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Proton, He^+ and He^{2+} ion Impact Electron Capture from Na Atom

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ABSTRACT Cross-Sections for single electron capture by protons He^+ and He^{2+} ions from Na atoms have been calculated in the Modified Binary Encounter Approximation. The Hartree –Fock velocity distribution has been taken into account throughout the calculations. The angular divergence factor has also been considered. The present calculations have fairly good agreement with the experimental observations.

KEYWORDS Electron Capture, Binary encounter approximation, Hartree-Fock Velocity distribution, Angular divergence factor.

INTRODUCTION

Charge exchange is a process which plays a vital role in the formation and decay of both astrophysical and Laboratory Plasma. In addition, state selective nature of charge exchange can be employed in diagnostic systems for laboratory plasmas, in pumping atomic levels which exhibits laser action and in some other applications (Bransden and Mc Dowell)[1]. Furthermore, the charge exchange processes are specially relevant to upper atmosphere researches. Bare nuclei present in low energy cosmic rays interact with the interstellar gas atoms and the electrons captured by the cosmic rays nuclei lead to the formation of atoms and ions in excited states. These formations yield x-rays through radiative decay and the x-rays so produced give a direct measure of the intersteller Cosmic ray intensity (see Belkic and Mc Carrol[2], Belkic and Gayat[3]). Charge changing processes provide valuable information about the radiation damage and design of radiation detectors. These processes are helpful in the production of negatively charged ions which play important role in accelerator technology, particularly in design of tandom accelerators. Moreover, the study of these processes is also important in thermonuclear fusion. Charge exchange is also useful in plasma diagnostics (See Mc Dowell and Ferendeci[4], Jochain and Post[5]). It also finds applications in the production of Vacuum ultra violet and x-radiation (Vinogradov and Soblemen[6], Bransden and Mc Dowell[1], Dixon and Elton[7]).

Due to a large number of applications, the interest has grown rapidly in studying charge transfer phenomena in recent years. Charge transfer process, the basic mechanism of rearrangement collision, is rather a complicated problem so far its theoretical as well as experimental studies are concerned (see Shevelko[8]). Despite the complexities existing therein, the charge transfer process due to impact of different positively charged particles has been investigated experimentally and theoretically by a number of workers but still are less and limited especially for heavier targets. In recent past Bates and Mc Carrol[9], Bransden[10], Bates and Kigston[11], Mapleton[12], Biswas et al[13], F. Fremon[14A], Basu et al[14B], A Amaya-Tapiya et al[14C] etc. have reviewed the theoretical investigations of charge exchange processes in different quantal and semiquantal approximations.

Fully quantal and semi-classical calculations of cross sections require large scale numerical computations. Due to inherent numerical complexities these calculations are restricted to the lighter targets only. For this reason there has always been an interest in thinking of models for ion-atoms collisions based on classical picture which can be expected to provide cross sections of at least moderate accuracy. Among the classical models, the classical trajectory Monte Carlo (CTMC) method and the Binary Encounter model have been found to the most successful. In case of CTMC, still the numerical complexities are more or less similar to the quantum formalism.

On the other hand, a theoretical model was constructed by Thomas[15] based on classical considerations as early as 1927. Later on it was improved and extended by Bates and Mapleton[16] and Mapleton[12]. The original as well as modified theories are based on the theories of two binary encounters-one between the incident ion and the target electron and the other between the ejected electron and the target nucleus to account for electron capture. Use of the original and the modified models of Thomas[15] is found to give satisfactory estimates of cross sections for electron capture from heavy atoms by fast light nuclei. Later on a classical model for electron capture involving single binary encounter between the incident ion and the target electron was proposed by Bates and Snyder[17] in which the idea of finite characteristic collision time was introduced. However, they themselves have expressed doubt about the suitability of the model in case of capture from heavier targets. Later on a classical model for charge transfer with single binary encounter was proposed by Gryzinski[18]. In recent past Roy and Rai[19] have derived new limits for energy transfer depending on the Thomas[15] condition and gave a detailed discussion of the Model for calculating charge transfer cross sections in GryZinski's[18] model. They have calculated single electron capture cross sections for noble gas due to proton impact & found satisfactory agreement with experiments. Their modified binary encounter model was then also applied by Kumar and Roy[20], Shrivastava and Roy[21], Chatterjee & Roy[22], S. Kumari et al[23] etc. Similar modified version of binary encounter was also given by Tan and Lee[24] independently which may be considered as the generalisation of the modified version of Roy and Rai[19].

