have an eikonal approximation to the exchange amplitude in a form suitable for numerical calculations.

In this paper we wish to point out that the eikonal approximation to the exchange amplitude for electron-hydrogen scattering can be reduced to two-dimensional expressions suitable for numerical integration. As a demonstration of this approximation we have numerically evaluated the electron-hydrogen elastic differential and total cross sections for 50-, 100-, and 200-eV electrons.

The scattering amplitude for the process e^--H$(i \to f)$ in which electron exchange occurs is related to the "post" and "prior" forms of the t matrix by the equation[9]

$$\begin{aligned} G_{(+)}(i\to f) &= (-1/2\pi)\langle \phi_f(\vec{r},\vec{R})\,|\,U_{(+)}\,|\,\psi_i^{(+)}(\vec{R},\vec{r})\rangle \\ &= G_{(-)}(i\to f) \\ &= (-1/2\pi)\langle \psi_f^{(-)}(\vec{r},\vec{R})\,|\,U_{(-)}\,|\,\phi_i(\vec{R},\vec{r})\rangle, \end{aligned} \tag{1}$$

where $U_{(+)} = 1/R' - 1/r$, $U_{(-)} = 1/R' - 1/R$, $\vec{R}' = \vec{R} - \vec{r}$, and $\vec{R}, \vec{r}$ are the coordinates of the incident and bound electrons, respectively, before the collision. Atomic units are used here.

The eikonal approximation to the "post" and "prior" forms of the scattering wave function are respectively given by[10]

$$\psi_i^{(+)}(\vec{R},\vec{r}) \cong \exp\left(i\vec{K}_i\cdot\vec{R} - \frac{i}{K_i}\int_{-\infty}^{Z} U_{(-)}(\vec{R},\vec{r})\,dZ\right)\phi_i(\vec{r}) \tag{2a}$$

and

$$\psi_f^{(-)}(\vec{r},\vec{R}) \cong \exp\left(i\vec{K}_f\cdot\vec{r} + \frac{i}{K_f}\int_{z}^{\infty} U_{(+)}(\vec{r},\vec{R})\,dz\right)\phi_f(\vec{R}). \tag{2b}$$

Performing the integrations in the eikonal phase factors and substituting the "post" and "prior" scattering wave functions into the "post" and "prior" forms of the t matrix, respectively, results in the "post" and "prior" eikonal exchange amplitudes:

$$\begin{aligned} G_{(+)}(i\to f,\vec{K}_i,\vec{K}_f) = \frac{-1}{2\pi a_0} C_f^* C_i D_i(\mu,\vec{\gamma}) D_f(M,\vec{\Gamma}) \int d\vec{R}\,d\vec{r}\,[\exp(-MR - i\vec{\Gamma}\cdot\vec{R} + i\vec{K}_i\cdot\vec{R})]\left(\frac{1}{R'} - \frac{1}{r}\right) \\ \times [\exp(-\mu r + i\vec{\gamma}\cdot\vec{r} - i\vec{K}_f\cdot\vec{r})]\left(\frac{R'-Z'}{R-Z}\right)^{in_i} \end{aligned} \tag{3a}$$

and

$$G_{(-)}(i\to f,\vec{K}_i,\vec{K}_f)=\frac{-1}{2\pi a_0}C_f^*C_iD_i(\mu,\vec{\gamma})D_f(M,\vec{\Gamma})\int d\vec{R}\,d\vec{r}\,[\exp(-MR-i\vec{\Gamma}\cdot\vec{R}+i\vec{K}_i\cdot\vec{R})]\left(\frac{1}{R'}-\frac{1}{R}\right)$$
$$\times[\exp(-\mu r+i\vec{\gamma}\cdot\vec{r}-i\vec{K}_f\cdot\vec{r})]\left(\frac{R'-Z'}{r+z}\right)^{i\eta_f} \tag{3b}$$

where $\eta_i=1/K_i$ and $\eta_f=1/K_f$. In Eqs. (3a) and (3b) above, we have made use of the fact that the initial and final bound-state wave functions can be written in the forms

$$\phi_i(\vec{r})=D_i(\mu,\vec{\gamma})C_ie^{-\mu r+i\vec{\gamma}\cdot\vec{r}}\big|_{\vec{\gamma}=0} \tag{4a}$$

$$\phi_f^*(\vec{R})=D_f(M,\vec{\Gamma})C_f^*e^{-MR-i\vec{\Gamma}\cdot\vec{R}}\big|_{\vec{\Gamma}=0}, \tag{4b}$$

where C_i and C_f are normalization constants, and $D_i(\mu,\vec{\gamma})$ and $D_f(M,\vec{\Gamma})$ are the appropriate differential operators which generate the required wave functions.

