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Elastic scattering of electrons by hydrogen atoms at intermediate energies

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The elastic scattering of electrons with hydrogen atoms at incident electron energies of 200–680 eV is studied using a two-potential method and the variable-charge Coulomb-projected Born approximation. Effects of exchange and polarization are included. The results obtained are found to be in reasonable agreement with recent experimental measurements. Comparison is made with other available theoretical calculations.

I. INTRODUCTION

The study of the scattering of electrons by hydrogen atoms has been made quite frequently in recent years. In the intermediate and high energies, there is much current interest in the study of electron-hydrogen scattering, as the absolute measurements for the cross sections have been performed over the last few years. Several attempts have been made to study the intermediate-energy region by suitably extending the range of the high-energy methods towards intermediate energy. The eikonal-Born-series (EBS) method[1] developed by Byron and Joachain has been applied with much success to study the electron-atom scattering problem in the high- and intermediate-energy region. Another approach apparently very similar to EBS and referred to as the modified Glauber approach, suggested by Byron and Joachain[2] and exploited recently by Gien,[3] has also been quite successful in predicting the electron-hydrogen and helium elastic and inelastic collision cross sections in the same energy region. In the study of inelastic scattering of electrons at intermediate energies, the distorted-wave method has been used with considerable success by Madison and Shelton,[4] Calhoun *et al.*,[5] Meneses *et al.*,[6] Baluja and McDowell,[7] Baluja *et al.*,[8] and Scott and McDowell.[9] Following Bransden and Coleman,[10] Bransden *et al.*,[11] and Winters *et al.*[12] have used a second-order-potential (SOP) method in the study of the elastic and inelastic scattering of hydrogen and helium atoms by charged-particle impact. Following Burke *et al.*,[13] Kingston *et al.*,[14] and Fon *et al.*[15] have used the close-coupling method and the pseudostate approximation in the study of the scattering of electrons by hydrogen atoms. Very recently, Fon *et al.*[16,17] have followed the R-matrix approach to study the elastic scattering of electrons from inert gases and atomic hydrogen. Kingston and Walters[18] have recently used a distorted-wave second-Born approximation (DWSBA) to study the elastic and inelastic scattering of electrons with hydrogen atoms.

Among the first-order theories, the first-Born approximation (FBA) is known to be inadequate in the intermediate-energy region. Attempts to improve the FBA by including the second-order effects have been made by Jhanwar *et al.*,[19] Geltman,[20] and Geltman and Hidalgo[21] introduced the Coulomb-projected Born approximation by taking the complete Coulomb interaction of the incident particle with the target nucleus in the unperturbed part of the Hamiltonian and treating all other interactions as perturbation. Recently, Junker[22] has suggested a more general class of distorted-wave Born approximation known as the modified-Born model in which the screening due to the bound electron has been taken into account by introducing a screening parameter. Stauffer and Morgan[23] proposed a generalization of the Coulomb-projected Born approximation (GCPBA) by allowing only part of the nuclear charge to act directly on the incident particle. Gupta and Mathur[24] used the method of Junker[22] to study the elastic scattering of electrons by hydrogen atoms. They included exchange (through Ochkur approximation) and polarization following the polarized-orbital method of Temkin and Lamkin.[25] Also, Gupta and Mathur[26] and Sharma *et al.*[27] have used a two-potential modified-Born model with considerable success in the study of excitation of hydrogen and helium atoms by electron impact. Recently, Schaub-Shaver and Stauffer[28] have modified the GCPBA by introducing a screening parameter which varies with the distance of the incident particle leading to a variable-charge Coulomb-projected Born approxi-

mation (VCCPBA). They have calculated the total cross sections for the elastic and total as well as differential cross sections for the inelastic electron-hydrogen collisions.

In the present paper we have extended the approach of Schaub-Shaver and Stauffer.[28] We follow a two-potential method[29] where we take the scattering-particle wave functions to be distorted both in the initial and final channels (Schaub-Shaver and Stauffer[28] in their method consider distortion only in the final channel). Further, we also consider the polarization effects besides exchange. For calculating the distorted waves we, however, adopt the same procedure as suggested by Schaub-Shaver and Stauffer.[28]

II. THEORY

The Hamiltonian for the electron plus hydrogen-atom system is given by (atomic units are used throughout)

$$H=-\tfrac{1}{2}\nabla_1^2-\tfrac{1}{2}\nabla_2^2-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{r_{12}}\ , \tag{1}$$

where $\vec{r}_1$ and $\vec{r}_2$ are the position coordinates of the atomic and incident electrons, respectively, and ∇_1^2 and ∇_2^2 are the respective kinetic energy operators.

