Elastic scattering of electrons with hydrogen atoms using the polarized Glauber approximation

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(Received 22 June 1973)

The Glauber theory for electron-atom collisions is extended to include the polarization effects. The results for the differential and the total elastic-scattering cross sections are presented, and it is observed that the agreement with the available data is improved with the inclusion of such effects.

I. INTRODUCTION

The Glauber approximation[1] has been used in recent years with considerable success for predicting elastic and inelastic scattering of electrons with atoms.[2] Although this approximation is more suited for high-energy scattering, it yields good results in the intermediate energy range where the other theories are either not good or get very complicated. Applications of the Glauber theory in the electron and proton scattering from the hydrogen atom have been extensive. Thomas and Gerjuoy[3] have obtained the closed-form expressions of the scattering amplitudes in hydrogen. An attempt to include the electron exchange was recently made by Tenny and Yates,[4] where the post and prior form of the Glauber exchange amplitudes were reduced using Bonham-Ochkur expansions. Extensions of the Glauber theory to the electron scattering from complex atoms have been reported.[5-9]

Byron[6] and Bransden and Coleman[10] have shown the relationship of the Glauber approximation with the close coupling and the impact-parameter methods, respectively. Bransden and Coleman made an allowance for the states omitted in the close-coupling method by constructing second-order potential and using closure. The effective energy parameter occurring in their calculations was chosen such that in the adiabatic limit the correct long-range interaction is obtained in the incident channel. Such long-range polarization effects are not included explicitly in the Glauber approximation. The need for introducing the polarization effects and their importance in electron-atom scattering has long been recognized.[11,12] For electron-helium scattering Khare and Moiseiwitsch[13] and LaBahn and Callaway[12] have noted a considerable improvement in the agreement of the theoretical differential cross sections with the experiment for low-scattering angles; and up to high enough incident electron energies (≈ 400 eV) when the polarization effects were included. Several attempts have been recently made to include polarization within the framework of the first Born and the close-coupling approximations.[14-18] One way of taking the polarization effects explicitly into the Glauber theory, in a simple way, is to treat the target eigenfunction perturbed by the field of static charge. In this paper we present the method of including perturbation effects in the Glauber theory for elastic electron-hydrogen scattering, so that our method will have the characteristics of the close-coupling method (implicit in the Glauber theory[6]) and the polarized-orbital theory.

II. THEORY

The scattering amplitude for a collision between a charged particle and an atom in the Glauber approximation is given by

$$F_{fi}(\vec{q}) = \frac{-1}{2\pi}\int d\vec{r}_1\, d\vec{r}_2 \Phi_f^*(\vec{r}_1) \times \Phi_i(\vec{r}_1) V(\vec{b}, z_2;\vec{r}_1) e^{i\vec{q}\cdot\vec{r}_2} \times \exp\left(\frac{-i}{k_i}\int_{-\infty}^{z_2} V(\vec{b}, z_2';\vec{r}_1)\, dz_2'\right), \qquad (1)$$

where $\vec{r}_1 = \vec{s} + \vec{z}_1$ and $\vec{r}_2 = \vec{b} + \vec{z}_2$ denote, respectively, the position vectors of the target and incident electrons. $\vec{b}$ is the impact-parameter vector and $\vec{s}$ is the projection of $\vec{r}_1$ on the plane of $\vec{b}$. Φ_i and Φ_f are the initial- and final-state wave functions of the target atom and $\hbar\vec{q}$ is the momentum imparted by the incident electron of initial momentum $\hbar\vec{k}_i$. $V(\vec{b}, z_2;\vec{r}_1)$ is the potential seen by the incident electron.