Keeping in view the above mentioned facts, I think it worthwhile to investigate electron capture cross sections of Na due to impact of Proton, $^3He^+$ and $^3He^{2+}$ ions for which the experimental results are available.

THEORETICAL CONSIDERATIONS

The theoretical descriptions for calculating ion impact single electron capture cross sections of atoms have been outlined in detail by Roy and Rai[19] and Shrivastava et al[25]. We now introduce two dimensionless variables s and t (see also Catlow and McDowell[26]) defined by $s^2 = \frac{v_1^2}{v_0^2}$ and $t^2 = \frac{v_2^2}{v_0^2}$ where $v_0^2 = U_i$ is the binding energy of the target atom in rydbergs and v_1 and v_2 are respectively the velocities of the projectile and the target electron in atomic units. In terms of these dimensionless variables, the lower and upper limits of energy transfer for electron cap lure can be given respectively by

$$\Delta E_l = (s^2+1)U_i + g - 2s(U_i g)^{\frac{1}{2}} \quad (1)$$

and $$\Delta E_u = (s^2+1)U_i + g + 2s(U_i g)^{\frac{1}{2}} \quad (2)$$

where $$g = {2zs}\Big/{r(s^2+t^2)^{\frac{1}{2}}} \quad (3)$$

Here z is the charge and r is the modules of the position vector of the bound electron with respect to the target nucleus which may be taken to be the radius of the Shell considered. It is exprened in atomic units.

Here, 'g has been used in place of f as mentioned by Roy and Rai[19].

The electron capture cross sections have been found by integrating Vrien's expression for $6_{\Delta E}$ and found six expressions for cross sections, denoted by Q (s, t), corresponding to various values of ΔE_l and ΔE_u falling under different energy ranges (see Shrivastava et. Ql[25], Chatterjee and Roy[22], see also Tan and Lee[24]). In order to take the effect of angular divergence into account, the solid angle correction factor is given by

$$c = \frac{1}{2}\left\{1 - \left(1 - \frac{g}{s^2 u}\right)^{\frac{1}{2}}\right\} \quad (4)$$

(See Tan and Lee[24])

For $s^2U<g$, electron capture is possible even if the energy transferred by the projectile to the target electron is less than ΔE_l (or ΔE_u). Corresponding to various values of ΔE_l and ΔE_u relative to the values of quantities s, $4su\ (s-t)$ and $4su\ (s+t)$ there are ten expressions for electron capture (see Chatterjee and Roy[22]). In all those ten expressions, it has been assumed that the Projectile captures all the electrons ejected due to energy transfer ΔE satisfying the condition $U \leq \Delta E \leq \Delta E_u$. Where only half of the ejected electrons, corresponding to $\Delta E_l \leq \Delta E \leq \Delta E_u$ are captured by the projectile (See Tan and Lee[24]).

The expressions so obtained are integrated over the Hartree-Fock Velocity distribution for the target electron in the Shell under consideration so that the electron capture cross-section reduces to

$$Q(s) = n_e \int_0^\infty Q(s,t)\, f(t) U^{\frac{1}{2}} dt \quad (5)$$

Where n_e is the no. of equivalent electrons in the shell; $f(t)$ is the momentum distribution function constructed by making use of the Hartree-Fock radial functions given by Clementi and Roetti[28]. The atomic radii and shell radii have been taken from Lotz[29] and Desclaux[30] respectively.

Thus the final expression for electron capture
is given by $Q = Q(s) \times c$ (6)

Where C is the solid angle correction factor (Eqn. 4).

RESULTS AND DISCUSSIONS

I have calculated the cross sections for electron capture due to impact of protons, He^+ and He^{2+} for Na[31] atoms along the lines discussed in sec. 2. The present results along with the experimental observations have been shown in the figures 1, 2, 3 and Tables 1, 2, 3 respectively. For the Sake of Comparison, other available theoretical calculations are also given in the figures & tables.