The "post" and "prior" eikonal exchange amplitudes $G_{(+)}$ and $G_{(-)}$ given by Eqs. (3a) and (3b) above are reduced to two-dimensional integral expressions by use of the techniques similar to those employed to reduce the direct amplitude[11]; consider first the "post" amplitude $G_{(+)}$. First, the factor $(R'-Z')^{i\eta_i}$ is replaced by its gamma function representation,[12] and then the Fourier transform of the factors containing R' is taken. This allows the $\vec{r}$ integral to be done analytically. Next, the integral over the Fourier-transform variable $\vec{k}$ is done using Feynman integration. Finally, the $\vec{R}$ integral is done using parabolic coordinates[13]; the result is the desired double-integral expression for $G_{(+)}$,

$$G_{(+)}(i\to f,\vec{K}_i,\vec{K}_f)=\frac{-\pi 2^{4-i\eta_i}}{a_0}\frac{\Gamma(1-i\eta_i)}{\Gamma(-i\eta_i)}C_f^*C_iD_i(\mu,\vec{\gamma})D_f(M,\vec{\Gamma})$$
$$\times\int_0^\infty d\lambda\,\lambda^{-i\eta_i-1}\int_0^1 d\chi\,\chi^{-1}\left[\mu\left(\frac{d}{d\mu^2}\right)^2\mathfrak{F}_{(+)}(1,0,0,0,0)-\chi^{-1}\left(\frac{d}{d\mu^2}\right)^2\mathfrak{F}_{(+)}(1,0,0,1,0)\right]\bigg|_{\vec{\gamma}=\vec{\Gamma}=0}, \tag{5a}$$

where

$$\mathfrak{F}_{(+)}(m,p,r,s,t)=\lambda^s(1-\chi)^s\Lambda_{(+)}^{-p}[\beta_{(+)}^2+Q_{(+)}^2]^{i\eta_i-m}[\beta_{(+)}-iQ_{(+)z}]^{-i\eta_i-r}\beta_{(+)}^t, \tag{5b}$$

$$\beta_{(+)}=\Lambda_{(+)}+M, \tag{5c}$$

$$\Lambda_{(+)}=[\lambda^2(1-\chi)^2+\mu^2\chi+(\vec{K}_f-\vec{\gamma})^2\chi(1-\chi)-2i\lambda\chi(1-\chi)(K_{fz}-\gamma_z)]^{1/2}, \tag{5d}$$

$$\vec{Q}_{(+)}=\vec{K}_i-\chi\vec{K}_f-i\lambda(1-\chi)\hat{z}+\chi\vec{\gamma}-\vec{\Gamma}. \tag{5e}$$

The "prior" exchange amplitude $G_{(-)}$ can be reduced in a similar manner; the result is

$$G_{(-)}(i\to f,\vec{K}_i,\vec{K}_f)=\frac{-\pi 2^{4-i\eta_f}}{a_0}\frac{\Gamma(1-i\eta_f)}{\Gamma(-i\eta_f)}C_f^*C_iD_i(\mu,\vec{\gamma})D_f(M,\vec{\Gamma})$$
$$\times\int_0^\infty d\lambda\,\lambda^{-i\eta_f-1}\int_0^1 d\chi\,\chi^{-1}\left[M\left(\frac{d}{dM^2}\right)^2\mathfrak{F}_{(-)}(1,0,0,0,0)-\chi^{-1}\left(\frac{d}{dM^2}\right)^2\mathfrak{F}_{(-)}(1,0,0,1,0)\right]\bigg|_{\vec{\gamma}=\vec{\Gamma}=0}, \tag{6a}$$

where

$$\mathfrak{F}_{(-)}(m,p,r,s,t)=\lambda^s(1-\chi)^s\Lambda_{(-)}^{-p}[\beta_{(-)}^2+Q_{(-)}^2]^{i\eta_f-m}[\beta_{(-)}-iQ_{(-)z}]^{-i\eta_f-r}\beta_{(-)}^t, \tag{6b}$$

$$\beta_{(-)}=\Lambda_{(-)}+\mu, \tag{6c}$$

$$\Lambda_{(-)}=[\lambda^2(1-\chi)^2+M^2\chi+(\vec{K}_i-\vec{\Gamma})^2\chi(1-\chi)-2i\lambda\chi(1-\chi)(K_{iz}-\Gamma_z)]^{1/2}, \tag{6d}$$

$$\vec{Q}_{(-)}=\vec{K}_f-\chi\vec{K}_i-i\lambda(1-\chi)\hat{z}+\chi\vec{\Gamma}-\vec{\gamma}. \tag{6e}$$