Writing $H=H_0+V$, one expresses ϕ_n and ψ_n as the solutions of the following equations:

$$H_0\phi_n=E\phi_n\ ,$$

$$H\psi_n=E\psi_n\ .$$

E is the total energy. H_0 is the unperturbed Hamiltonian and $V(=1/r_{12}-1/r_2)$ is the total interaction potential of the incident electron with the target. The T-matrix element for the excitation of the target atom from an initial state i to a final state f is given by

$$T_{i-f}=\langle\phi_f\mid V\mid\psi_i^{(+)}\rangle\ . \tag{2}$$

The superscripts $(\pm)$ refer to the outgoing and incoming wave boundary conditions, respectively.

In the two-potential model (TPMB), we divide the Hamiltonian as

$$H=H_2+W\ ,$$

where $H_2=H_0+U$ with $U=-\zeta(r_2)/r_2$ and

$$W=-\frac{[1-\zeta(r_2)]}{r_2}+\frac{1}{r_{12}}\ .$$

$\zeta(r_2)$ is a screening parameter which depends on the location of the incident particle.

Let χ_n be the solution of the Schrödinger equation

$$H_2\chi_n=E\chi_n\ . \tag{3}$$

Writing

$$\chi_n(\vec{r}_1\vec{r}_2)=F_n(\vec{r}_2)u_n(\vec{r}_1)\ ,$$

Eq. (3) becomes

$$(H_0+U)F_n(\vec{r}_2)u_n(\vec{r}_1)=E\,F_n(\vec{r}_2)u_n(\vec{r}_1)\ , \tag{4}$$

$u_n(\vec{r}_1)$ are the target wave functions and $F_n(\vec{r}_2)$ are the distorted-wave functions for the scattered particle, which satisfy the equation,

$$\left[\frac{1}{2}\nabla_2^2+\frac{\zeta(r_2)}{r_2}+\frac{1}{2}k_n^2\right]F_n(\vec{r}_2)=0\ . \tag{5}$$

The T-matrix element in the TPMB approximation is then written as[29]

$$T=\langle\phi_f\mid U\mid\chi_i^{(+)}\rangle+\langle\chi_f^{(-)}\mid W\mid\psi_i^{(+)}\rangle\ , \tag{6}$$

where

$$\phi_f(\vec{r}_1\vec{r}_2)=e^{i\vec{k}_f\cdot\vec{r}_2}u_f(\vec{r}_1)\ . \tag{7}$$

The first matrix element on the right side in Eq. (6) will vanish for excitation process due to the orthogonality of the target wave functions.

Considering the perturbation of the target system by the incident particle, we express the trial wave function $\psi_i^{(+)}$ of Eq. (6) (which includes both exchange and polarization terms) in the following form:

$$\psi_i^{(+)}(\vec{r}_1\vec{r}_2)=F_i^{(+)}(\vec{r}_2)[u_i(\vec{r}_1)+u_{\rm pol}(\vec{r}_1\vec{r}_2)]\pm F_i^{(+)}(\vec{r}_1)[u_i(\vec{r}_2)+u_{\rm pol}(\vec{r}_1\vec{r}_2)]\ , \tag{8}$$

where F_n's (when expanded in spherical harmonics) can be written as

$$F_n^{(\pm)}(\vec{r}_2)=k_n^{-1/2}r_2^{-1}\sum_{l=0}^{\infty}(2l+1)i^l\exp[\pm i\delta_l(k_n^2)]u_l(k_n,r_2)P_l(\cos\hat{k}_n\cdot\hat{r}_2)\ . \tag{9}$$

δ_l is the phase shift of the lth partial wave, u_l are the radial functions, and P_l are the Legendre polynomials.

