ELASTIC SCATTERING OF ELECTRONS BY SOME LIGHT ATOMS AND MOLECULES IN THE FORWARD DIRECTION

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ABSTRACT

Elastic scattering of electrons by hydrogen, helium and lithium atoms are studied in the forward direction within the framework of Born approximations. Using the independent atom model and independent united atom model, the forward differential scattering cross-sections for hydrogen molecule are studied from the present hydrogen and helium results. The present results are more accurate when compared with other results.

INTRODUCTION

In recent years a number of theoretical models[1,2] have been proposed to study the electron-atom scattering processes. Though these models[1,2] are expected to be accurate, yet practically all the results are found to deviate from model to model in the forward direction (q or $\theta = 0$) and a few of these models are difficult to extend the studies for other atoms. Especially, in the forward direction, a good comparison of differential cross-sections (DCS) is not only important from theoretical point of view but also useful for experimentalists to interpret their results. Motivated by this and encouraged by the author's earlier work[3], the scattering of electrons by H, He, Li and H_2 in the forward direction has been studied.

In the present study an analytical expression for the forward elastic scattering amplitude is derived within the framework of Born approximations[4]. The forward elastic DCS for scattering of electrons by H, He, Li and H_2 are studied by using the present scattering amplitude at incident energy $(E) \leq 1000$ eV. The independent atom model (IAM) and the independent united atom model (IUAM) are used to obtain the H_2 results through H and He results. Ochkur[5] exchange effects are considered in the present studies. The present DCS results for H, He, Li and H_2 are shown in table 1 along with other recent results[1,6,7]. In table 2, we present the real part of the forward elastic scattering amplitude for electron –He as compared with other results[8,9]. The present results are in good agreement with earlier results[7]. In table 3, individual contributions of the Born and exchange terms for H, He, Li are given.

THEORY

Throughout the work automic units ($\hbar = m = e = 1$) are used[4]. Basic formulation of the Born theory was discussed earlier[4]. The direct scattering amplitude in this Born approximation can be given as:

$$F(\theta) = F_{B1} + F_{B2} + F_{B3} \pm F_{BE} \qquad (1)$$

where F_{B1}, F_{B2}, F_{B3} and F_{BE} terms in (1) are the Born approximations and first order Ochkur[5] Born exchange term respectively. In the forward direction (q or $\theta = 0$) the F_{B3} term in (1) becomes zero[10]. Now the scattering amplitude (1) can be written as

$$F(0) = F_{B1} + \mathrm{Re}\ F_{B2} + \mathrm{Im}\ F_{B2} \pm F_{BE}, \qquad (2)$$

where the second and third terms in (2) are the real and imaginary parts of the second Born approximation. The + or − before F_{BE} in (2) corresponds to singlet and triplet states of the target, these signs and other multiple factors are adjusted properly in the final calculations. The second Born term in the forward direction can be obtained in the closed form by putting momentum transfer (q) equal to zero in the second Born approximation[4]. Now the closed form of the real and imaginary parts of the second Born can be written as

$$\mathrm{Re}\ F_{B2} = \frac{4\pi}{K_i} \sum_{m=0}^{n'} \sum_{l=1}^{n} D'''(y_l) N(l) \left[\frac{8}{y_l^5} + \frac{1}{K_i} \left\{ \frac{3}{y_l^4} - \frac{20}{y_l^6} DE \right\} \right] \qquad (3)$$

$$\mathrm{Im}\ F_{B2} = \frac{8}{K_i} \sum_{m=0}^{n'} \sum_{l=1}^{n} D'''(y_l) N(l) \left[\frac{1}{y_l^4} \log \left\{ 1 + \left(\frac{K_i y_l}{DE} \right)^2 \right\} \right], \qquad (4)$$

where, $N(l)$'s, Y_l's and n, n' in (3) and (4) are constants related to the normalization and exponential parameters of the target wavefunctions[11–13] all

Table 1 *Forward elastic DCS (a_0^2 sr^{-1}) for scattering of electrons by H, He, Li and H_2*

E	Hydrogen		Helium		Lithium	Hydrogen molecule		
(in eV)	Present	Ref. 1	Present	Ref. 11	present	Present IAM	Ref. 7	Present IUAM
100	8 033	8.22	4.787	4 03	284.31	12.516	8.25	9.574
200	5.382	5.59	3 106	2.99	191 05	8.600	7.37	6 212
300	4.344	4 50	2.496	2.48	153.33	7.036	7.09	4.992
400	3.766	3.88	2.155	2.18	132.21	6.148	6.95	4.310
500	3.390	—	1.946	1.98	118.48	5.564	—	3.892
600	3.122	—	1.792	—	108.75	5.148	—	3.584
700	2.920	—	1.685	1.72	101.43	4.824	6.77	3.370
800	—	—	1.591	—	—	—	—	3.182
900	—	—	1.518	—	—	—	—	3.036
1000	—	—	1.460	—	—	—	6.70	2.920

