IOSR Journal of Applied Physics (IOSRJAP)
ISSN – 2278-4861 Volume 1, Issue 2 (July-Aug. 2012), PP 08-13
www.iosrjournals.org

Charge transfer cross-sections in $H^+ - Li(2s)$ collisions

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Abstract: *Single charge transfer cross-section in $H^+ - Li(2s)$ collisions has been studied in the frame work of the Coulomb-Born Distorted Wave approximation (CBDWA). The differential as well as total cross-sections have been calculated in the energy range from 10keV to 1MeV.The results so obtained have been compared with other's available results.*

Key words: *Coulomb-Born distorted wave approximation. Differential cross-sections, Electron captureTotal cross-sections,*

I. INTRODUCTION

Over decades, the charge transfer collisions from proton with alkali metal atoms have been studied extensively. Theoretically the study of proton-alkali metal atoms becomes very complicated due to the multi electron character of the target atoms. For many practical processes the alkali atoms can be considered as one electron system just like hydrogen atom. We have also considered only the valence electron with single particle Slater orbital wave functions. The charge of the alkali metal has been taken as unity in this case.

Ferrante et al [1] have studied the valence and core electron capture in proton-lithium ($H^+ - Li$) collisions using the Oppenheimer Brinkman Kramer's (OBK) approximation. Ferante et al [2] have also studied electron capture process in proton-alkali atom collisions using the Eikonal approximation to obtain the total cross-sections. In another approach Daniel et al [3] have used the Eikonal approximation treatment to obtain the total charge transfer cross-section for high energy proton-alkali atoms charge transfer problem. Erolamaev [4] studied electron capture by proton from L to K shells of Li- atoms using two centre orbital methods. A modified two centre atomic orbital expansion method has been applied by Fritsch et al [5] for electron capture in ($H^+ - Li$) collisions. Sato and Kimura [6] have used a multi state perturbed stationary state method for charge transfer cross-sections at low energy to intermediate impact energy. Very recently Lur and Saenz [7] have studied proton-anti-proton collisions with alkali atoms Li, Na and K and calculated only ionization and excitation and have not considered the charge transfer in the energy range from 2 to 1000keV by using a time-dependent channel-coupling approach.

In this paper we have studied only single charge transfer collisions in proton-lithium atom collisions by using the Coulomb-Born Distorted wave approximation (CBDWA) which has been recently used by Gharban-Adivi [8] in proton-Helium collisions. In this approximation the distortion produced by the Coulomb potential are included in the T-matrix formalism. As the differential cross-sections give more extensive information of collision dynamics, we have calculated differential cross-section for wide range of energy for the process we have under taken.

Throughout this paper, we have used the atomic units in which (m=e=$\hbar$ =1) except for the cross-sections which has been calculated in unit of πa_0^2.

II. Theory:

We have considered the process

$$H^+ + Li(2s) \rightarrow H(1s) + Li^+ \tag{1.1}$$

The coordinate systems for the process (1) are as: $\vec{R}_i$ is the position vector of hydrogen atom relative to the centre of mass of electron and target ion. $\vec{R}_f$ is the position vector of the target ion with respect to the centre of mass of proton and electron. $\vec{r}\,'$ and $\vec{r}$ are the vector separation of the electron from Li atom and H respectively. $\vec{R}$ is the inter-nuclear separation.

The transition matrix T_{if} from an initial state i to a final state f in the CBDW approximation for the process (1) are given by

$$T_{if} = \int d\vec{r} d\vec{R}_f \Psi_f^* V_f^* \Psi_i \quad (1.2)$$

Where Ψ_i and Ψ_f are the wave functions for the process (1.1) in the initial and final channels respectively and are given by

$$\Psi_i = \Phi_i(\vec{r}\,')\varphi_i(\vec{R}_i) \quad (1.3)$$

and

$$\Psi_f = \Phi_f(\vec{r})\varphi_f(\vec{R}) \quad (1.4)$$

Where again,

$\Phi_i(\vec{r}\,')$ = wave function of the Li-atom in the ground state.

$\Phi_f(\vec{r})$ =wave function of the hydrogen atom in $1s$ state $= \dfrac{e^{-r}}{\sqrt{\pi}}$ (1.5)

$\varphi_i(\vec{R}_i) = e^{i\vec{k}_i.\vec{R}_i}$ is a plane wave in the initial channel.

$\varphi_f(\vec{R}_f) = e^{-\pi\alpha/2}\Gamma(1-i\alpha)e^{i\vec{k}_f.\vec{R}_f}\,{}_1F_1(i\alpha;-ik_fR_f - i\vec{k}_f.\vec{R}_f)$ is Coulomb wave

Where $\vec{k}_i$ and $\vec{k}_f$ are the momentum vectors in the initial and final channels respectively.