$u_{\text{pol}}(\vec{r}_1,\vec{r}_2)$ is defined by Temkin and Lamkin.[25] We include the dipole term only. Exchange polarization is neglected and the Bonham-Ochkur[30,31] approximation is used for the first-order exchange term.

Our numerical methods were checked by reproducing Tables I and II of Schaub-Shaver and Stauffer.[28] The infinite summations over partial waves involved in any of the matrix elements, for example, M, in Eq. (6) are carried out exactly up to a value l (say l_0) for which a matrix element M_{l0} becomes nearly equal to the corresponding Born matrix element $M^B_{l_0}$. We can thus write M in the following standard way:

$$M=\sum_{l=0}^{l_0} M_l+M^B-\sum_{l=0}^{l_0} M_l^B\,, \tag{10}$$

where M^B is the usual full-Born result.

The differential cross section for a collision in which the hydrogen atom is excited from an initial state i to a final state f is obtained by

$$\frac{d\sigma}{d\Omega}=\frac{1}{4\pi^2}\frac{k_f}{k_i}\left(\tfrac{1}{4}\,|\,T_+\,|^2+\tfrac{3}{4}\,|\,T_-\,|^2\right), \tag{11}$$

where the subscripts correspond to the $\pm$ signs in Eq. (8) and $\vec{k}_i$ and $\vec{k}_f$ are the momentum vectors of the incident and the scattered particle, respectively.

The total cross section is given by

$$\sigma=\int \frac{d\sigma}{d\Omega}d\Omega\,. \tag{12}$$

III. RESULTS AND DISCUSSION

Figures 1–4 and Tables I and II show the results of our calculations for the elastic scattering of electrons by atomic hydrogen at incident particle energies of 200, 300, 400, and 680 eV. In the figures we have compared our results (P with polarization and $P1$ without polarization) for the differential cross sections (DCS) with the available experimental data of Williams[32] and van Wingerden *et al.*[33] We also show a comparison with the calculations of Kingston and Walters[18] obtained in the distorted-wave second-Born approximation (DWSBA) and the available eikonal-Born-series (EBS) calculations of Byron and Joachain.[34] For the sake of clarity of the figures, we give some of the other available theoretical results for the differential cross sections in Table I at 200 eV.

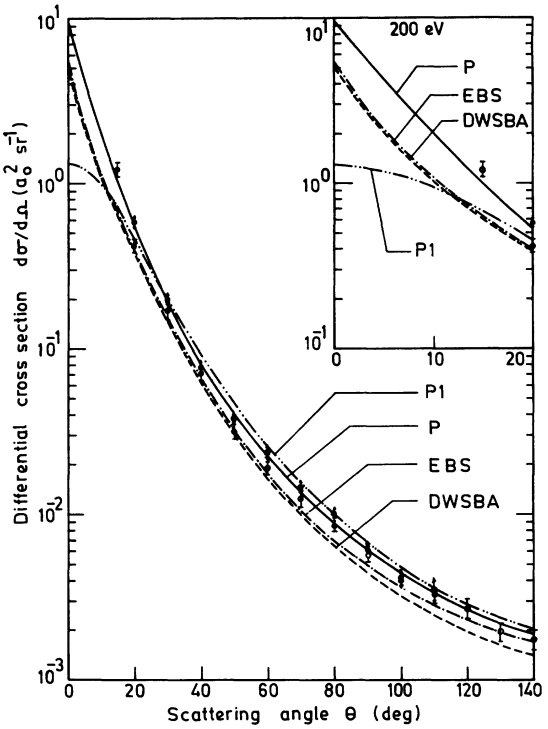

FIG. 1. Differential cross section for e^--H elastic scattering at an incident electron energy of 200 eV. ——, present calculation (curve P); —··—··—, present calculation without polarization (curve $P1$); — — —, distorted-wave second-Born approximation (curve DWSBA); —·—·—·, eikonal-Born-series approximation (curve EBS); ⊕, experimental data of Williams (Ref. 32); ⊕ experimental data of Wingerden *et al.* (Ref. 33).

