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Electron-hydrogen elastic scattering in the eikonal approximation

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Differential and total cross sections for elastic scattering of electrons from atomic hydrogen have been calculated using the full eikonal approximation. The eikonal results for 50-, 100-, and 200-eV incident electrons are compared with other theoretical calculations and with recent experimental data. It is found that the full eikonal approximation predicts both small-angle differential cross sections and total cross sections, which are in better agreement with experiment than either the Born or Glauber results.

I. INTRODUCTION

In recent years there has been much interest in eikonal-type approaches to electron-atom scattering problems.[1] In particular, electron scattering from atomic hydrogen has been the subject of extensive study since the e-H system is the simplest one.[2] The full eikonal scattering amplitude for electron-hydrogen scattering has been derived by a number of authors in various ways[3]; it is given by

$$F_{fi}(\vec{q}) = \frac{-2m}{4\pi\hbar^2}\int e^{i\vec{q}\cdot\vec{R}}\, V(R,R')\exp\left[-\frac{i}{\hbar v}\int_{-\infty}^{Z} V(R,R')\,dZ\right] \times u_f^*(\vec{r})u_i(\vec{r})\,d\vec{R}\,d\vec{r}, \tag{1}$$

where $\vec{R}$ and $\vec{r}$ are the coordinates of the incident and bound electrons, respectively, $\vec{R}' = \vec{R}-\vec{r}$, and $V(R,R') = e^2(1/R' - 1/R)$ is the interaction potential between the target atom and the incident electron. Here $m\vec{v} = \hbar\vec{k}$ is the incident electron's momentum, $\vec{q} = \vec{k}-\vec{k}'$ is the momentum transfer to the target, and u_f and u_i are the final and initial bound states of the target atom. In the above expression, $\vec{k}$ is along the z axis.

In order to simplify the six-dimensional integral in Eq. (1) to a form amenable to calculations, the additional approximation $\vec{q}\perp\vec{k}$ (i.e., $q_z = 0$) is often made in Eq. (1). The assumption $q_z = 0$ allows the Z integration to be done immediately, and in addition allows the resulting expression for the scattering amplitude to be simplified considerably,[4] not only for electron-hydrogen scattering but for electron–heavy-atom collisions as well.[5] This neglect of the longitudinal component of the momentum transfer in Eq. (1) above is known as the Glauber approximation. The Glauber approximation has been widely used in electron-atom collision studies to calculate both differential and total scattering cross sections. In many cases, this approximation appears to give very good results when compared to experimental data and other theoretical calculations, especially in the intermediate energy ranges where the Born approximation is known to fail and where close-coupling calculations would be intractable.[6]

However, some unrealistic physical consequences arise from the assumption $q_z = 0$. In particular, this assumption leads to the prediction that the Lyman-α decay radiation (produced by $1s \to 2p$ electron excitation of hydrogen) is linearly polarized. Moreover, the approximation $q_z = 0$ is, in principle, valid only for small-angle elastic scattering and high-energy intermediate-angle inelastic scattering.[7] Hence it would seem to be useful to utilize the full eikonal scattering amplitude given by Eq. (1) to study electron-hydrogen collisions.

Recently, Gau and Macek[8] showed that the six-dimensional integral in Eq. (1) above can be reduced in the case of arbitrary hydrogenic states to a two-dimensional integral by using the fact that the bound-state wave function product can be written as

$$u_f^*(\vec{r})u_i(\vec{r}) = D(\mu,\vec{\gamma})\,C_{fi}\,e^{-\mu r + i\vec{\gamma}\cdot\vec{r}}\Big|_{\vec{\gamma}=0}\,. \tag{2}$$

Here, C_{fi} is a normalization constant and $D(\mu,\vec{\gamma})$ is the differential operator which generates the required wave functions when operating on the exponential in Eq. (2) above.

