Charge Transfer in Nitrogen Ion - Hydrogen Atom Interaction in Intermediate and High Energies

Dr Rakesh Samanta

Assistant Professor, Department of Physics, Raja Rammohun Roy Mahavidyalaya, Radhanagar, P.O- Nangulpara, Hooghly, Pin-712406,West Bengal, India.

Abstract : In this paper the main attention has been given mainly on the projectile energies of ionic nitrogen in collision between atomic hydrogen as target in intermediate and high energies. Boundary Corrected Continuum Intermediate State Approximation (BCCIS) formulism has been taken to study the present problem. Theoretical calculation using quantum mechanics has been taken into account in this formulism. The important feature of this method lies in the fact that proper boundary condition is satisfied and intermediate continuum states are accounted properly into the formalism. It may easily be extended to non-coulombic potential as well. We have calculated the charge transfer collision cross sections for different degree ions of nitrogen from atomic hydrogen by reducing the charge exchange amplitude to arbitrary states to a one dimensional integral form. Projectile energies are limited in between 40 keV/ amu and 200 keV/ amu in the present work. Cross sectional data of charge transfer of the collision problem have been given in graphical representation. The calculated cross sections are in good agreement with the other experimental theoretical and experimental available results. The success of the present investigation lies on the fact that the careful construction of the model potential in such a way that the potential parameters are unambiguously determined on imposing several checks. It may be pointed out that in such a formulation the dynamic correlation of the active electrons is absent. Only the static correlations of the electrons have been included. However, the charge transfer dynamics at low energies is very complex even on quantum mechanical framework. Collisions cross sectional data are important in studies of reactors, explanation of astrophysical phenomenon, investigation of ionization radiation and high energy particle transport in inertial controlled fusion (ICF) radiobiology.

***Index Terms* - BCCIS Approximation, Charge transfer, Ion- Atom Collision, Total Collision Cross sections.**

I. INTRODUCTION

Collision cross sectional data is very much important now a day in various fields of Physics as well as different fields of sciences [1]. So the researches on the topic of charge transfer may be single or double are important both for practical and academic point of view. The possible significance of the collision cross sectional data are widely used in Tokamac fusion devices [2,3]. Electron captures by partially or fully stripped heavy ions from ground state atomic hydrogen or helium takes place mainly into excited states due to energy resonance. The charge transfer into excited state by emission of radiation [4] generally belongs to the soft x-ray region. This property of interest may also lead to the possibility of production of an x-ray laser [5-7]. Under these circumstances Boundary Corrected Continuum Intermediate State (BCCIS) approximation successfully formulated by Mandal et al [8] has been incorporated for the study of present problem. The special features of the framework are (i) intermediate continuum states have been introduced (ii) boundary conditions are satisfied properly (iii) This formulation can be incorporated easily to non-coulombic interactions also. In the present paper the systematic and rigorous quantum mechanical investigation on charge transfer has been studied for the collision,

$$N^{Q+} + H\,(1s) \rightarrow N^{(Q-1)+}\,(nlm) + H^{+}$$

where Q=1-5 and n, l, m are the principal, angular and magnetic quantum number of exchanged electron respectively. The range of energy studied is 40 to 200 keV/amu. In this formalism, the static correlation has only been taken, but the dynamic correlation which originates from the electron-electron Coulomb interaction during the collision, was ignored. When many active electrons are involved in ion-atom collisions, one has to face the question of the influence of electronic correlations on the magnitude of the process. Due to the rapid expansion of computer facilities, increasing theoretical attention has been paid in the last ten years to atomic collisions involving many-electron process.

The outline of this article is as follows. In section II, theoretical formulations are given. In section III, results and discussion are the contents. Finally section IV, concluding remarks are given. Atomic unit is used as usual.

II. THEORETICAL FORMULATIONS

The total Hamiltonian for the collision system may be written as

$$H = H_i + V_i = H_f + V_f \tag{1}$$

where, $H_i = -\frac{1}{2\mu_i}\nabla^2_{R_T} + \frac{Z_P(Z_T-1)}{R_T} - \frac{1}{2a}\nabla^2_{r_T} - \frac{Z_T}{r_T}$, $\qquad V_i = \frac{Z_P}{R_T} - \frac{Z_P}{r_P}$

and $\quad H_f = -\frac{1}{2\mu_f}\nabla^2_{R_P} - \frac{1}{2b}\nabla^2_{r_P} - \frac{Z_P}{r_P}$, $\qquad V_f = \frac{Z_P Z_T}{R_T} - \frac{Z_T}{r_T}$

$$\mu_i = \frac{M_P(1+M_T)}{1+M_P+M_T},\ \mu_f = \frac{M_T(1+M_P)}{1+M_P+M_T},\ a = \frac{M_T}{1+M_T},\ b = \frac{M_P}{1+M_P}.$$