$\alpha = \dfrac{\mu_f}{\vec{k}_f}$ is the repulsive Coulomb parameter and

${}_1F_1(i\alpha;-ik_fR_f - i\vec{k}_f.\vec{R}_f)$ = confluent hyper-geometric function.

For Li-atom we have used single particle wave functions of Simsic and Williamson Jr [9] of the type

$$\Phi_i(\vec{r}\,') = \frac{1}{2\sqrt{\pi}}\left(C_2e^{-S_2r'} + C_1r'e^{-S_1r'}\right) \quad (1.6)$$

Where $S_1 = 0.65, C_1 = 0.39888$

$S_2 = 2.7, C_2 = -1.496099$

Now the transition matrix element for the process (1) will be obtained by putting (1.5) and (1.6) in equation (1.2), we get

$$T_{if} = \int d\vec{r} d\vec{R}_f e^{i(\vec{k}_i.\vec{R}_i - \vec{k}_f.\vec{R}_f)}\frac{e^{-r}}{\pi}e^{-\pi\alpha/2}\Gamma(1+i\alpha)\,{}_1F_1(i\alpha;-ik_fR_f - i\vec{k}_f.\vec{R}_f)$$
$$\times\left(-\frac{1}{r'}\right)\frac{1}{2\sqrt{\pi}}\left(C_2e^{-S_2r'} + C_1r'e^{-S_1r'}\right)$$

$$T_{if} = \int d\vec{r} d\vec{R}_f e^{i(\vec{k}_i.\vec{R}_i - \vec{k}_f.\vec{R}_f)}e^{-\pi\alpha/2}\Gamma(1+i\alpha)\,{}_1F_1(i\alpha;-ik_fR_f - i\vec{k}_f.\vec{R}_f)$$
$$\times\left(-\frac{1}{r'}\right)\frac{1}{2\sqrt{\pi}}\left(C_2e^{-S_2r'} + C_1r'e^{-S_1r'}\right)$$
$$T_{if} = = e^{-\pi\alpha/2}\Gamma(1+i\alpha)I \quad (1.7)$$

Where

$$I = -\int d\vec{r} d\vec{R}_f e^{i(\vec{k}_i.\vec{R}_i - \vec{k}_f.\vec{R}_f)}\frac{e^{-r}}{\sqrt{\pi}}\,{}_1F_1(i\alpha;-ik_fR_f - i\vec{k}_f.\vec{R}_f)\left(\frac{1}{r'}\right)\frac{1}{2\sqrt{\pi}}\left(C_2e^{-S_2r'} + C_1r'e^{-S_1r'}\right)$$

$$= -\frac{2\pi C_2}{\mu_a^6}\int_0^1 xdx\frac{1}{g^3}\frac{1}{\lambda_2}\frac{d}{d\lambda_2}\frac{1}{\lambda_2}\frac{d}{d\lambda_2}\phi(\lambda_2) + \frac{2\pi S_1C_1}{\mu_a^8}\int_0^1 x(1-x)dx\frac{1}{g^4}\frac{1}{\lambda_1}\frac{d}{d\lambda_1}\frac{1}{\lambda_1}\frac{d}{d\lambda_1}\frac{1}{\lambda_1}\frac{d}{d\lambda_1}\phi(\lambda_1) \quad (1.8)$$

Where

$$g = x + \frac{(1-x)}{\mu_a^2}$$

$$\phi(\lambda_2) = \left(\frac{q^2+\lambda_2^2}{2}\right)^{-i\alpha-1}\left(\frac{q^2+\lambda_2^2}{2} + \vec{k}_f.\vec{q} - i\lambda_2 k_f\right)^{i\alpha}$$

$$\phi(\lambda_1) = \left(\frac{q^2+\lambda_1^2}{2}\right)^{-i\alpha-1}\left(\frac{q^2+\lambda_1^2}{2} + \vec{k}_f.\vec{q} - i\lambda_1 k_f\right)$$

$$\vec{q} = \frac{\vec{k}_i}{\mu_a} + \frac{\vec{K}_0}{\mu_a} - \vec{k}_f,\ \vec{K}_0 = \frac{(1-x)(\mu_a\mu_b - 1)}{g\mu_a^2}\vec{k}_i$$

$$\mu_a = \frac{M_P}{M_P+1} \text{ and } \mu_b = \frac{M_T}{M_T+1}, M_P = \text{mass of projetile and } \mathrm{M}_T = \text{mass of target atom}$$

Putting equation (1.8) in the equation (1.7), the matrix elements are obtained.

