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ANGULAR AND TOTAL SCATTERING OF ELECTRONS BY H-ATOMS AND H_2-MOLECULES IN DEBYE PLASMA

[1]Hitesh S. Modi*, [2]Manish J. Pindariya and [3]K.N. Joshipura

[1]*Shree Sardar Patel Higher Secondary School, Patan - 384265 (N.G.)*

[2]*Physics Department, Sheth M.N. Science College, North Gujarat University, Patan - 384 265*

[3]*Sardar Patel University, Vallabh Vidyanagar - 388 120*

ABSTRACT

Elastic scattering of electrons by atomic as well molecular hydrogen is studied here at intermediate and high incident energies at and above 50 eV. Although the problem is very well investigated in literature, the aim of our present theoretical work is to examine the effect of weak external Debye plasma on the angular and total scattering of electrons with the said targets. The basic calculations are carried out in the 'eikonal-Born-series' (EBS) approach suitable for atomic hydrogen, along with the 'independent atom-in-molecule' (IAiM) model for molecular hydrogen target. The effect of the weak coupling of the plasma on the scattering is considered through the Debye screening length Λ_D. Reduction in the forward differential cross sections (FDCS) and the total (complete) cross sections (TCS) is studied quantitatively at Λ_D = 5, 7.5 and 10 Bohr radii a_0. Compared to the TCS, the FDCS are more sensitive to the effect of plasma screening, but even in that case, the effect dwindles beyond say 25 a_0.

INTRODUCTION

Atomic and molecular hydrogen - the most abundant astrophysical species - are the well-known targets of electron scattering investigations since long. H - atoms offer an exact wave function and charge-density and therefore offer a standard target for testing theoretical models and methods for electron scattering processes. About four decades back Byron and Joachain [1] developed a high energy method called *'eikonal-Born-series'* (EBS) theory to derive e^- - H elastic scattering cross sections accurately. The direct elastic scattering amplitude f^d_{EBS} considered through O (k^{-1}) with k as the electron wave-vector magnitude, is given in the EBS theory as follows.

$$f^d_{EBS} = f_{B1} + \mathrm{Re}\, f_{B2} + f_{G3} + i\,\mathrm{Im}\, f_{B2} \qquad (1)$$

Where subscripts B1 and B2 stand for the first and the second Born approximations, while G3 indicates the third Glauber approximation. Details of this theory along with the inclusion of electron exchange through the high energy Ochkur amplitude g_{och} are discussed by Joachain [2]. All the above scattering amplitudes depend on the scattering angle θ through the elastic wave-vector transfer

$$\Delta = \left| \vec{k}_I - \vec{k}_f \right| = 2k \sin\frac{\theta}{2}$$

with $\vec{k}_I$ and $\vec{k}_f$ as the initial and the final wave-vectors of the external electron. Cross sections of e^- - H scattering are described reasonably well in the EBS method, employed for fast electrons. Electron scattering from H_2 molecules has also been extensively studied in theory, as discussed in [3,5]. Our present interest is in the range of high incident energies $Ei \geq 50\,eV$. Therefore we invoke a high energy formalism, called *'Independent Atom-in-Molecule'*, (IAiM) approximation [3,5]. The electron charge density of ground-state Hydrogen atom is given in au by the simple expression $\rho(r) = 1/\pi .\exp(-\lambda r)$, with λ =2Z and the atomic number Z =1. But in the IAiM approximation, the H-atom in H_2 molecule, Z is assigned the variational value Z*=1.193, to account for the covalent bonding in the molecule, and e^- - H_2 cross sections are calculated approximately, by taking λ =2Z*. Further details are discussed in [3 - 5].

In the above theoretical outline the target atoms or molecules are supposed to be free or isolated as usual, say in a beam experiment. Our special interest in this paper is in the target atoms or molecules embedded in a weak plasma. The so-called Debye plasma has property of screening the coulomb potential by a factor exp ($-r/\Lambda_D$), where Λ_D is the characteristic Debye screening length, which depends on the electron concentration n_e and electron - temperature T_e of the plasma. The length Λ_D is conveniently expressed in the unit of Bohr radius 'a_0'. The infinitely long range coulomb potential (+q/r) of a point test-charge (+q) embedded in plasma, becomes the short range screened coulomb potential

$$Vsc\,(r; \Lambda_D) = +\,(q/r).\exp(-\,r/\Lambda_D) \qquad (2)$$

with r as a radial distance. For the present purpose we work with plasma parameter $\lambda_D = \frac{1}{\Lambda_D}$ expressed in a_0^{-1}. Atomic scattering of electrons or positrons in plasma has been investigated by several authors e.g. [6, 7].