Their double-integral expression for the full eikonal amplitude in Eq. (1) is[9]

$$F_{fi}(\vec{q}) = \frac{-2^{4-i\eta}}{a_0}\pi\frac{\Gamma(1-i\eta)}{\Gamma(-i\eta)}C_{fi}D(\mu,\vec{\gamma})\mu\left(\frac{d}{d\mu^2}\right)^2\left[\int_0^\infty d\lambda\,\lambda^{-i\eta-1}\int_0^1 d\chi\,\chi^{-1}[\mathfrak{F}(1,0,0,0)-\mathfrak{F}(1,1,0,1]\right]\Bigg|_{\vec{\gamma}=0}, \tag{3a}$$

where

$$\mathfrak{F}(m,p,r,s)=\lambda^{s}(1-\chi)^{s}\Lambda^{-p}(\Lambda^{2}+q'^{2})^{i\eta-m}(\Lambda-iq'_{z})^{-i\eta-r}, \tag{3b}$$

$$\Lambda=[\lambda^{2}(1-\chi)^{2}+\mu^{2}\chi+2i\lambda\chi(1-\chi)\gamma_{z}+\gamma^{2}\chi(1-\chi)]^{1/2}, \tag{3c}$$

and

$$\vec{q}'=\vec{q}-i\lambda(1-\chi)\hat{z}+\chi\vec{\gamma}. \tag{3d}$$

In the above expression, a_0 is the Bohr radius and $\eta=e^2/\hbar v=1/k$. When dealing with λ integrals which diverge at $\lambda=0$, η is given a small imaginary part $i\delta$; one then integrates by parts and sets $\delta=0$.

Gau and Macek have examined large-angle $1s\to 2p$ electron-hydrogen scattering by expanding Eq. (3a) above for large $\vec{q}$ in order to obtain an approximate scattering amplitude. They find, among other things, that the Lyman-α decay radiation is, in general, elliptically polarized. Their large-angle approximate results show that the use of the full eikonal scattering amplitude Eq. (1) does predict physical phenomena not obtainable when the assumption $q_z=0$ is used.

However, no numerical calculations for elastic or inelastic electron-hydrogen scattering have as yet been reported, using the full eikonal amplitude as given by the double-integral expression Eq. (3a). See *Added note* at the end of this paper.

We have done numerical calculations for electron-hydrogen elastic scattering using the full eikonal amplitude in Eq. (3a), and we report here our results for the differential cross section vs electron scattering angle for incident electron energies of 50, 100, and 200 eV. Comparison is made with recent experimental data and other theoretical calculations.

II. ELECTRON-HYDROGEN ELASTIC SCATTERING AMPLITUDE

To evaluate Eq. (3a) for electron-hydrogen elastic scattering, we note that

$$u_f^*u_i=\pi^{-1}e^{-2r}\ (r \text{ in units of } a_0) \tag{4}$$

for $1s\to 1s$ scattering. Thus we have

$$\mu=2, \tag{5a}$$

$$C_{fi}=\pi^{-1}, \tag{5b}$$

$$\vec{\gamma}=0, \tag{5c}$$

and

$$D(\mu,\vec{\gamma})=1. \tag{5d}$$

Inserting the quantities given by Eqs. (5a)–(5d) into the scattering amplitude Eq. (3a) results in the following expression for $F_{1s\to 1s}(\vec{q})$:

$$F_{1s\to 1s}(\vec{q})=\frac{-2^{4-i\eta}}{a_0}\frac{\Gamma(1-i\eta)}{\Gamma(-i\eta)}\mu\left(\frac{d}{d\mu^2}\right)^2\left[\int_0^\infty d\lambda\,\lambda^{-i\eta-1}\int_0^1 d\chi\,\chi^{-1}\,[\mathfrak{F}(1,0,0,0)-\mathfrak{F}(1,1,0,1)]\right]. \tag{6}$$

In order to carry out the differentiations implied in the above, the following recursion formula is needed[10]:

$$\frac{d}{d\mu^2}\mathfrak{F}(m,p,r,s)=\chi[-\tfrac{1}{2}p\,\mathfrak{F}(m,p+2,r,s)+(i\eta-m)\mathfrak{F}(m+1,p,r,s)-\tfrac{1}{2}(i\eta+r)\mathfrak{F}(m,p+1,r+1,s)]. \tag{7}$$