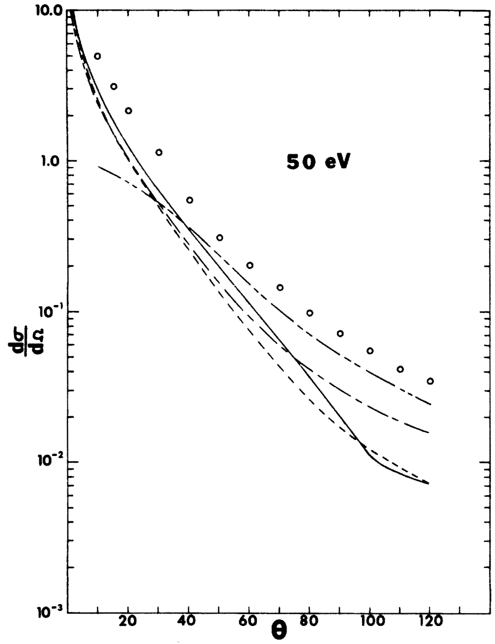

FIG. 1. Differential cross section $d\sigma/d\Omega$ vs scattering angle θ for the elastic scattering of 50-eV electrons from atomic hydrogen. The eikonal results corrected for exchange (solid line) are compared with the eikonal results without exchange (dotted line) (Ref. 7), the Glauber results without exchange (dash-dotted line) (Ref. 14), the Born results without exchange (dash-double-dotted line) (Ref. 15), and the recent experimental results of Williams (open circles) (Ref. 16). $d\sigma/d\Omega$ is in units of a_0^2/sr, and θ is in deg.

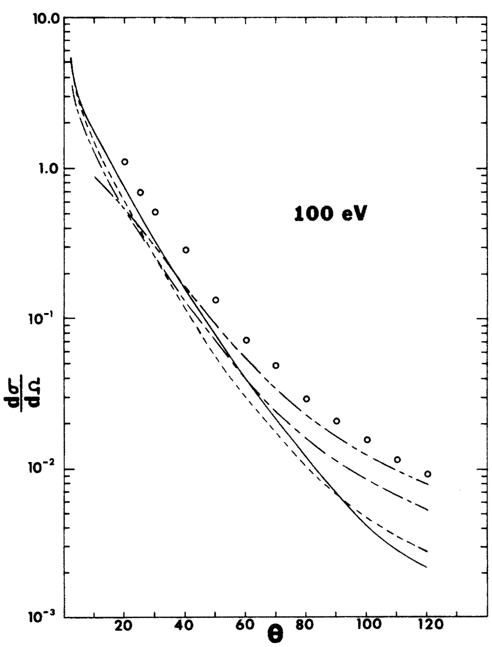

FIG. 2. Same as Fig. 1 but for 100-eV incident electrons.

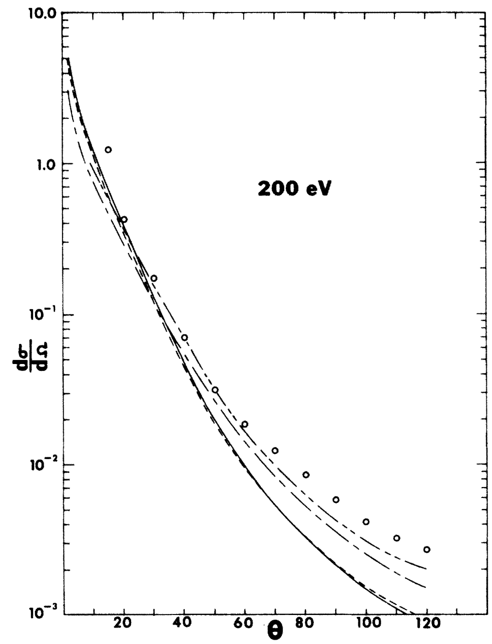

FIG. 3. Same as Fig. 1 but for 200-eV incident electrons.