The single electron capture cross sections for Na due to Proton impact have been calculated up to impact energy 1000 KeV. The present calculations for cross sections have been plotted as a function of incident energy shown in fig. 1. The fig.1 includes, in addition to the present cross sections, the theoretical results of Fritsch[32] and experimental observations of Dubois and Toburen[31]. For the sake of comparison, the graph has been taken only up to 70.0 KeV because the theoretical results of Fritsch are only limited up to 15 KeV whereas the experimental results are limited up to 70.0 KeV. The present calculated cross sections are always within a factor of 2 of the experimental results, except in the energy range below 2 KeV. The theoretical calculation of Fritsch[32] in case of proton impact is always in better agreement with experiment than the present one. However, the results of Fritsch are available only upto 15.0 KeV. Its agreement with experiment can't the predicted in still higher energy range whereas the present calculated cross sections are agreeing well with the experimental observations beyond 15.0 KeV. The discrepancy in low energy range in case of Proton impact may partly be attributed to the non-suitability of Binary Encounters Approximate (BEA). The fairly good agreement of the present results with experiment is the general feature of the BEA.

Table 1: Proton impact electron captures cross sections for Na.

(in units of 10^{-17} cm^2)

Impact energy (KeV)	Present Calculations	Calculations Fritsch[32]	Experiment DuBois & Toburen[31]
1.0		259.00	
2.00	222.00	590.00	664.00
3.0		680.00	852.00
4.0	478.00	689.00	689.00
5.0	593.00		
6.0	536.00	580.00	621.00
8.00	363.00	425.00	454.00
10.0	235.00	270.00	308.00
15.0	74.90	105.00	93.70
20.0	38.30		50.30
30.0			12.50
40.0	9.3		9.66
50.0			5.75
60.0	4.95		3.72
70.0	4.0		3.63
80.0	3.3		
100.0	2.5		
110.0	2.1		
150.0	1.43		
200.0	0.69		
250.0	0.40		
300.0	0.242		
400.0	0.103		
500.0	0.050		
700.0	0.016		
900.0	0.007		
1000.0	0.004		

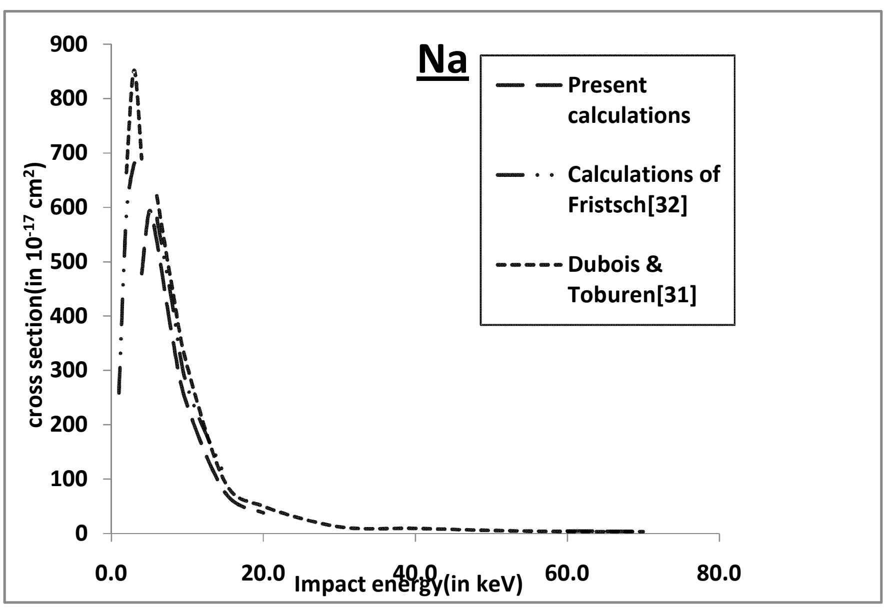

Figure 1: Proton impact electron capture cross sections for Na

In case of $^3He^+$ ion impact single electron capture cross – sections for Na atom have been presented in fig. 2 and Table 2. The present calculation of cross-sections have been done up to 1000.0 KeV but graph has been plotted only upto 100.0 KeV for comparison with the available experimental results. In the case of $^3He^+$ ion impact I have calculated the cross sections taking Z_{eff}=1.0 and Z_{eff}=1.22. In ionisation processes the He^+ ion can be considered equivalent to an effective charge, Z, lying somewhere between actual net charge and the total nuclear charge (see Martin et all[33]). As pointed out by Martin et al, a He^+ ion at high energy (corresponding to 800 KeV) can be considered equivalent to a point charge with Z=1.22. However, the value of Z_{eff} is slightly energy dependent but I have taken Z_{eff}=1.22 throughout the energy range considered, as suggested by Martin et al[33] and also supported by de Heer at el[34]. The same calculations have been repeated with Z_{eff}=1.0 throughout the same energy range. In fig. 2, the present calculated cross sections have been compared with the experimental observations of Dubois and Toburen[31]. However, the experimental results are available only upto 100.0 KeV, so the comparison is restricted up to 100 KeV . I have not compared the present results with other theoretical calculations because no other theoretical results are available in this energy range.