With this introductory background, the aim of the present paper is to examine the effect of weak plasma, on the differential and the total cross sections of e^- - H and e^- - H_2 elastic scattering at intermediate and high incident energies. Atomic units (au) are used presently. Sample results are obtained and shown here to draw quantitative conclusions about the effect of different Debye plasmas on the cross sections of atomic as well as molecular hydrogen.

THEORETICAL METHODOLOGY

We begin with the elastic scattering of fast electrons by hydrogen atoms considered as free or isolated. In that case, the differential cross section (DCS)

*Corresponding author: *hmsir2010@gmail.com*

including exchange, is given exactly by the following expression [2].

$$\frac{d\sigma}{d\Omega}(\theta,k)=\frac{3}{4}\left| f_{EBS}^{d}-g_{och}\right|^2+\frac{1}{4}\left| f_{EBS}^{d}+g_{och}\right|^2 \quad (3)$$

The high energy elastic DCS are peaked in the forward direction i.e. θ=0 (Δ=0). The forward DCS (FDCS) is dominated by target polarization effects, and is represented by the real part of the second Born amplitude Re f_{B2}, vide equation (1). Detailed expressions for the different terms of equation (1) are given in [1]. For example the first Born scattering amplitude derived through the H - atom static potential V_{st} (r), is given by formula

$$f_{B1}=2\,\frac{(\Delta^2+2\lambda^2)}{(\Delta^2+\lambda^2)^2} \quad (4)$$

Where λ =2Z=2 corresponding to H (1s) - atoms. Details of the DCS calculations in the EBS theory are omitted here, but the obtained results are in a good accord with experimental data, as shown in [1,2].

The total (complete) cross section, which was referred to as the Bethe-Born cross section σ_{tot}^{BB} in earlier literature [1,2], is denoted presently by the symbol Q_T (E_i), and this quantity is related to the imaginary part of the forward scattering amplitude O(k^{-1}) through the optical theorem, viz.,

$$Q_T\ (E_i)=\frac{4\pi}{k}\,\mathrm{Im}\,f_{B2}\ (\theta=0) \quad (5)$$

Now, if the target atoms are surrounded by a weak plasma medium, the e^- - H interactions are influenced through the Debye screening factor exp $(-r/\lambda_D)$, as mentioned above. We assume the external plasma to be so weak that it does not alter the basic target properties like the charge- distribution, ionization energy etc. In that case the amplitude f_{B1} for H- atoms in plasma, is given again by equation (4), but with λ=2 replaced by λ' viz.,

$$\lambda'=\lambda+\lambda_D \quad (6)$$

This replacement accounts for the presence of plasma medium characterized by the inverse-length parameter λ_D (in a_o^{-1}).

Now, it is known that the plasma tends to curtail long range interactions like polarization potential. This potential dominates the electron - atom/molecule DCS in the forward direction. Therefore, in order to see the maximum effect of the plasma on the DCS we calculate presently the forward elastic e^- - H (and H_2) scattering at energies from 50 eV onwards. Expressions for various scattering amplitudes [1, 8] needed to calculate the atomic FDCS, incorporating θ=0, Δ=0, are as hereunder.

$$f_{B1}=\frac{4}{\lambda'^2} \quad (7a)$$

$$Ref_{B2}=\pi\,/\,k.Z'^2 \quad (7b)$$

$$\mathrm{Im}\,f_{B2}=\frac{2}{kZ'^2}\left[\ell n\left(\frac{2Z'k}{\omega}\right)-\frac{1}{4Z'^2}\right] \quad (7c)$$

$$f_{G3}=0 \quad (7d)$$

$$g_{och}=-\frac{2}{k^2Z'^4} \quad (7e)$$

The third Glauber amplitude is zero in the forward direction, as was shown by Dewangan [9]. The parameter λ' =2Z' is chosen through equation (6), for a particular plasma. Further ω= 0.465 au is the average excitation energy of H- atom. The TCS (Q_T) are obtained through equation (5).