Considering the perturbation of the target atom due to the field of the incident charge, the perturbed wave function in the initial state is given by

$$\Phi_i'(\vec{r}_1) = \Phi_0(\vec{r}_1) + \Phi_{\rm pol}(\vec{r}_1, \vec{r}_2)\,. \qquad (2)$$

$\Phi_0(\vec{r}_1) = (\pi)^{-1/2} e^{-r_1}$ is the ground-state wave function of the hydrogen atom. $\Phi_{\rm pol}(\vec{r}_1, \vec{r}_2)$ represents the polarized part of the target wave function and, in the dipole approximation, is expressed, following Temkin,[11] by

$$\Phi_{\mathrm{pol}}(\vec{r}_1,\vec{r}_2) = -\epsilon(r_1,r_2)\Phi_0(\vec{r}_1)(1/r_2^2)\times(r_1+\tfrac{1}{2}r_1^2)\cos\theta_{12},$$

$$\cos\theta_{12} = (\hat{r}_1\cdot\hat{r}_2), \tag{3}$$

where $\epsilon(r_1,r_2)$ is a unit step function introduced to express the fact that polarization will be meaningful only when $r_2>r_1$, and so

$$\epsilon(r_1,r_2)=\begin{cases}1 & \text{if } r_2>r_1,\\ 0 & \text{if } r_2<r_1.\end{cases}$$

Duxler *et al.*[19] have made a detailed study of the polarized-orbital method and investigated the effect of the unit step function $\epsilon(r_1,r_2)$ on the cross sections. They have demonstrated that the results obtained by performing the integrations in the full range of r_2 do not differ appreciably from those obtained by limiting the range of integration to $r_2>r_1$. Similar remarks have been made by Stilley and Callaway[20] and McIlveen.[21] The step function can therefore be just ignored and taken equal to unity in the whole region.

Thus in the prescription of polarized-orbital approximation we replace the wave function Φ_i in Eq. (1) by the perturbed wave function Φ_i' given by equation (2). The elastic scattering amplitude in the polarized Glauber approximation is then given by

$$F_{ii}(\vec{q}) = f_1(\vec{q}) + f_2(\vec{q}), \tag{4}$$

with

$$f_1(\vec{q}) = (ik_i/2\pi^2)\int e^{-2r_1}\Gamma(\vec{b},\vec{r}_1)e^{i\vec{q}\cdot\vec{b}}\,d^2b\,d\vec{r}_1 \tag{5}$$

and

$$f_2(\vec{q}) = -(1/2\pi)\int d\vec{r}_1\,d\vec{r}_2\,\phi_f^*(\vec{r}_1)\times\Phi_{\mathrm{pol}}(\vec{r}_1,\vec{r}_2)V(\vec{b},z_2;\vec{r}_1)e^{i\vec{q}\cdot\vec{r}_2}\times\exp\left[-(i/k_i)\int_{-\infty}^{z_2}V(\vec{b},z_2';\vec{r}_1)dz_2'\right], \tag{6}$$

where

$$\Gamma(\vec{b},\vec{r}_1) = 1-\exp\left[(-i/k_i)\int_{-\infty}^{+\infty}V(\vec{b},z_2,\vec{r}_1)\,dz_2\right]. \tag{7}$$

Equation (5) has been obtained by writing

$$\vec{q}\cdot\vec{r}_2 = \vec{q}\cdot\vec{b}+\vec{q}\cdot\hat{k}_i z_2 \approx \vec{q}\cdot\vec{b} \tag{8}$$

and performing the integration over the z_2 coordinate of the incident electron. The amplitude f_1 has been evaluated by Franco[2] and yields

$$f_1(\vec{q}) = 2ik_i\int_0^{\pi/2}\sin^3\theta\cos\theta(\sin^2\theta-\tfrac{1}{2}q^2\cos^2\theta)\times(\sin^2\theta+\tfrac{1}{4}q^2\cos^2\theta)^{-4}\times[1-(|\cos2\theta|/\cos\theta)^{2in}|\cos2\theta|\times{}_2F_1(\tfrac{1}{2}+\tfrac{1}{2}in,1+\tfrac{1}{2}in;1;\sin^2 2\theta)]\,d\theta, \tag{9}$$

where $n=e^2/\hbar v_i$ and v_i is the velocity of incident electron.