Here e, T and P present active electron, target ion and projectile ion respectively. $\vec{R}_T$ and $\vec{R}_P$ be the position vector of P and T relative to the centre of mass of (T, e) and (P, e) respectively. The initial non-perturbed wave function is given by

$$\psi_i = \varphi_i(\vec{r}_T)\chi_i^+(\vec{R}_T) \tag{2}$$

where $\varphi_i(\vec{r}_T)$ is the initial bound state wave function. The function $\chi_i^+(\vec{R}_T)$ is an outgoing Coulomb continuum wave function representing the projectile ion moving in the field of an effective ion of charge (Z_T-1), so the Schrodinger equation is

$$(E - H_i')\chi_i^+ = 0$$

where $\chi_i^+(\vec{R}_T) = e^{-\frac{\pi}{2}\alpha_3}\Gamma(1+i\alpha_3)e^{i\vec{k}_i\cdot\vec{R}_T}\,{}_1F_1\{-i\alpha_3;1;i(k_iR_T - \vec{k}_i\cdot\vec{R}_T)\}$, $\quad \alpha_3 = \frac{Z_P(Z_T-1)}{v_i}$.

Here $\vec{k}_i$ is the initial wave vector.

The prior form of the transition matrix element, $\quad T_{if}^{(-)} = \langle \psi_f^- | V_i | \psi_i \rangle \qquad (3)$

$$\approx \langle \psi_f^{BCCIS-3B} | V_i | \psi_i \rangle.$$

We write the final wave function,

$$\Psi_f^{BCCIS-3B} = e^{\frac{\pi}{2}(\alpha_1-\alpha_2)}\Gamma(1+i\alpha_1)\Gamma(1-i\alpha_2)e^{i\vec{k}_f\cdot\vec{R}_P}\varphi_f(\vec{r}_P)\,{}_1F_1\{-i\alpha_1;1;-ia(v_f r_T + \vec{v}_f\cdot\vec{r}_T)\}\times$$
$${}_1F_1\{i\alpha_2;1;-ib(k_fR_T + \vec{k}_f\cdot\vec{R}_T)\} \tag{4}$$

where $\qquad \alpha_1 = \frac{Z_T}{v_f}, \qquad \alpha_2 = \frac{Z_P Z_T}{v_f}.$

The transition amplitude can be written as

$$T_{if}^{(-)} = N\iint d\vec{r}_T d\vec{R}_T e^{i\vec{k}_i\cdot\vec{R}_T - i\vec{k}_f\cdot\vec{R}_P}\varphi_f^*(\vec{r}_P)\left(\frac{Z_P}{R_T} - \frac{Z_P}{r_P}\right){}_1F_1\{i\alpha_1;1;ia(v_f r_T + \vec{v}_f\cdot\vec{r}_T)\}\times$$

$${}_1F_1\{-i\alpha_2;1;ib(k_fR_T + \vec{k}_f\cdot\vec{R}_T)\}\varphi_i(\vec{r}_T)\,{}_1F_1\{-i\alpha_3;1;i(k_iR_T - \vec{k}_i\cdot\vec{R}_T)\} \tag{5}$$

where $N = e^{\frac{\pi}{2}(\alpha_1-\alpha_2-\alpha_3)}\Gamma(1-i\alpha_1)\Gamma(1+i\alpha_2)\Gamma(1+i\alpha_3)$.

Using integral representation ${}_1F_1(i\alpha;1;z)=\dfrac{1}{2\pi i}\oint d\tau\,\tau^{i\alpha-1}(\tau-1)^{-i\alpha}\,e^{\tau z}$ .The transition amplitude of equation (5) may be written as

$$T_{if}=\frac{AN}{(2\pi i)^3}\lim_{\varepsilon_1\to 0}D(\varepsilon_1,\lambda,\beta)\oint dt_1 t_1^{i\alpha_1-1}(t_1-1)^{-i\alpha_1}\oint dt_2 t_2^{-i\alpha_2-1}(t_2-1)^{i\alpha_2}\oint dt_3 t_3^{-i\alpha_3-1}(t_3-1)^{i\alpha_3}\,J$$