Table 2 *Present real part of the scattering amplitude (a.u.) for electron-Helium elastic scattering at $E \leq 1000$ eV*

E (in eV)	Present results	Ref. 9	Ref. 8
100	1.911	1.91	1.91
200	1.519	1.54	1.71
300	1.365	1.39	1.48
400	1.275	1.30	1.36
500	1.216	1.24	1.29
600	1.176	—	—
700	1.143	—	—
800	1.118	—	—
900	1.096	—	—
1000	1.078	—	—

these constants are given earlier[14] and K_i in (3, 4) is the incident momenta of the scattered electron. $D^m(Y_l)$ stands for the mth other differentiation with respect to Y_l and DE is excitation energy for H, He and Li atoms[11-13]. Similarly the analytical expressions for F_{B1} and F_{BI} in the forward direction can be obtained as

$$F_{B1} = -\frac{1}{2\pi}\int \psi_i^*(r)\ v\ \psi_i(r)\ dr \tag{5}$$

$$F_{BI} = -\frac{2}{K_i^2}\int \psi_i^*(r)\ \psi_i(r)\ dr, \tag{6}$$

where $\psi_i(r)$, $\psi_i(r)$ and v in (5) and (6) are the initial and final state wavefunctions of the target and interaction potential between the incident electron

Table 3 *Individual contributions of scattering amplitude (2) in a.u. for elastic scattering of electrons by H, Li and He atoms at $E \leq 1000$ eV*

E	Hydrogen			Lithium			Helium		
(in eV)	Re F_{B2}	Im F_{B2}	F_{BE}	Re F_{B2}	Im F_{B2}	F_{BE}	Re F_{B2}	Im F_{B2}	F_{BE}
100	1.182	1.632	0.272	2.265	14.464	0.273	0.848	1.066	0.272
200	0.830	1.333	0.136	1.596	11 322	0.136	0.592	0.894	0.136
300	0 677	1.174	0 091	1.300	9.767	0.091	0.480	0.799	0.091
400	0.585	1.069	0.068	1.125	8.780	0.069	0.415	0.729	0.068
500	0.523	0.994	0.054	1.005	8.076	0.055	0.370	0 685	0.054
600	0.477	0.935	0.045	0.917	7.539	0 046	0.337	0.645	0.045
700	0.441	0.887	0.039	0.849	7.110	0.039	0.312	0.617	0.038

F_{B1} values for hydrogen, lithium and helium atoms are 1.0, 6.265 and 0.792 at all E values and target atom. Using (2), (3), (4), (5) and (6) the DCS in the forward direction can be obtained as

$$d\sigma/d\Omega|_{\theta=0} = |F(0)|^2. \quad (7)$$

The DCS for H, He and Li atoms are obtained at $E \leqslant 1000$ eV, $\bar{e}$-H_2 results are also studied by using IAM[6] and IUAM[6]. These present results[1,7,11]. In table 2 the real part of the present forward elastic scattering amplitude (3) for electron Helium scattering is given along with other results[8,9]. In table 3, individual terms of (2) are given.

RESULTS AND DISCUSSION

The present DCS results for H, He, Li and H_2 molecule are given in tables 1, 2 and 3 along with other results. Unfortunately, experimental data are not available to compare our results. The present results are discussed below with other theoretical studies.

Hydrogen: These results are given in table 1, along with the unitarized eikonal Born series (UEBS) results[1]. The present H results are slightly smaller than the UEBS[1] and approaches to the eikonal Born series (EBS) results[9] (not shown in table). Higher order exchange terms are considered in UEBS[1] whereas in the present studies only the first order exchange term is considered, because of this reason the present results are slightly smaller than the UEBS[1] results.

Helium: In table 2, the real part of the present scattering amplitude (2) for helium is compared with the EBS[9,11] and dispersion relation results[8]. The present real part is found to be in good agreement with these compared results. In table 1. DCS for He are compared with the optical model results[11]. The present He results are in good agreement with these compared optical model results[11].

Hydrogen molecule: In table 1, the present IUAM and IAM results for H_2 are compared with the other Born results[7]. The present IAM values are higher than the IUAM values and nearer to the compared results. Basically, IUAM was found[3,6] to be better than the IAM. The compared Born results are smaller than the experimental results[7] at $\theta \leq 20$. In spite of the simplicity of the present approach, it is expected that it would provide a reasonable description of the e-H_2 scattering processes.

Lithium: These results are given in table 1 at $E \leq 1000$ eV. Unfortunately no other data are available at $E \leq 1000$ eV to compare our present results. It is expected that the Li results would compare nicely with the future experimental results.

Finally by comparing the present results with other results[1,7,9] (tables 1 and 2), we are led to the conclusion that the present Born technique is computationally simple and contains an additional term of order K_i^2 in the real part (3). Due to this term, the present method accurately describes the collision cross-sections in the small angle region[4]. The present expressions (3), (4), (5) and (6) can be used to study the DCS for other light atoms like Sodium and Potassium. The present results can be improved by the inclusion of higher order exchange terms in the amplitude (2).

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