Figure 1 shows the results at incident electron energy of 200 eV. Our results are compared with the EBS and DWSBA calculations and also with the experimental data. The results (P) are in fair agreement with the data over a wide angular range. In the small-angle region (below 20°) both EBS and DWSBA (which are almost identical) estimate the cross sections much lower than the experiment as well as our calculations (P). We also see that our results (P) are in better agreement with the experimental results of van Wingerden *et al.*[33] than with the data of Williams[32] in the lower-angle region. The EBS and DWSBA both are in satisfactory agreement with the experimental data of Williams[32] from 20° to 50°. Beyond 50° our results (P) show a better agreement with the data compared to EBS and DWSBA calculations. From the figure we notice that for angles ($\approx$ up to 20°) there is a substantial difference in the curves P and $P1$,

TABLE I. Comparison of experimental and theoretical differential cross sections (in units $a_0^2 sr^{-1}$) for the elastic scattering of electrons by atomic hydrogen at 200-eV energy. [$a^{-b}=a\times10^{-b}$. The numbers in the parenthesis are the total errors in the last significant digits. The results for EBS, SOP, and the calculation of Jhanwar and Khare, have been taken from the paper of van Wingerden *et al.* (Ref. 33).]

Angle θ°	Williams[a]	van Wingerden *et al.*[b]	*P* present results	DWSBA Kingston and Walters[c]	Fon *et al.*[d]	CPBP Gupta and Mathur[e]	EBS Byron and Joachain[f]	Jhanwar and Khare	SOP Winters *et al.*[g]
10			2.05	1.05	8.42^{-1}	1.92			
20	0.419(40)	0.577(48)	5.37^{-1}	3.86^{-1}	3.76^{-1}	0.49	4.00^{-1}	3.79^{-1}	3.85^{-1}
30	0.172(17)	0.200(15)	1.86^{-1}	1.50^{-1}	1.59^{-1}	0.16	1.54^{-1}	1.56^{-1}	1.50^{-1}
40	0.0706(68)	0.0774(73)	7.98^{-2}	6.35^{-2}	7.09^{-2}	0.65^{-1}	6.57^{-2}	6.80^{-2}	6.21^{-2}
50	0.0314(32)	0.0379(32)	3.97^{-2}	3.05^{-2}	3.48^{-2}	0.31^{-1}	3.18^{-2}	3.29^{-2}	2.98^{-2}
60	0.0187(19)	0.0237(23)	2.20^{-2}	1.65^{-2}	1.89^{-2}	0.17^{-1}	1.74^{-2}	1.77^{-2}	1.64^{-2}
70	0.0125(14)	0.0145(13)	1.33^{-2}		1.13^{-2}	0.99^{-2}	1.05^{-2}	1.05^{-2}	9.69^{-3}
80	0.00859(92)	0.0100(10)	8.65^{-3}		7.24^{-3}	0.64^{-2}	6.89^{-3}	6.74^{-3}	6.25^{-3}
90	0.00584(61)	0.0062(8)	5.96^{-3}	4.35^{-3}	4.97^{-3}	0.44^{-2}	4.85^{-3}	4.63^{-3}	4.20^{-3}
100	0.00412(42)	0.00411(51)	4.34^{-3}		3.62^{-3}	0.32^{-2}	3.61^{-3}		3.12^{-3}
110	0.00323(31)	0.00347(60)	3.32^{-3}	2.45^{-3}	2.76^{-3}		2.82^{-3}		
120	0.00272(35)		2.65^{-3}	1.97^{-3}	2.20^{-3}	0.20^{-2}			

[a]Reference 32.
[b]Reference 33.
[c]Reference 18.
[d]Reference 15.
[e]Reference 24.
[f]Reference 34.
[g]Reference 12.

showing that the contribution of polarization is quite significant in this region. This feature is exhibited at all the energies studied here. For larger angles, there is only a slight difference between the curves P and $P1$, which become less as the energy increases.

In Table I we also compare our present results (P) at 200-eV energy with (i) the calculations of Winters *et al.*[12] based on the second-order-potential (SOP) method, (ii) the calculation of Gupta and Mathur[24] based on the Coulomb-projected Born-polarization (CPBP) approach, (iii) the calculation of Jhanwar and Khare (unpublished), and (iv) the calculations of Fon *et al.*[15] based on the pseudo-state approximation. We find that all the other calculations shown in table are below our present results (P) over the entire angular range. An overall comparison with experiment shows that in the entire angular range our results (P) yield satisfactory agreement with the data.