While solving equation (1.8), the technique used by Tiwari [10] and Gharban-Adivi [8] have been used. The differential cross-sections [11] for the charge transfer from Li-atom to 1 s state of hydrogen atom are given by

$$\frac{d\sigma}{d\Omega} = \frac{\mu_i\mu_f}{4\pi^2}\frac{k_f}{k_i}\left|T_{if}\right|^2 \tag{1.9}$$

Where $\vec{k}_i$ and $\vec{k}_f$ are related by the energy conservation relation

$$\frac{k_i^2}{2\mu_i} - \frac{k_f^2}{2\mu_f} = E_f - E_i = \Delta E \tag{1.10}$$

Where

E_i = Binding energy of Li-atom

E_f = Binding energy of the H-atom

are obtained from Moore's table[12].

$\mu_i = \frac{M_P(M_T+1)}{M_P+M_T+1}$ and $\mu_f = \frac{M_T(M_P+1)}{M_P+M_T+1}$ are the reduced masses of the system in the initial and final channels.

The total cross-sections are obtained by integrating equation (1.9)

$$\sigma = 2\pi\int_0^\pi \frac{d\sigma}{d\Omega}\sin\theta d\theta \tag{1.11}$$

Since, the charge transfer differential cross-sections for atomic collisions with heavy particle projectiles is strongly peaked in the forward direction and falls rapidly with increasing scattering angle θ, we have used suitable transformation of the integration variable instead of θ as

$$k_i^2(1-\cos\theta) = \frac{1+z}{1-z} \tag{1.12}$$

The values of z are supplied by Gaussian- quadrature points when convergence is insured. While

The one dimensional integration from 0 to 1 are done numerically by using the Gauss-Legendre quadrature formula. The convergences in both cases for differential and total cross-section have been insured by increasing the number of Gaussian points. In this way the value of cross-sections are obtained with sufficient accuracy.

III. Results and discussions:

We have calculated the charge transfer cross-sections in the frame work of CBDWA into the 1s state of hydrogen in proton-lithium atom collisions for the incident energy range varying from 10 keV to 1MeV. The total cross-sections of 1s state of hydrogen in the energy range 10 keV to 1 MeV in units of πa_0^2 have been compared with the results obtained in different approximations in table 1. The first Born approximation (FBA) and OBK results are considerably higher while the eikonal results are slightly higher than our results above 120 keV but between 70 to 100 keV our results are in good agreement with both FBA and eikonal results. Below 70 keV other results are not available for comparison.

Table : Total cross-sections for the process $H^+ + Li(2s) \rightarrow H(1s) + Li^+$ in units of πa_0^2.

Incident energy keV	σ_{CBDWA}	σ_{eik}	σ_{OBK}	σ_{FBA}
10	0.46736(2)	----------	----------	----------
15	0.17964(2)			
20	0.85041(1)			
30	0.43704(1)			
40	0.13476(1)			
50	0.18319(0)			
60	0.75029(-1)			
70	0.32055(-1)	0.11975(-1)	0.78162(-1)	0.51665(-1)
80	0.14092(-1)	0.86291(-2)	0.26978(-1)	0.17832(-1)
90	0.63179(-2)	0.64477(-2)	0.11458(-1)	0.75737(-2)
100	0.28816(-2)	0.48947(-2)	0.68400(-2)	0.45212(-2)
110	0.13522(-2)	0.37748(-2)	0.54443(-2)	0.35986(-2)
120	0.67719(-3)	0.29358(-2)	0.48988(-2)	0.32381(-2)
140	0.27040(-3)	0.18760(-2)	0.41165(-2)	0.27210(-2)
160	0.21481(-3)	0.12191(-2)	0.32779(-2)	0.21667(-2)
180	0.21048(-3)	0.83367(-3)	0.25032(-2)	0.16546(-2)
200	0.20210(-3)	0.56149(-3)	0.18730(-2)	0.12380(-2)
300	0.10355(-3)			
400	0.44827(-4)			
500	0.20484(-4)			
1000	0.10939(-5)			

σ_{CBDWA}: present the results in Coulomb-Born Distorted wave approximation, σ_{eik} : Daniele et al's results in eikonal approximation, σ_{OBK} : Ferrante et al's result in Oppenheimer-Brinkman and Kramer's approximation quoted by Daniele et al and σ_{FBA}: Estimated results on OBK. The bracketed numbers denote powers of ten by which each entry should be multiplied.

For charge transfer processes the usual form of the first Born approximation is not asymptotically correct at high energies [13]

Fig.1 shows the differential cross-sections for (p-Li) collisions at incident energies 10, 15 and 20 keV.