Where, $$J=\iint d\vec{r}_T d\vec{R}_T\; e^{i\vec{k}_i.\vec{R}_T-i\vec{k}_P.\vec{R}_P+ia\vec{v}_f.\vec{r}_T t_1+ib\vec{k}_f.\vec{R}_T t_2-i\vec{k}_i.\vec{R}_P t_3}\,\frac{e^{-\beta_1 r_T}}{r_T}\frac{e^{-\lambda r_P}}{r_P}\frac{e^{-\varepsilon R_T}}{R_T}, \qquad (6)$$

$$\beta_1=\beta-iav_f t_1 \quad\text{and}\quad \varepsilon=\varepsilon_1-ibk_f t_2-ik_i t_3.$$

Here the constant A is originating from the initial and final bound state wave functions. $D(\varepsilon_1,\lambda,\beta_1)$ is a parametric differential operator used to generate higher state wave functions. β and λ are the orbital exponent of the initial and the final bound state wave functions.

Taking the Fourier transform of equation (6) and using integral representation of general three denominator integration of Lewis [14], Sinha and Sil [15],

$$J=\frac{16\pi^2}{a^2}\int_0^\infty\frac{dx}{a'x^2+2b'x+c'}. \qquad (7)$$

Using equation (7), the transition matrix element now becomes

$$T_{if}=\frac{NA}{(2\pi i)}\frac{16\pi^2}{a^2}\lim_{\varepsilon_1\to 0}D(\varepsilon_1,\lambda,\beta)\oint dt_2 t_2^{-i\alpha_2-1}(t_2-1)^{i\alpha_2}\int_0^\infty K\,dx \qquad (8)$$

where $$K=\frac{1}{A}\left(\frac{A}{A+B}\right)^{i\alpha_1}\left(\frac{A}{A+C}\right)^{-i\alpha_3}{}_2F_1\{i\alpha_1;-i\alpha_3;1;z\},\qquad z=\frac{BC-AD}{(A+B)(A+C)}.$$

Now the complex integration of t_2 is converted to real integral [16,17], which is subdivided into a number of sub-intervals and each sub-interval is integrated numerically using Gauss Laguerre quadrature method. Lastly a single electron capture cross sections is obtained numerically over scattering angles with the Gauss Legendre quadrature method. The orders of two dimensional integral are varied until convergence to three decimal places is obtained for the total charge transfer cross sections.

III. RESULTS AND DISCUSSION

Cross sectional data of charge transfer of the collision problem $N^{Q+} + H(1s) \rightarrow N^{(Q-1)+}(nlm) + H^+$ have been given in graphical representation and is given from Fig.1 to Fig. 5. The projectile charge increase from Q=1 to Q=5. For charge transfer where in excited states short ranged potential have negligible effect. Total cross sections have been obtained by adding all the sub shell cross sectional data. Convergence improves with decreasing charge state of the projectile ion and approximately equals to 10% for Q=2. Charge transfer results are displayed in Fig. 1 to Fig. 5. The results are compared with the other theoretical and experimental results obtained. Finally cross section vs charge graph displayed in Fig. 6 at 100 KeV/ amu. In Fig. 1 the experimental results are depicted for collision of N^+ with atomic hydrogen in the intermediate and high energy region. We can see the discrepancy with the experimental data of Phaneuf et al [9] and OBK- approximation of Eichler et al [10] with increasing energies. The compared results are plotted for the collision of N^{2+} and N^{3+} also with atomic hydrogen in fig Fig. 2. We may find the magnitudes of the cross sections for N^{2+} ions have a good agreement with the experimental findings of Phaneuf et al at lower energies. Compared results are found a good agreement with the experimental results [9, 10] and we can see the total charge transfer collision collision depend on energy of impact and the charge state of the projectile ions. It has almost no dependence on the structure of the structure of incoming projectile ions. The computed results for projectile ions with charges Q= 4 and Q= 5 have good agreement with the CTMC results of Olson and Salop [11].