Examination of the above expressions shows that either form of the reduced eikonal exchange amplitude can be obtained from the other one by interchanging $\vec{K}_i$ with $\vec{K}_f$, η_i with η_f, μ with M, and $\vec{\gamma}$ with $\vec{\Gamma}$ everywhere except in the differential operators D_i and D_f. We note here that Glauber-type exchange amplitudes could be obtained by setting $q_z = (\vec{K}_i - \vec{K}_f)_z = 0$ in the above expressions; however, this approximation would not appreciably simplify the expressions further.

The above double-integral expressions for the eikonal exchange amplitudes should prove useful in electron-hydrogen exchange scattering studies; in particular, the exchange calculations for any transition of interest should require scarcely more effort than that required for the direct excitation calculations. Equations (5a) and (6a) may also be generalized for many-electron atoms with configuration interactions.

We have calculated the differential and total scattering cross sections for the elastic scattering of 50-, 100-, and 200-eV electrons on hydrogen using the "post" and "prior" forms of the exchange amplitude. The exchange-corrected differential and total cross sections are calculated using the familiar expressions

$$\frac{d\sigma}{d\Omega} = \tfrac{1}{4}|F+G|^2 + \tfrac{3}{4}|F-G|^2, \tag{7a}$$

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega, \tag{7b}$$

TABLE I. Elastic differential cross sections (in units of a_0^2/sr) vs scattering angle θ (in deg) for 50-eV incident electrons.

θ	Direct	"Post" exchange	"Prior" exchange	"Post" exchange corrected	"Prior" exchange corrected	Experimental
2	10.5	0.239	0.239	10.4	10.4	...
3	7.64	0.237	0.238	7.77	7.77	...
5	5.90	0.230	0.233	6.16	6.16	...
7	4.02	0.221	0.226	4.30	4.31	...
10	2.60	0.202	0.211	2.91	2.93	5.04
15	1.57	0.163	0.181	1.88	1.92	3.18
20	1.02	0.121	0.147	1.28	1.34	2.17
40	0.253	1.53×10^{-2}	4.55×10^{-2}	0.308	0.384	0.551
60	7.37×10^{-2}	3.06×10^{-5}	1.42×10^{-2}	7.23×10^{-2}	0.119	0.205
80	2.71×10^{-2}	2.40×10^{-3}	3.89×10^{-3}	2.27×10^{-2}	3.97×10^{-2}	9.93×10^{-2}
100	1.25×10^{-2}	3.76×10^{-3}	2.28×10^{-3}	1.06×10^{-2}	1.09×10^{-2}	5.58×10^{-2}
120	7.26×10^{-3}	3.96×10^{-3}	7.76×10^{-3}	6.71×10^{-3}	7.51×10^{-3}	3.49×10^{-2}

where F is the direct eikonal amplitude and G is the "post" or "prior" exchange amplitude. We wish to emphasize that no numerical convergence problems are encountered if Eqs. (5a), (6a), and the corresponding expression for the direct amplitude are integrated by parts before numerical evaluation is attempted. The results of the calculations are displayed graphically in Figs. 1, 2, and 3, while the numerical data are given in Tables I, II, and III.

The total cross sections are given in Table IV. It is apparent that the "prior" form of the eikonal approximation agrees with experimental differential cross sections better than the straight Glauber or Born approximations for scattering angles less than approximately 30°. At larger scattering angles both the "post" and "prior" forms of the eikonal approximation fail and the straight Glauber approximation appears to be closer to the data; however, the Born approximation seems to be the best. The total cross section for the "prior" form of the eikonal exchange amplitude (at 50 eV) seems to be in reasonable agreement with the inferred experimental result. At 100 eV the post-prior discrepancy is less than 3%, and at 200 eV the exchange correction is less than 9%.

From a classical point of view, the eikonal method gives poor results at large angles because the straight-line eikonal trajectory is a poor approximation to the actual electron trajectory for large-angle scattering.

It has been shown[18] that the Glauber approximation fails to adequately represent the second Born term (which would be present in an expansion of the exact direct scattering amplitude); presumably, the eikonal method used here to calculate the direct amplitudes also suffers from a similar defect. We believe, however, that for elastic scattering

TABLE II. Elastic differential cross sections (in units of a_0^2/sr) vs scattering angle θ (in deg) for 100-eV incident electrons.