If integration by parts is required to avoid divergences at $\lambda=0$, the following recursion formula is also needed[11]:

$$\begin{aligned}\frac{d}{d\lambda}\mathfrak{F}(m,p,r,s)=(1-\chi)[&s\,\mathfrak{F}(m,p,r,s-1)-p\mathfrak{F}(m,p+2,r,s+1)-ip\gamma_z\chi\mathfrak{F}(m,p+2,r,s)\\&-2iq_z(i\eta-m)\mathfrak{F}(m+1,p,r,s)+(i\eta+r)\mathfrak{F}(m,p,r+1,s)\\&-i\gamma_z\chi(i\eta+r)\mathfrak{F}(m,p+1,r+1,s)-(i\eta+r)\mathfrak{F}(m,p+1,r+1,s+1)].\end{aligned} \tag{8}$$

Evaluating the derivatives indicated in Eq. (6) and then setting $\mu=2$ results in the desired double-integral expression for $F_{1s\to 1s}(\vec{q})$:

$$F_{1s\to 1s}(\vec{q})=\frac{-2^{5-i\eta}}{a_0}\frac{\Gamma(1-i\eta)}{\Gamma(-i\eta)}\times\int_0^\infty d\lambda\,\lambda^{-i\eta-1}\int_0^1 d\chi\,\chi^{-1}\,\mathcal{G}(\lambda,\chi,\vec{q}), \tag{9a}$$

where

$$\mathcal{G}(\lambda,\chi,\vec{q})=\left(\frac{d}{d\mu^2}\right)^2[\mathfrak{F}(1,0,0,0)-\mathfrak{F}(1,1,0,1)], \tag{9b}$$

and

$$\Lambda=[\lambda^2(1-\chi)^2+\mu^2\chi]^{1/2}\quad(\mu=2), \tag{9c}$$

$$\vec{q}'=\vec{q}-i\lambda(1-\chi)\hat{z}. \tag{9d}$$

TABLE I. Electron-hydrogen elastic scattering differential cross section vs electron scattering angle for 50-, 100-, and 200-eV incident electrons.

Electron scattering angle (deg)	$d\sigma/d\Omega$ (a_0^2/sr) 50 eV	100 eV	200 eV
2	10.5	5.18	4.57
3	7.64	3.72	3.30
5	5.90	2.56	2.26
7	4.02	2.02	1.65
10	2.60	1.51	1.11
15	1.57	0.925	0.604
20	1.02	0.587	0.344
40	0.253	0.121	4.59×10^{-2}
60	7.37×10^{-2}	2.99×10^{-2}	9.59×10^{-3}
80	2.71×10^{-2}	1.02×10^{-2}	3.31×10^{-3}
100	1.25×10^{-2}	4.75×10^{-3}	1.57×10^{-3}
120	7.26×10^{-3}	2.80×10^{-3}	9.42×10^{-4}

III. RESULTS AND DISCUSSION

We have numerically integrated the eikonal scattering amplitude $F_{1s\rightarrow1s}(\vec{q})$ given by Eq. (9a) above, for incident electron energies of 50, 100, and 200 eV, and scattering angles from 2° to 120°. We find that integration of Eq. (9a) by parts is necessary to obtain numerical convergence.

In Table I our numerically computed differential cross sections are presented. The differential

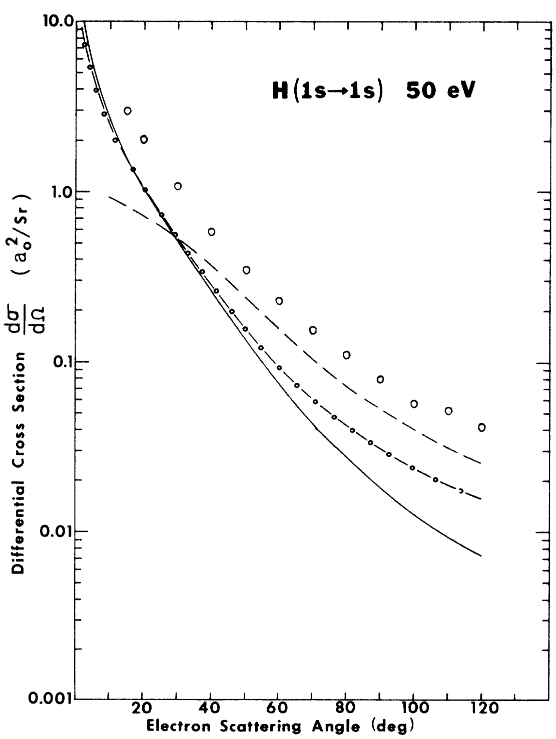

FIG. 1. Differential cross section for the elastic scattering of 50-eV electrons from atomic hydrogen. The present full eikonal results (solid line) are compared with the Born approximation (dashed line) (Ref. 13), the Glauber approximation (dash-dotted line) (Ref. 14), and recent experimental data (open circles) (Ref. 12).