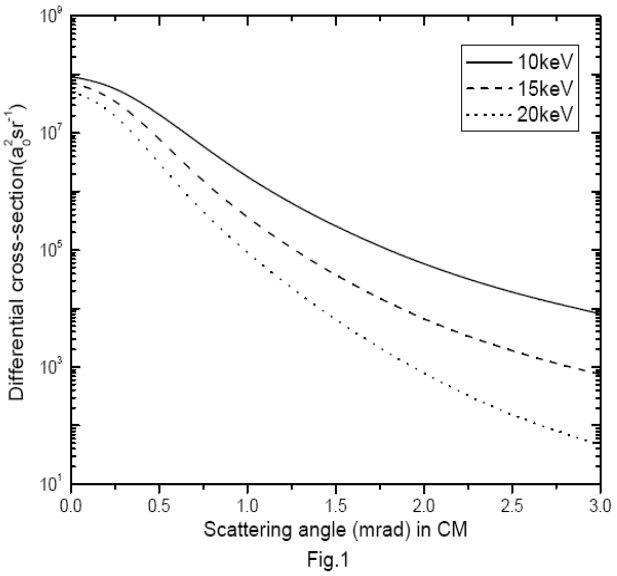

Fig.1. Differential cross-sections (CM system) for the charge transfer process $H^+ + Li(2s) \rightarrow H(1s) + Li^+$ at energies 10, 15 and 15 keV.

Fig.2 shows the differential cross-sections at energies 80,120 and 300 keV. Fig.3. shows the differential cross-sections at energies at 400 and 1000 keV.

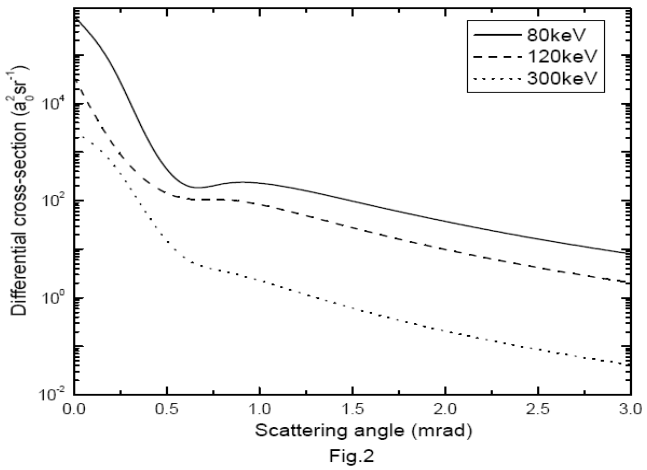

Fig.2 Differential cross-sections (CM system) for the charge transfer process $H^+ + Li(2s) \rightarrow H(1s) + Li^+$ at energies 80,120 and 300 keV.

In the fig.1 the nature of the curves are of the similar type. In fig 2. We have observed pronounced dip at energy 80 keV at about .6 mrad and similar nature with less dip have been observed at energies 120 and 300 keV. In fig3. The dip is found at .6 mrad at both the energies.

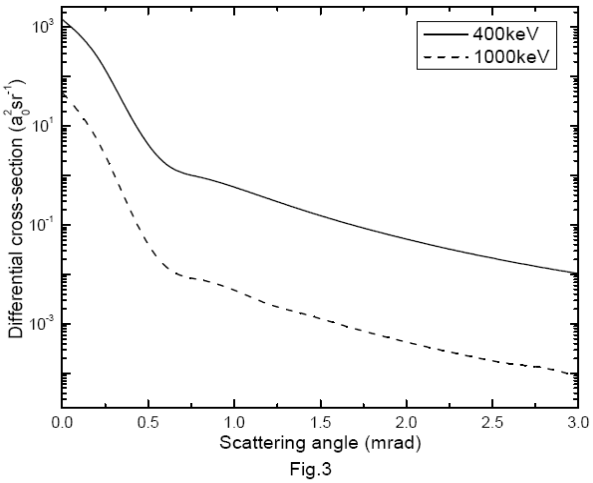

Fig.3. Differential cross-sections (CM system) for the charge transfer process $H^+ + Li(2s) \rightarrow H(1s) + Li^+$ at energies 400 and 1000 keV.

IV. Conclusions:

The study of charge transfer reactions in atomic collisions are of great interest both from scientific point of view as well as from its wide applications in the diverse fields of Physics. Studies of these reactions are helpful from plasma diagnostics. Many such atomic collisions processes are relevant to the problems associated with fusion reactors. We observe that CBDWA gives better results over OBK and FBA.More theoretical and experimental results are needed to compare the results at higher energies.

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