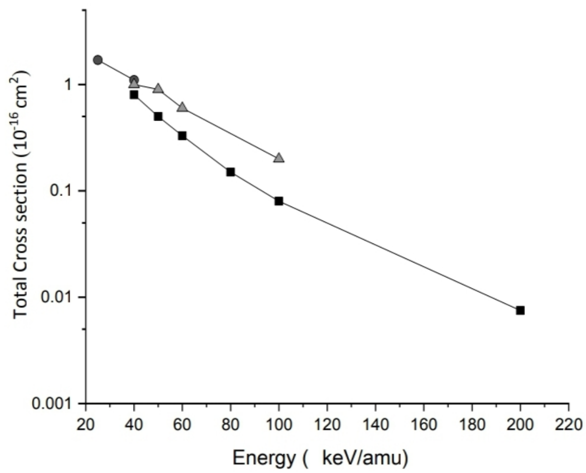

Fig 1. *N^+ + H (1s) Collisions. -■-, results of present work, -●-, Experimental result of Phaneuf et al, -▲-, OBK approximation of Eichler et al.*

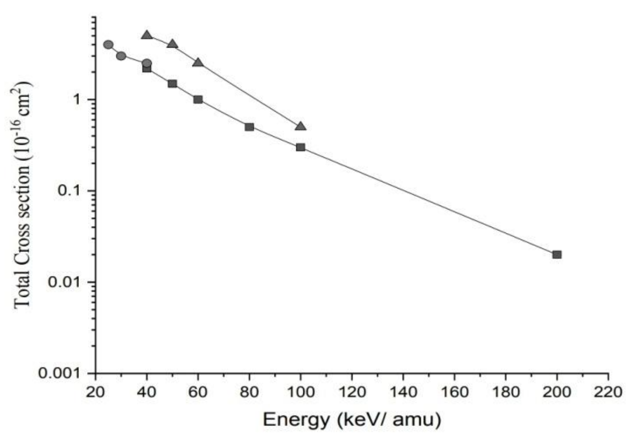

Fig 2. *N^{2+} + H (1s) Collisions. -■-, results of present work, -●-, Experimental results of Phaneuf et al, -▲-, OBK approximation of Eichler et al.*

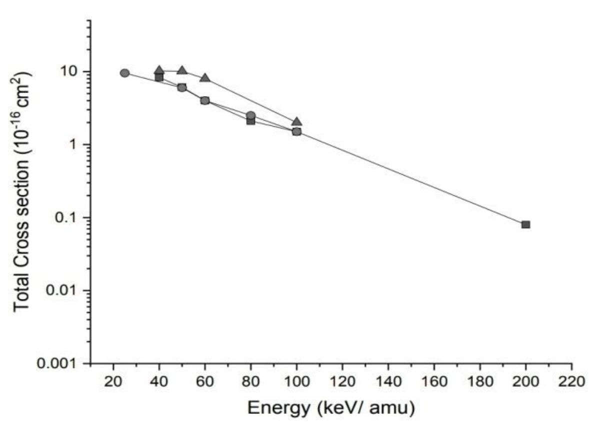

Fig 3. *N^{3+} + H (1s) Collisions. -■-, results of present work, -●-, Experimental results of Phaneuf et al, -▲-, OBK approximation of Eichler et al.*

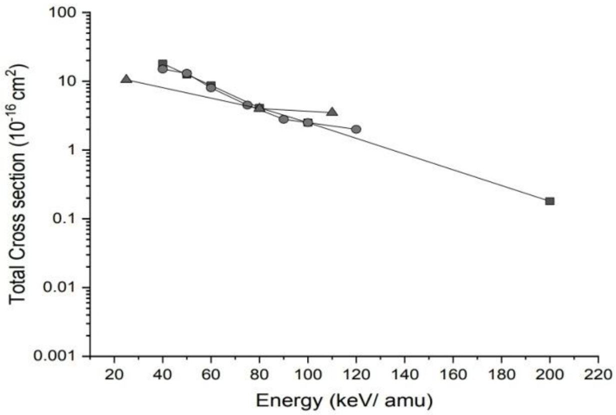

Fig 4. *N^{4+} + H (1s) Collisions. -■-, results of present work, -●-, Experimental results of Phaneuf et al, -▲-, CTMC results of Olson and Salop.*

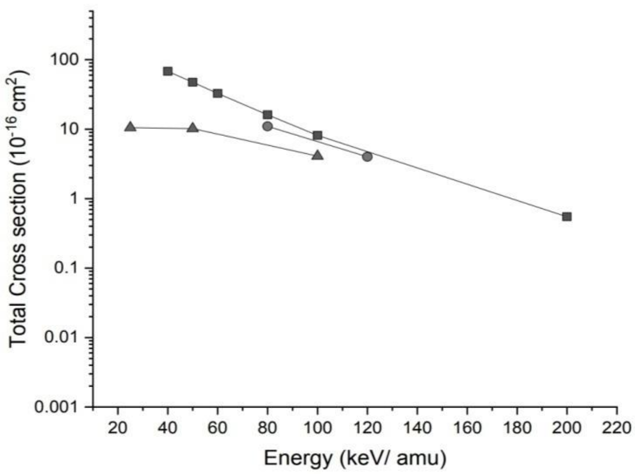

Fig 5. *N^{5+}+ H (1s) Collisions. -■-, results of present work, -●-, Experimental results of Phaneuf et al, -▲-, CTMC results of Olson and Salop.*