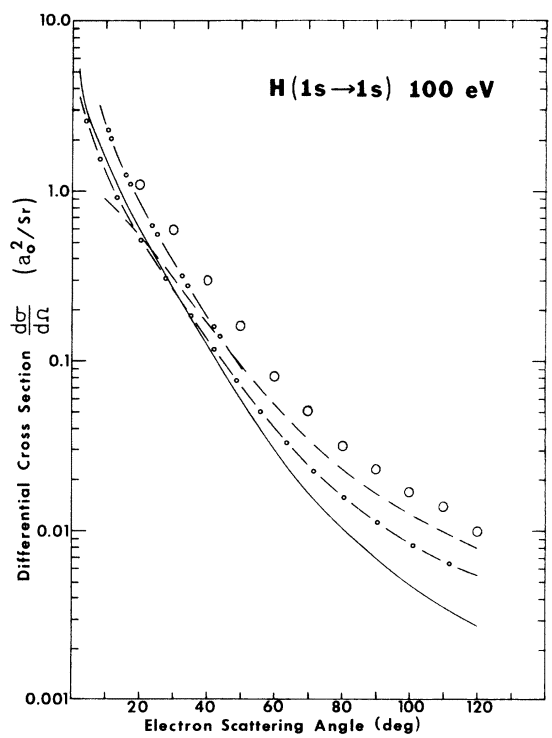

FIG. 2. Differential cross section for the elastic scattering of 100-eV electrons from atomic hydrogen. The present full eikonal results (solid line) are compared with the Born approximation (dashed line) (Ref. 13), the Glauber approximation (dash-dotted line) (Ref. 14), the eikonal-Born-series results (dash-double-dotted line) (Ref. 16), and recent experimental data (open circles) (Ref. 12).

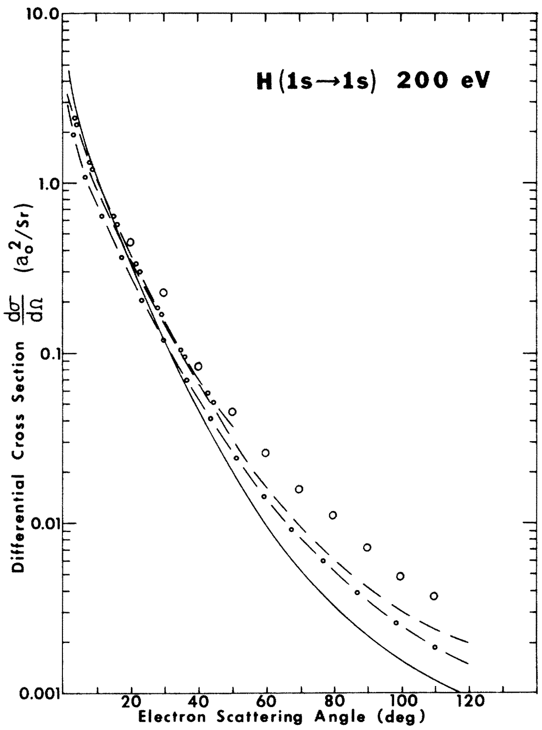

FIG. 3. Differential cross section for the elastic scattering of 200-eV electrons from atomic hydrogen. The present full eikonal results (solid line) are compared with the Born approximation (dashed line) (Ref. 13), the Glauber approximation (dash-dotted line) (Ref. 14), the eikonal-Born-series results (dash–double-dotted line) (Ref. 16), and recent experimental data (open circles) (Ref. 12).