Let us turn now to e^- - H_2 elastic scattering in the IAiM model which yields the following expression [4a,b] for the orientation-averaged elastic DCS including, the exchange effect, as yet without any plasma.

$$\bar{I}(\theta,k,Z^*)=2\left| f_{EBS}^{d}-\frac{1}{2}g_{och}\right|^2\left[1+\frac{\sin\Delta R}{\Delta R}\right] \quad (8)$$

In equation (8), the required scattering amplitudes for H - atom (within the modulus sign) are essentially the same as in [1, 2] but we have $\lambda=2Z^*$, and Z^*=1.193, representing the atom bound in the molecule. Of course this corresponds to e^- - H_2 system without any plasma. The factor in the square bracket in equation (8), with R=1.4 a_o as the bond-length in H_2 molecule, arises from the interference of electron-waves scattered by two H - atoms in this molecule. Note that this factor simply becomes 2 in the forward direction.

Next, considering the target H_2 molecules in plasma, we replace $\lambda=2Z^*$ by $\lambda'=2Z^*+\lambda_D$, along the line of arguments presented above, i. e. equation (6). Thus, the e^- - H_2 cross sections are calculated essentially in the EBS method, and the Debye screening is introduced via λ_D. Specific values are chosen for the plasma parameter λ_D, and we return to this point in section 3.

RESULTS, DISCUSSIONS AND CONCLUSIONS

In this paper the elastic scattering of fast electrons is studied for atomic as well as molecular hydrogen targets. The differential and the total (complete) cross sections are calculated, initially without any plasma medium. The usual DCS and TCS for free atoms/molecules well reproduce the experimental data at high energies, and not shown here. The EBS being a high energy method, does not yield accurate results at a lower energy like 50 eV. However, even at such energies it is still meaningful to calculate and make relative comparisons of results with and without plasma.

Our aim is to examine quantitatively how the FDCS, $\frac{d\sigma}{d\Omega}(\theta=0)$ and the TCS (Q_T) are affected when the targets are in the midst of plasma.

Choice of parameter λ_D

In order to choose the parameter λ_D representing the strength of the plasma, we note that the average radius of H(1s) - atom is well-known to be <r> = 1.5 a_o. Hence to ensure that the plasma is weak enough, we choose the model values of the Debye length Λ_D to be typically larger than 3<r>. Thus our calculations are carried out at three different Debye lengths Λ_D = 5.0, 7.5 and 10 (all in a_o), and λ_D is set accordingly in equation (6). If the Debye length is chosen to be smaller, it would mean stronger plasma, which may alter the basic properties of the target, and the Debye screening model itself would not be reliable. For large values of Λ_D the cross sections are hardly influenced by the plasma.

Let us now discuss the obtained results for atomic and molecular hydrogen.

e^- - H, H_2 elastic scattering in plasma

The present FDCS and TCS for e^- - H scattering without and with plasma confinement are exhibited in table 1, at selected electron energies from 50 eV to 10 keV. The usual cross sections of e^- - H (free) scattering are compared with the theoretical values of [1,2] at the first two energies. The agreement is quite good, and the small difference in the cross sections is due to the choice of the average excitation energy ω.

Table 1: FDCS and TCS of electron-H atom elastic scattering at selected energies. Here, * indicates compared data from ref [1,2]. The percentage decrease in plasma ($\Lambda_D = 7.5$ $a_0 = 5\langle r\rangle_H$) is shown relative to no-plasma case.

Energy	FDCS	FDCS	TCS	TCS	FDCS	TCS
E_i (eV)	Without Plasma	With Plasma	Without Plasma	With Plasma	% Decrease	% Decrease
		$\Lambda_D = 7.5$ a_0		$\Lambda_D = 7.5$ a_0		
50	13.96 (14.20)*	11.46	12.69 (12.20)*	11.58	Approx. 21%	Approx. 10 %
100	8.55 (8.25)*	6.92	7.53 (7.49)*	6.83		
200	5.58	4.47	4.35(4.39)*	3.94		
300	4.46	3.55	3.13(3.17)*	2.82		
400	3.85	3.06	2.47(2.50)*	2.23		
500	3.45	2.73	2.06	1.85		
600	3.17	2.51	1.77	1.59		
700	2.96	2.34	1.55	1.39		
800	2.8	2.21	1.39	1.25		
1000	2.55	2.01	1.15	1.03		
2000	1.99	1.56	0.63	0.57		
5000	1.56	1.21	0.28	0.25		
7000	1.45	1.13	0.21	0.19		

* compared data from [1, 2].

Now, the effect of external weak plasma is to reduce the electron-target interaction strength, resulting into a decrease of the cross sections compared to free (or no-plasma) case. Out of the three typical values of Λ_D chosen presently, the smallest value i. e. 5.0 a_0 has the strongest influence on the FDCS of e^- - H scattering at all energies considered here. Thus we find that, with $\Lambda_D = 5.0$ a_0 the FDCS of H-atoms are reduced by as much as 30%, while the TCS are reduced by about 13%, compared to no-plasma situation. It was shown in [6] that DCS of electron scattering by a polar molecule like H_2O in plasma are considerably reduced in the forward direction, since the long range dipole potential is effectively curtailed by the Debye screening. The reduction trend is also observed in the elastic positron - Hydrogen calculations carried out by Ghoshal et al [7].