θ	Direct	"Post" exchange	"Prior" exchange	"Post" exchange corrected	"Prior" exchange corrected	Experimental
2	5.18	0.105	0.105	5.29	5.29	...
3	3.72	0.103	0.103	3.80	3.80	...
5	2.56	9.86×10^{-2}	9.97×10^{-2}	2.77	2.77	...
7	2.02	9.24×10^{-2}	9.44×10^{-2}	2.31	2.31	...
10	1.51	8.07×10^{-2}	8.43×10^{-2}	1.75	1.76	...
15	0.925	5.85×10^{-2}	6.47×10^{-2}	1.11	1.12	...
20	0.587	3.81×10^{-2}	4.60×10^{-2}	0.722	0.743	1.10
40	0.121	3.02×10^{-3}	8.47×10^{-3}	0.139	0.158	0.288
60	2.99×10^{-2}	2.20×10^{-5}	1.83×10^{-3}	3.07×10^{-2}	3.88×10^{-2}	7.22×10^{-2}
80	1.02×10^{-2}	7.69×10^{-5}	4.13×10^{-4}	9.59×10^{-3}	1.22×10^{-2}	2.95×10^{-2}
100	4.75×10^{-3}	1.40×10^{-4}	2.55×10^{-4}	4.23×10^{-3}	4.03×10^{-3}	1.55×10^{-2}
120	2.80×10^{-3}	1.51×10^{-4}	4.75×10^{-4}	2.41×10^{-3}	2.17×10^{-3}	9.2×10^{-3}

TABLE III. Elastic differential cross sections (in units of a_0^2/sr) vs scattering angle θ (in deg) for 200-eV incident electrons.

θ	Direct	"Post" exchange	"Post" exchange corrected	Experimental
2	4.57	3.71×10^{-2}	4.73	···
3	3.30	3.62×10^{-2}	3.48	···
5	2.26	3.34×10^{-2}	2.43	···
7	1.65	2.97×10^{-2}	1.81	···
10	1.11	2.33×10^{-2}	1.24	···
15	0.604	1.34×10^{-2}	0.687	1.22
20	0.344	6.68×10^{-3}	0.391	0.419
40	4.59×10^{-2}	1.87×10^{-4}	4.90×10^{-2}	7.06×10^{-2}
60	9.59×10^{-3}	9.20×10^{-6}	9.66×10^{-3}	1.87×10^{-2}
80	3.31×10^{-3}	1.27×10^{-5}	3.21×10^{-3}	8.59×10^{-3}
100	1.57×10^{-3}	1.23×10^{-5}	1.49×10^{-3}	4.12×10^{-3}
120	9.42×10^{-4}	1.06×10^{-5}	8.77×10^{-4}	2.72×10^{-3}

TABLE IV. Total cross sections (units of πa_0^2) for 50-, 100-, and 200-eV incident electrons.[a]

E(eV)	σ_B [b]	σ_G [b]	σ_E	$\sigma_{E\text{-post}}$	$\sigma_{E\text{-prior}}$	σ_{expt}
50	0.51	0.64	0.72	0.84	0.94	1.2
100	0.29	0.29	0.39	0.43	0.44	···
200	0.15	0.15	0.22	0.24	···	···

[a] σ_B is for the Born approximation (Ref. 17); σ_G, Glauber approximation (Ref. 17); σ_E, full eikonal approximation (Ref. 7); $\sigma_{E\text{-post}}$, exchange-corrected eikonal approximation using the post form of the amplitude (this work); $\sigma_{E\text{-prior}}$, exchange-corrected eikonal approximation using the prior form of the amplitude (this work); σ_{expt}, experimental (Ref. 1).

[b] Exchange not included.

the results of this paper clearly demonstrate that exchange effects are important for incident energies below about 100 eV.

Added note: Since submission of this paper for publication it has been brought to our attention that R. Madan [Phys. Rev. A 12, 2631 (1975)] has derived a similar expression for the eikonal exchange amplitude and has evaluated the elastic exchange-corrected differential and total cross sections for electron-hydrogen scattering at 50 eV, using both the Ochkur approximation and the Glauber form of the exchange amplitude (i.e., with $\vec{q}\cdot\hat{z}=0$).

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