cross section is given by

$$\frac{d\sigma}{d\Omega} = |F_{1s\to 1s}(\vec{q})|^2 . \qquad (10)$$

In Figs. 1–3, we have plotted our eikonal results for $d\sigma/d\Omega$ vs scattering angle θ, along with recent experimental data[12] and other theoretical calculations. Examination of Figs. 1–3 shows that our full eikonal differential cross sections fall somewhat below the experimental data at all angles for which data are available; however, the agreement between the two is seen to improve as the angle decreases. For large-angle scattering, the Born[13] and Glauber[14] cross sections are in better agreement with the data than our eikonal results; however, for small-angle scattering, which makes the major contribution to the total cross section, the eikonal results are in the best agreement with experiment. At large angles, the full eikonal results are depressed relative to the Glauber values due to a damping effect resulting from inclusion of the longitudinal component of momentum transfer.[15] The eikonal-Born-series results of Byron and Joachain[16] for 100- and 200-eV incident electrons are also shown here for comparison; these results agree somewhat better with the data than our eikonal cross sections at all angles. However, the eikonal-Born-series calculations include exchange effects which are not included in our full eikonal calculations.

By using Newton-Cotes open-ended numerical integration[17] to integrate our values of $d\sigma/d\Omega$ over θ we have also obtained total elastic cross sections for e-H scattering at 50-, 100-, and 200-eV incident energies. These results, compared with the Glauber and Born[18] total cross sections and with experiment,[19] are shown in Table II.

TABLE II. Total electron-hydrogen elastic scattering cross sections for 50-, 100-, and 200-eV incident electrons.

Incident electron energy (eV)	Total scattering cross section (πa_0^2) Present eikonal	Glauber	Born	Experiment
50	0.72	0.64	0.51	1.2
100	0.39	0.29	0.29	···
200	0.22	0.15	0.15	···

IV. SUMMARY AND CONCLUSIONS

We have calculated, using the full eikonal approximation, both differential and total cross sections for electron-hydrogen elastic scattering for 50-, 100-, and 200-eV incident electrons. We obtain results in reasonable agreement with experiment. In particular, for small-angle scattering, which gives the dominant contribution to the total cross section, our differential cross sections represent an improvement over both the Born and Glauber results, and give rise to total cross sections in somewhat better agreement with available experimental values.

We, therefore, feel the two-dimensional integral expression for the full eikonal scattering amplitude, which is made use of in the present paper, to be a useful technique for electron-hydrogen scattering studies.

Added note: It has been brought to our attention that J. N. Gau and J. Macek have calculated inelastic electron-hydrogen scattering in the unrestricted Glauber approximation [Phys. Rev. A **12**, 1760 (1975)]. Although some of our work duplicates some of their results for elastic scattering, we do not find any difficulties with numerical convergence. We wish to emphasize that in order to avoid the difficulties our Eq. (9a) must be integrated by parts. The integration by parts allows us to integrate numerically down to a 2° scattering angle without difficulty, and hence to obtain total elastic scattering cross sections. At 100 eV (the only incident energy common to both calculations) the two calculations agree to within 4% for scattering angles larger than 20°; however, for 10° our result for $d\sigma/d\Omega$ is smaller than the Gau-Macek result by 40%.

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[1]Extensive lists of references involving the application of Glauber and eikonal-type theories to electron-atom scattering can be found in the following: E. Gerjuoy and B. K. Thomas, Rep. Prog. Phys. 37, 1345 (1974); W. Williamson, Jr., and G. Foster, Phys. Rev. A 11, 1472 (1975).

[2]See E. Gerjuoy and B. K. Thomas, pp. 1383–1409 in Ref. 1 above, for a detailed review of the application of Glauber theory to electron-hydrogen scattering. See W. Williamson, Jr., and G. Foster, Ref. 1 above, for a list of references involving related eikonal-type approaches to electron-hydrogen scattering.

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[8]Reference 7, pp. 524–525.

[9]Reference 7, p. 525, Eq. (17a).

[10]Reference 7, p. 525, Eq. (18a).

[11]This recursion formula is not given by Gau and Macek; we have therefore derived it ourselves for the present work.

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[19]E. Gerjuoy and B. K. Thomas (in Ref. 1 above) extrapolate the 50-eV experimental data of Ref. 12 to angles <15° and >130° in order to estimate the experimental total cross section; they assign an uncertainty of ±50% to this result. They did not make this estimate for the 100- and 200-eV data, which were not available when Ref. 1 was published.