To evaluate the polarized part of the total scattering amplitude we differentiate Eq. (6) twice with respect to q:

$$\frac{\partial^2 f_2}{\partial q^2} = -\frac{1}{2\pi^2}\int e^{-2r_1}(r_1+\tfrac{1}{2}r_1^2)(\hat{q}\cdot\hat{r}_2)^2\times e^{i\vec{q}\cdot\vec{r}_2}\cos\theta_{12}V(\vec{b},z_2,\vec{r}_1)\times\exp\left(-\frac{i}{k_i}\int_{-\infty}^{z_2}V(\vec{b},z_2',\vec{r}_1)\,dz_2'\,d\vec{r}_1\,d\vec{r}_2\right). \tag{10}$$

Using Eq. (8) and performing the z_2 integration in the integral on the right-hand side, we get

TABLE I. Differential cross-section for the elastic scattering of electrons with hydrogen atoms.

Momentum transferred squared $q^2(a_0^{-2})$	Differential cross-section $\frac{d\sigma}{d\Omega}$ (πa_0^2)		
	50 eV	100 eV	200 eV
1,−3[a]	1.7,1	1.4,1	1.3,1
5,−3	7.8,0	6.5,0	5.7,0
1,−2	5.4,0	4.5,0	4.0,0
5,−2	2.1,0	1.8,0	1.6,0
1,−1	1.3,0	1.2,0	1.0,0
5,−1	3.6,−1	3.6,−1	3.5,−1
1,0	1.8,−1	1.9,−1	2.0,−1
5,0	1.8,−2	2.5,−2	3.0,−2
1,1	5.4,−3	7.6,−3	9.1,−3

[a]Notation: $a,b = a\times10^b$.

TABLE II. Total cross section for the elastic scattering of electrons with hydrogen.

Energy of the incident electron (eV)	Total cross-section (πa_0^2)
5	7.5,0[a]
10	3.8,0
20	2.0,0
50	8.3,−1
80	5.3,−1
100	4.3,−1
200	2.2,−1

[a]Notation: $a,b = a\times10^b$.

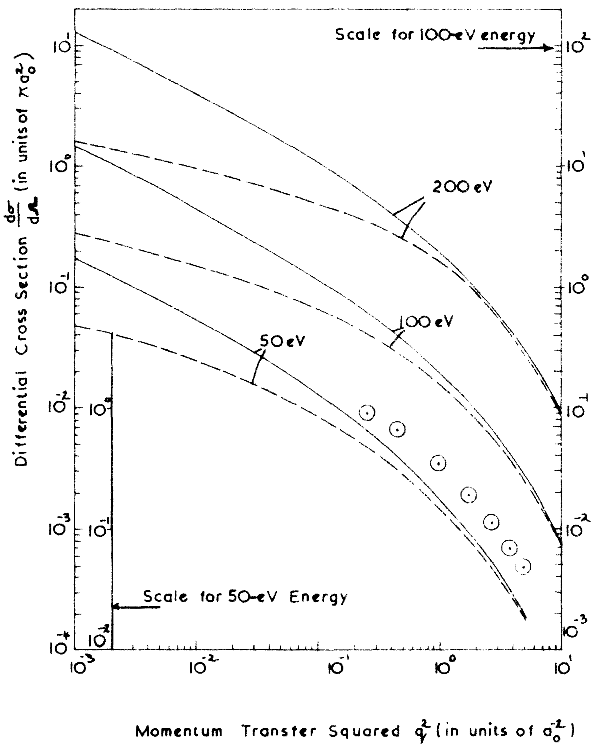

FIG. 1. Differential elastic scattering cross sections for electrons on hydrogen atoms. Solid line: present calculations using the polarized Glauber approximation; dashed line: unpolarized Glauber calculations.