We have shown in table 1 the numerical values of e^- - H cross sections at a typically moderate Debye length Λ_D= 7.5 a_0, at selected energies. In the usual no-plasma situation, our calculated values of FDCS and TCS agree with those of [1, 2]. For FDCS, the difference between the free and plasma cases is about 21%while for the TCS it is about 10%. Further, figure 1 is the graphical plot for the FDCS of e^- - H scattering over a very wide range of energy, without and with plasma (at three different Λ_D). With H - atoms again, the TCS (Q_T) are also reduced in the presence of plasma, and these are also shown at three different Λ_D in figure 2.

Figure 1: FDCS of e^- - H elastic scattering plotted vs. incident electron energy, at different Debye screening lengths, the top most curve showing free or no-plasma case

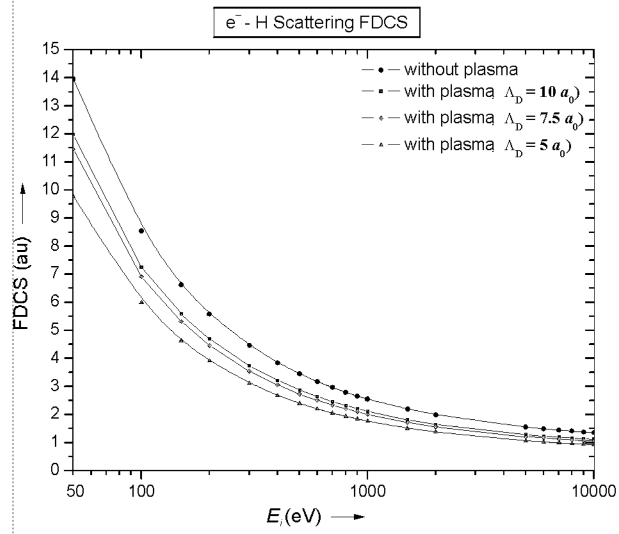
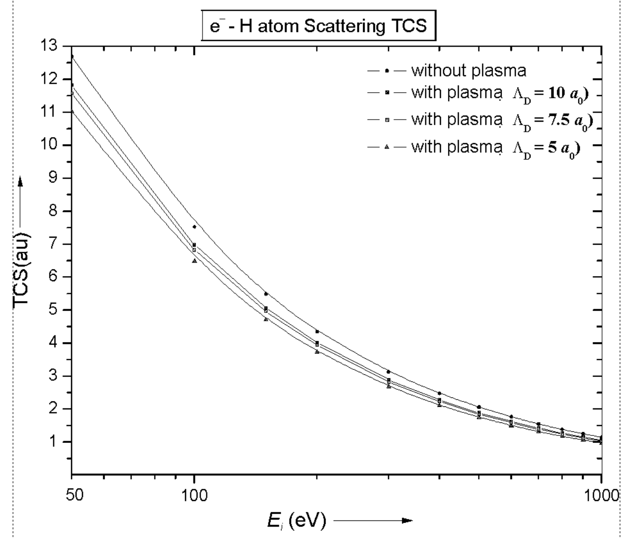


Figure 2: TCS Q_T (in a_0^2) of e^- - H elastic scattering plotted vs. incident electron energy, at different Debye screening lengths, the top most curve showing free or no-plasma case