Table 2: $^3He^+$ impact electron capture cross sections for Na

(in units of 10^{-17} cm^2)

Impact energy (KeV)	**Present Calculations**		**Experiment DuBois & Toburen[31]**
	Z=1.0	**Z=1.22**	
10.0	203.00	328.0	
15.0	255.00	423.0	
20.0	247.00	410.0	
30.0	201.00	323.0	
40.0	153.00	253.0	136.00
50.0	81.40	194.0	
60.0	52.00	111.0	44.6
70.0	35.50	75.1	
80.0	25.50	53.8	23.4
90.0	19.20	40.2	
100.0	15.00	31.1	18.5
120.0	10.0	20.4	
150.0	6.9	13.4	
160.0	6.29	12.2	
180.0	5.43	10.4	
200.0	4.35	9.27	
250.0	3.44	7.40	
300.0	2.55	5.56	
400.0	1.60	3.42	
500.0	1.05	2.25	
600.0	.70	1.52	
700.0	.482	1.05	
800.0	.338	0.741	
900.0	.245	0.536	
1000.0	.180	0.395	

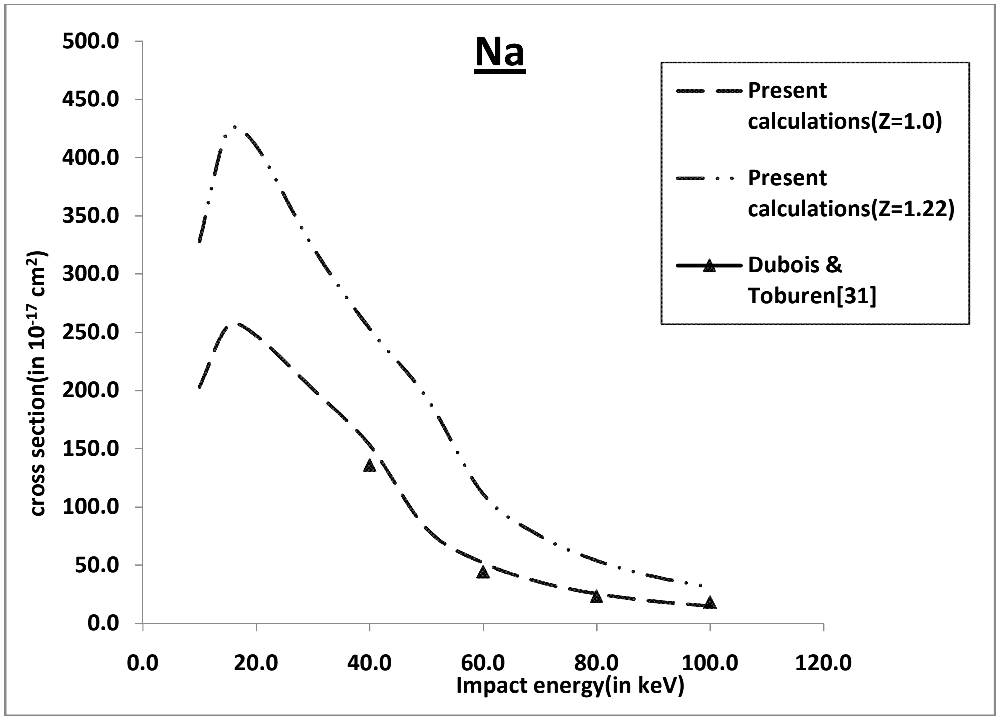

Figure 2: 3He+ impact electron capture cross sections for Na

From the close inspection of the present results it is quite clear that the cross sections when Zeff=1.0 agree well with the experimental observations while when Z_{eff}=1.22 the calculated cross sections overestimate on the experimental data always within a factor of 2 throughout the energy range available (See Martin et al[33]). For still higher energy it can't be compared with experimental observations, as no results are available.