$$\frac{\partial^2 f_2}{\partial q^2}=\frac{ik_i}{2\pi^2}\left(-\frac{\partial}{\partial\lambda}+\frac{1}{2}\frac{\partial^2}{\partial\lambda^2}\right)\int(\hat{q}\circ\hat{b})^2 e^{-\lambda r_1}$$

$$\times\cos\theta_{12}\Gamma(\vec{b},\vec{r}_1)e^{i\vec{q}\cdot\vec{b}}(b\,db\,d\phi_b)(s\,ds\,d\phi_s\,dz_1) \tag{11}$$

for $\lambda=2$.

Expressing $\cos\theta_{12}=\cos(\phi_s-\phi_b)$ and integrating over $d\phi_s$, $d\phi_b$, and dz_1, respectively, we get

$$\frac{\partial^2 f_2}{\partial q^2}=-\frac{ik_i}{\pi}\left(-\frac{\partial}{\partial\lambda}+\frac{1}{2}\frac{\partial^2}{\partial\lambda^2}\right)I\,, \tag{12}$$

where

$$I=\int[J_0(qb)-J_2(qb)]K_1(\lambda s)bs^2(2s/by)^{in}N\,db\,ds\,, \tag{13}$$

with

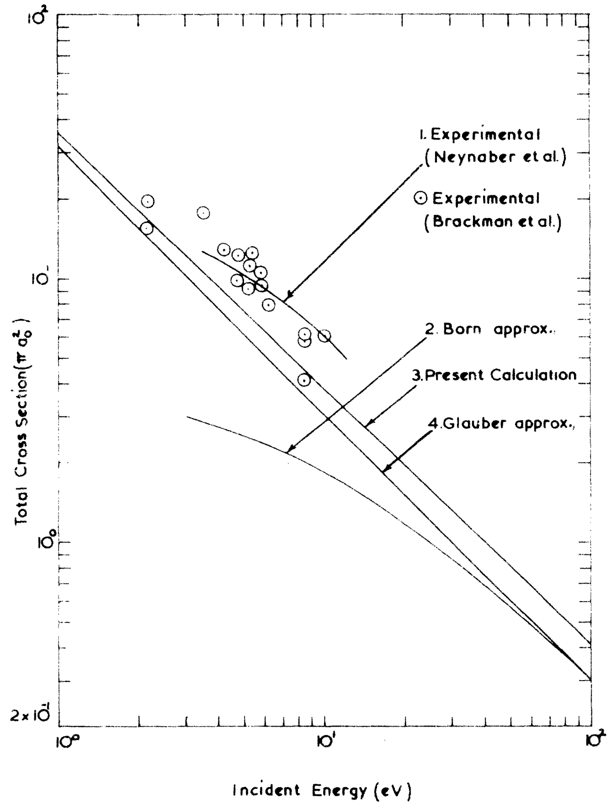

FIG. 2. Total elastic scattering cross sections for electrons on hydrogen atoms. ⊙: Experimental data, Brackman *et al.* (Ref. 27); Curve 1: Experimental data, Neynaber *et al.* (Ref. 26); Curve 2: First Born approximation calculations (Ref. 2); Curve 3: present calculations using the polarized Glauber approximation; Curve 4: unpolarized Glauber-approximation calculations of Franco (Ref. 2).

$$N=\int_0^{2\pi}d\phi_s\,\cos\phi_s(1-y\cos\phi_s)^{in} \tag{14}$$

and

$$y=2bs/(b^2+s^2)\,.$$

J_n and K_n are the Bessel and the modified Bessel functions, respectively. Following Tai *et al.*,[2] N is expressed in an analytic form

$$N=-in\pi y(1-y^2)^{in+\frac{1}{2}}\,{}_2F_1(\tfrac{1}{2}in+1,\,\tfrac{1}{2}in+\tfrac{3}{2};2;y^2)\,. \tag{15}$$