Figure 2 shows the results at 300-eV energy where we compare our results (P) with the DWSBA calculation. Here also the DWSBA results are below our results in the entire angular range. In the lower-angle region (up to 20°) the present calculation differs considerably from the DWSBA, whereas in the larger-angle region (beyond 20°) this difference is small.

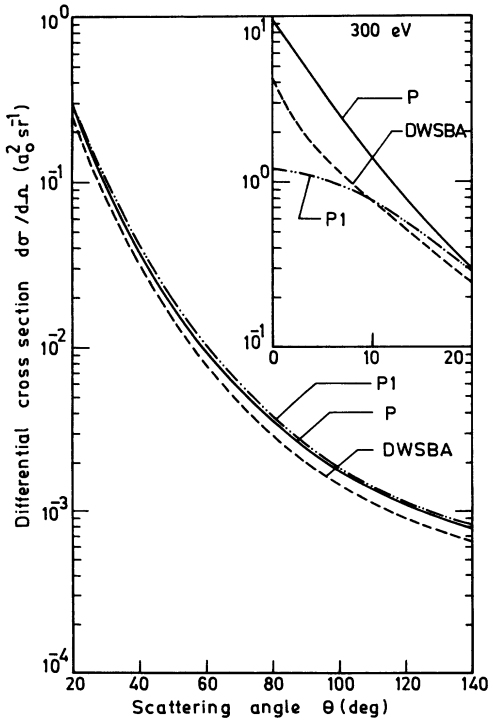

FIG. 2. Differential cross section for e^--H elastic scattering at incident electron energy of 300 eV. Caption is the same as described for Fig. 1.

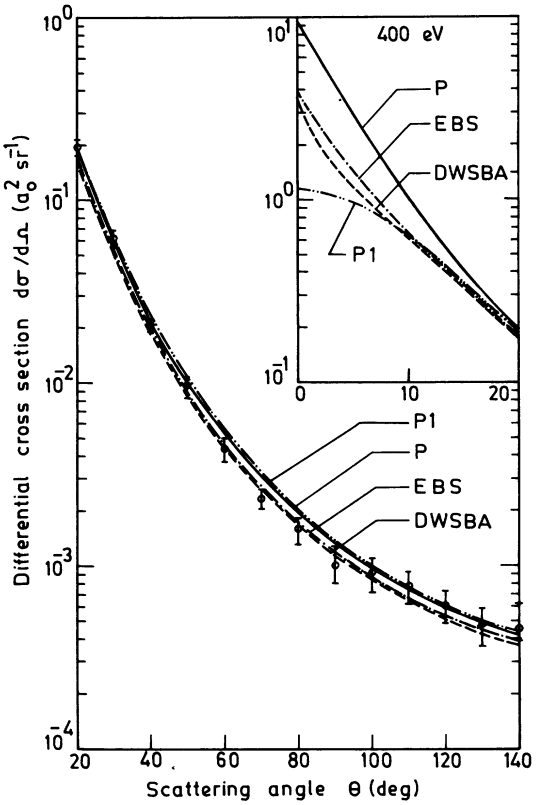

FIG. 3. Differential cross section for e^--H elastic scattering at an incident electron energy of 400 eV. Caption is the same as described for Fig. 1.

In Figs. 3 and 4 we show our results at 400 and 680-eV energy, respectively. At 400 eV we compare our results (P) with the DWSBA and EBS calculations and also with the data of Williams.[32] Our results (P) are in close agreement with the data for all angles except for the angular range 50°—90°. At 680-eV energy, also, where we compare our results (P) with the available DWSBA calculation and the data of Williams,[32] the present calculation (P) yields a good agreement with the data. There seems to be no particular reason for the discrepancy between our results (P) and the data at 400 eV for the angular range 50°—90°. As we have seen that, at other energies (200 and 680 eV) our results (P) are in fairly good agreement with the data in the whole angular range, we expect our calculation to be reasonable at 400 eV in the whole range. We feel that the above discrepancy at 400 eV for the angular range 50°—90° can be