The single electron capture cross sections have been calculated for Na atom due to $^3He^{2+}$ ion impact upto 1000 KeV. The present calculated cross sections have been compared with only experimental results of Dubois and Toburen[31]. The present results and the experimental observations have been given in table 3 as well as in fig. 3. For the sake of comparison I have plotted the graph only up to 200 KeV, because of the availability of the experimental observations. Since no theoretical calculations are available in this energy range. So I have not compared my results with other theoretical calculations.

From the observations of the table – 3 & fig. 3 it is quite clear that the present results of $^3He^{2+}$ ion impact of single electron capture cross sections are in excellent agreement with the experiment.[31]

Table 3: $^3He^{2+}$ impact electrons capture cross sections for Na.

(in units of 10^{-16} cm^2)

Impact energy (KeV)	Present Calculations	Experiment DuBois & Toburen[31]
2.0	1.56	
3.0	9.3	
4.0	27.8	
6.0	68.9	
8.0	99.8	125.00

10.0	128.0	
12.0		163.00
15.0	168.0	
16.0		136.00
20.0	142.0	142.00
30.0	113.0	113.00
40.0	81.4	79.6
50.0	59.3	45.9
60.0	40.1	28.1
80.0	19.9	13.6
100.0	12.2	
120.0	8.32	5.22
150.0	5.73	
160.0		3.83
200.0	3.8	3.39
250.0	2.86	
300.0	2.5	
500.0	1.85	
600.0	1.56	
800.0	0.598	
1000.0	0.335	

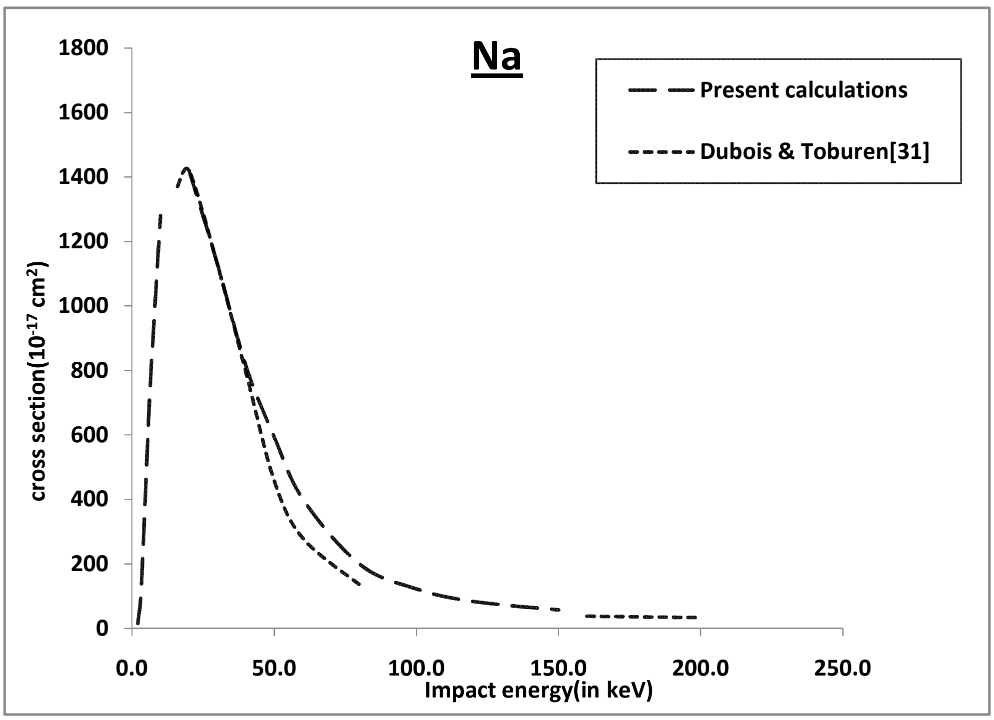

Figure 3: 3**He^{2+} impact electron capture cross sections for Na**

Since there is no experimental results available below energy range 8 KeV, so I can't compare the present calculated results. Also beyond 200 KeV, the comparison is not possible. Overall it can be said that the agreement excellent. The success of the present model may be attributed to the increase in charge state of the projectile.

CONCLUSION

Thus, it can be concluded that the Modified BEA gives a good account of the experimental observations in case of charge transfer process. It has also been noticed that the agreement with experiment improve with increase in charge state of the projectile. Further it is observed that the present model is well suited for heavier atomic targets compared to other quantal or semi quantal approximations. Also it has been found that the present Model is more favourable for more massive projectiles.

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