Performing the integration in I we get

$$\frac{\partial^2 f_2}{\partial q^2}=-\tfrac{1}{8}nk_i\int_0^{\pi/2}\sin^3\theta\cos\theta[\sin^2\theta+\tfrac{1}{4}q^2\cos^2\theta]^{-6}[25\sin^6\theta-57q^2\cos^2\theta\sin^4\theta-\tfrac{3}{16}q^4\cos^4\theta\sin^2\theta+\tfrac{5}{32}q^6\cos^6\theta]$$

$$\times\sin2\theta|\cos2\theta|(|\cos2\theta|/\cos\theta)^{2in}\,{}_2F_1(\tfrac{1}{2}in+1,\tfrac{1}{2}in+\tfrac{3}{2};2;\sin^2 2\theta)d\theta\,. \tag{16}$$

The differential cross section for elastic scattering is defined as

$$\frac{d\sigma}{d\Omega}(q) = |F_{ii}(\vec{q})|^2 \tag{17}$$

and the total elastic scattering cross section is

$$\sigma = \frac{2}{k_i^2}\int_0^{2k_i} q\,\frac{d\sigma}{d\Omega}(q)\,dq \quad (\pi a_0^2)\,. \tag{18}$$

Equations (17) and (18) have been used to evaluate the differential and total cross sections for electron-hydrogen elastic scattering. The inhomogeneous differential equation (16) has been solved using Numerov's method[22] and with the following boundary conditions

$$\left.\begin{aligned} f_2(q) &= 0, \\ f_2'(q) &= 0, \end{aligned}\right\} \quad q \to \infty\,. \tag{19}$$

The solution of Eq. (16) is therefore started from a large value of q and continued inwards.

III. RESULTS AND DISCUSSION

The results for the differential and the total cross sections are given in Tables I and II. As a check to our calculations we have reproduced the results of Franco[2] using Eq. (9).

In Fig. 1 we show a plot of the differential cross sections with respect to the momentum transfer squared for three incident energies 50, 100, and 200 eV. The essential features for all the three energies are seen to be similar. We observe that the inclusion of polarization effects in Eq. (1) causes a large increase in the differential cross sections at low values of the momentum transfer. Beyond a value of $q \approx 2a_0^{-1}$, the two curves with and without the polarization tend to merge. The relative differential cross sections for the elastic scattering of hydrogen were measured by Tai *et al.*[23] and compared with the theory.[24] Recently, absolute differential cross sections have been measured by Teubner *et al.*[25] at 50-eV energy. The experimental data of Teubner *et al.* are subject to a ±35% error and are shown in Fig. 1. We note that in the range of angles in which the data are available the present calculations are in better agreement with the data compared to the Glauber-approximation calculation without the polarization included. A better comparison would be possible if the data are obtained at lower values of the scattering angles. However, the rise in differential cross sections at low-scattering angles with the inclusion of polarization effects is consistent with the other theoretical predictions for hydrogen and helium.[11-13]

The total integrated elastic scattering cross sections are shown in Fig. 2. The Born calculations and the experimental data of Neynaber *et al.*[26] and Brackman *et al.*[27] are also plotted. We observe that the present polarized-orbital Glauber calculations are in better agreement with the data compared to the ordinary Glauber calculations, in the range of energies in which the data are available. At high energies (not shown in the Fig. 2) the two Glauber calculations merge showing that the polarization effects become less important when the incident energy is very large.

ACKNOWLEDGMENTS

The author is grateful to Professor D. R. Bates for providing the facilities and for the hospitality and to Professor P. G. Burke for helpful discussions. Financial assistance from Leverhulme Trust is acknowledged.

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*Leverhulme visiting fellow: on leave of absence from Physics Department, University of Roorkee, Roorkee, India.

*Work supported by the U. S. Office of Naval Research, under Contract No. N00014-69-C-0035.

[1]R. J. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1959) Vol. 1, p. 315.