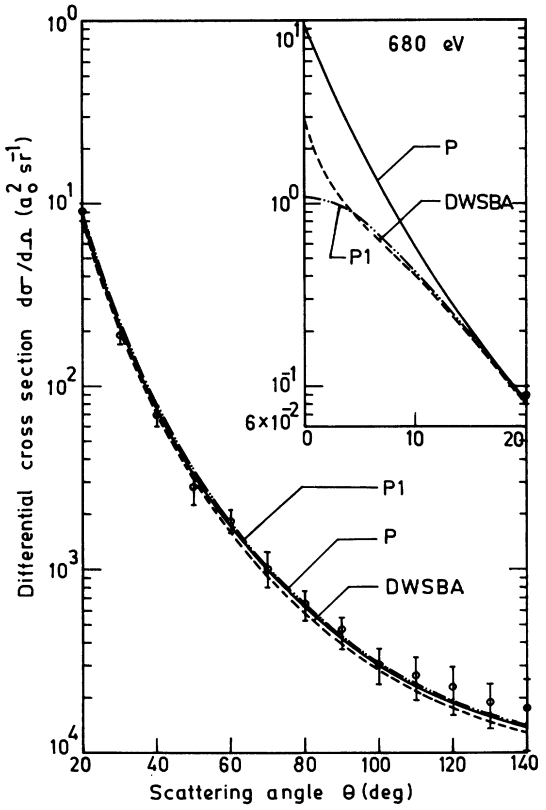

FIG. 4. Differential cross section for e^--H elastic scattering at an incident electron energy of 680 eV. Caption is the same as described for Fig. 1.

clarified if some other data become available at this energy in future.

From the figures we notice that the difference between our calculations and those under DWSBA and EBS narrow down (in the large-angle region) as energy increases from 200 to 680 eV. The large difference between the present calculations and the DWSBA and EBS calculations at lower angles may be due to the absorption effects which have not been considered in the present calculation. The forward peak in the present calculations arises from the polarization contribution.

In Table II we show our results for the electron-hydrogen total elastic scattering cross sections obtained by integrating the DCS over all angles [Eq. (12)]. Here we compare our present results at 200, 300, 400, and 680-eV energies (at lower energies the present method of calculation is not expected to be reliable since the VCCPBA is essentially a high-energy approximation) with the available experimental data of Williams[32] and van Wingerden *et al.*,[33] and theoretical calculations of (i) the VCCPBA calculation of Schaub-Shaver and Stauffer[28] (SSS), (ii) DWSBA calculation of Kingston and Walters,[18] (iii) pseudostate approximation calculation of Fon *et al.*,[15] (iv) EBS results of Byron and Joachain,[34] (v) SOP calculation of Winters *et al.*,[12] and (vi) the Born approximation results. For the sake of comparison with SSS results, we also show our results obtained without exchange. Our results at 200 eV are in better accord

TABLE II. Comparison of total cross sections for the elastic scattering of electrons by atomic hydrogen (in units of πa_0^2).

Energy (eV)	Williams[a]	van Wingerden *et al.*[b]	Present Without exchange	Present With exchange	VCCPBA Schaub-Shaver and Stauffer[c]	DWSBA Kingston and Walters[d]	Fon *et al.*[e]	EBS Byron and Joachain[f]	SOP Winters *et al.*[g]	First Born[h]
200	0.20	0.25	0.29	0.31	0.67	0.19	0.18	0.20	0.18	0.15
300			0.19	0.20		0.12		0.12		0.10
400	0.06		0.14	0.14		0.09		0.09		0.08
680			0.08	0.08		0.05				0.04

[a]Reference 32.
[b]Reference 33.
[c]Reference 28.
[d]Reference 18.
[e]Reference 15.
[f]Reference 34.
[g]Reference 12.
[h]Reference 18.

with the experimental data of van Wingerden *et al.*[33] than with the data of Williams.[32] At all the energies our results are slightly higher than the experimental data. The SSS calculation yields a very high value of the cross section. The reason for this may be that in the SSS calculations the total cross sections are obtained from the phase shifts [Eq. (46) of their paper] and not by integrating the DCS over all angles. Since the phase shifts are calculated from the potential U alone, the effect of the remaining interaction potential W does not seem to be accounted in their calculations for the total elastic cross sections.

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