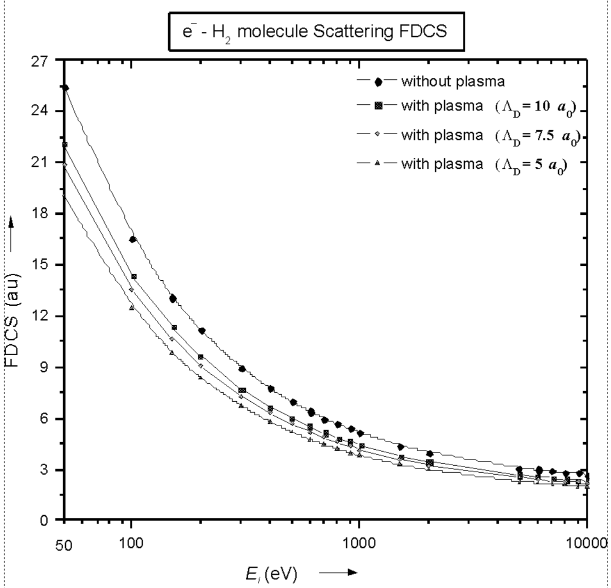


Next we consider e^- - H_2 scattering cross sections calculated in the IAiM approximation. The approximate method holds better when the de Broglie wave length (λ_{dB}) of incident electrons is smaller than the bond-length R=1.4 a_0 of H_2. In other words the method is reliable above E_i = 270 eV, which corresponds to λ_{dB} = R. At lower energies, the IAiM approximation together with the EBS theory gives overestimated results, but still a relative comparison of cross sections without and with plasma can be made. Therefore, we have shown in table 2, the FDCS and TCS of molecular hydrogen from E_i = 50 eV onwards. In this case the decrease in FDCS and TCS, brought about by plasma with Λ_D= 7.5 a_0 is almost similar to that in the respective H atom cases. Increasing Λ_D results into lesser and lesser decrease in these cross sections, as against no-plasma case, and that is expected. Table 2 exhibits the present results for e^- - H_2 scattering by considering Λ_D= 7.5 a_0. For molecular hydrogen, the reduction in the FDCS and TCS is nearly 19% and 8% respectively. Figure 3 is the graphical plot for the FDCS of e^- - H_2 scattering over a very wide range of energy, without and with plasma at three different Λ_D.

Table 2: The present FDCS and TCS of electron - H_2 molecule scattering at selected energies. The percentage decrease in plasma (Λ_D = 7.5 a_0) is shown relative to no-plasma case

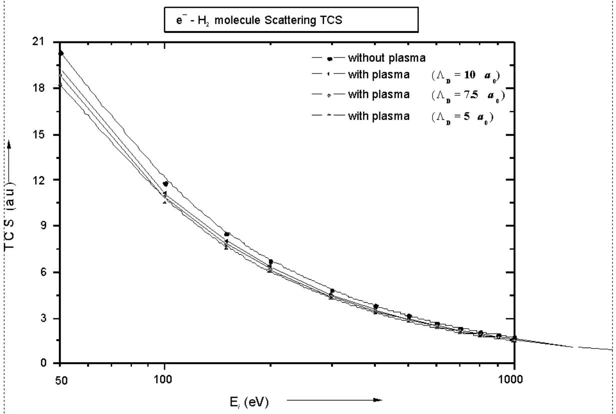
Energy E_i(eV)	FDCS Without Plasma	FDCS With Plasma	TCS Without Plasma	TCS With Plasma	FDCS % Decrease	TCS % Decrease
		Λ_D = 7.5 a_0		Λ_D = 7.5 a_0		
50	25.47	20.84	20.37	18.89	Approx. 19 %	Approx. 8 %
100	16.57	13.56	11.85	10.93		
200	11.13	9.1	6.75	6.21		
300	8.97	7.32	4.83	4.43		
400	7.76	6.32	3.79	3.48		
500	6.97	5.67	3.14	2.88		
600	6.4	5.21	2.69	2.47		
700	5.98	4.86	2.36	2.16		
800	5.64	4.58	2.1	1.93		
1000	5.14	4.17	1.74	1.59		
2000	4	3.24	0.95	0.87		
5000	3.1	2.5	0.42	0.39		
7000	2.89	2.33	0.31	0.29		
10000	2.71	2.18	0.23	0.20		

Figure 3: FDCS of e^- - H_2 elastic scattering plotted vs. incident electron energy, at different Debye screening lengths, the top most curve showing free or no-plasma case



In conclusion the influence of external plasma medium is rather more on the FDCS of elastic electron scattering from H and H_2, while the TCS (Q_T) are affected to a lesser degree, (figure 4) as discussed in this paper. The reduction effects decrease as the Debye length increases. The Debye length corresponding to weakly coupled plasma chosen here is arbitrary but it is taken to be sufficiently larger than the average atomic radius 1.5 a_0 of the H atom.

Figure 4: TCS Q_T (in a_0^2) of e - H_2 elastic scattering plotted vs. incident electron energy, at different Debye screening lengths, the top most curve showing free or no-plasma case



Our calculations in this paper lead to an interesting question; can we ascertain a limit, in terms of Λ_D, beyond which the Debye plasma becomes practically ineffective in influencing the electron interactions and hence the cross sections? Our present findings indicate that, even the FDCS, more sensitive to plasma screening, are reduced by less than 5% in a plasma with Λ_D more than 25 a_0 or so.

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