[2]V. Franco, Phys. Rev. Lett. 20, 709 (1968); H. Tai, R. H. Bassel, E. Gerjuoy, and V. Franco, Phys. Rev. A 1, 1819 (1970); A. S. Ghosh and N. C. Sil, Indian J. Phys. 43, 490 (1969); Indian J. Phys. 44, 153 (1970); A. S. Ghosh, P. Sinha, and N. C. Sil, J. Phys. B 3, L58 (1970); A. N. Tripathi, K. C. Mathur, and S. K. Joshi, Phys. Lett. A 36, 161 (1971).

[3]B. K. Thomas and E. Gerjuoy, J. Math. Phys. 12, 1567 (1971).

[4]A. Tenny and A. C. Yates, Chem. Phys. Lett. 17, 324 (1972).

[5]V. Franco, Phys. Rev. A 1, 1705 (1970); Phys. Rev. Lett. 26, 1088 (1971).

[6]F. W. Byron, Jr., Phys. Rev. A 4, 1907 (1971).

[7]A. C. Yates and A. Tenny, Phys. Rev. A 6, 1451 (1972).

[8]K. C. Mathur, A. N. Tripathi, and S. K. Joshi, Phys. Rev. A 5, 746 (1972); J. Phys. B 4, L39 (1971).

[9]A. N. Tripathi, K. C. Mathur, and S. K. Joshi, J. Chem Phys. 58, 1384 (1973).

[10]B. H. Bransden and J. P. Coleman, J. Phys. B 5, 537 (1972).

[11]A. Temkin, Phys. Rev. 116, 358 (1959); A. Temkin and J. C. Lamkin, Phys. Rev. 121, 788 (1961).

[12]R. W. LaBahn and J. Callaway, Phys. Rev. 135, A1539 (1964); Phys. Rev. 147, 28 (1966); Phys. Rev. 180, 91 (1969).

[13]S. P. Khare and B. L. Moiseiwitsch, Proc. Phys. Soc. Lond. 85, 821 (1965).
[14]M. D. Llyod and M. R. C. McDowell, J. Phys. B 2, 1313 (1969).
[15]S. P. Khare and P. Shobha, J. Phys. B 4, 208 (1971); Phys. Lett. A 31, 571 (1970).
[16]K. C. Mathur, A. N. Tripathi, and S. K. Joshi, Phys. Lett. A 38, 159 (1972).
[17]A. N. Tripathi, K. C. Mathur, and S. K. Joshi, Phys. Rev. A 4, 1873 (1971).
[18]Vo Ky Lan, N. Feautrier, M. Le. Dourneuf, and H. Van Regemorter, J. Phys. B 5, 1506 (1972).
[19]W. M. Duxler, R. T. Poe, and R. W. LaBahn, Phys. Rev. A 4, 1935 (1971).
[20]J. L. Stilley and J. Callaway, Ap. J. 160, 245 (1970).
[21]W. A. McIlveen, Ph.D. thesis (Queen's University, Belfast, Northern Ireland, 1972) (unpublished).
[22]D. R. Hartree, *The Calculation of Atomic Structures* (Wiley, New York, 1957), p. 71.
[23]H. Tai, P. J. Teubner, and R. H. Bassel, Phys. Rev. Lett. 22, 1415 (1969); Phys. Rev. Lett. 23, 453(E) (1969).
[24]The calculations of Tai *et al.* based on the Glauber theory do not seem to agree with the corresponding results of Franco (Ref. 2).
[25]P. J. O. Teubner, C. R. Llyod, and E. Weigold, J. Phys. B 6, L134 (1973).
[26]R. H. Neynaber, L. L. Marino, E. W. Rothe, and S. M. Trujillo, Phys. Rev. 124, 135 (1961).
[27]R. T. Brackman, L. W. Fite, and R. H. Neynaber, Phys. Rev. 112, 1157 (1958).