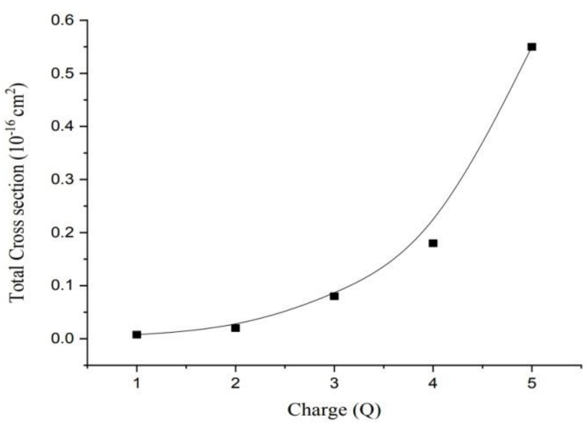

Fig 6. *Total cross section vs Charge graph at collision energy 200 keV/ amu of present work.*

Oscillations in charge dependence of the total charge transfer cross sections have been observed by Kim et al [12]. They explained the interference between the amplitudes obtained from the short-range part and the long-range part of the potential experienced by the electron with the projectile ion. But there is no such oscillations have been found [13] in collisions of projectiles like Si^{9+}, Fe^{9+}, Mo^{9+} etc. From Fig. 6, the theoretical observation of this work no such oscillations have been found. We cannot expect the interference term is significant because as the charge state of the projectile increases, charge transfer into excited state dominates. So the influence of short-range part of the potential is negligibly small in comparison to the long range part.

IV. CONCLUSION

The results so obtained are reasonably encouraging over the entire range of energy. This may be due to the fact that: (i) the continuum state of the active electron with the stronger charge has been taken into account; (ii) the scattering wavefunction satisfies the boundary condition; and (iii) the transition potential is faster falling than the coulomb potential. Electron correlation effect has been underestimated in our formalism. However, for single-electron capture process in an asymmetric collision ($Z_P > Z_T$) in a multi-electron environment, the accurate study of correlation effect is important to test the validity of the BCCIS approximation.

The computed results are compared with the available experimental observations. It is evident that, for the study of collisions problem of very low charged ions with neutral atoms, all the possible interaction possibility has to be taken in the interaction of the active electron with projectile ion. It is also seen from the total collision cross section data that if the projectile energies increases, the capture cross section gradually decreases. The oscillatory structure of the charge dependence of the total capture cross sections is not found in the present work using BCCIS formalism. Under this circumstance, more works should be carried out in studies of charge transfer in collision problems of partially stripped ions with neutral atoms.

REFERENCES

1. Osterbrock D E. Astrophysics of Gaseous Nebulae and Active Galactic Nuclei: Mill Valley: University Science Book, 1989.
2. Coleman J P. Case Studies in Atomic Collision Physics. Vol. 1, Ch. 3. North-Holland, 1969.
3. Marinković BP, Pejčev V, Filipović DM, Šević D, Milosavljević AR, Milisavljević S, Rabasović MS, Pavlović D, Maljković JB. Cross section data for electron collisions in plasma physics. *Journal of Physics: Conference Series*. 2007; 86, 012006 (1-8). DOI:10.1088/1742-6596/86/1/012006.
4. Isler RC, Crume EC. Charge-transfer excitation of impurity ions in Tokamaks. *Physical Review Letters.* 1978; 41, 1296-1300. DOI:https://doi.org/10.1103/PhysRevLett.41.1296.
5. Joachain CJ, Post DE. Atomic and Molecular Physics of Controlled Thermonuclear Fusion, Plenum Publishing Company. 1983.
6. Elton Raymond C. X-Ray Lasers, Academic Press, 1990.
7. Marrus Richard. Physics of Highly-Ionized Atoms, NATO Science Series B: Volume 201, 1989.
8. Mandal CR, Mandal M, Mukherjee SC. Excited-state positronium formation from positron–atomic-hydrogen collisions, *Physical Review A*. 1991; 44, 2968-2974. DOI: https://doi.org/10.1103/PhysRevA.44.2968.
9. Phaneuf RA, Mayer FW, McKnight RH. Single-electron capture by multiply charged ions of carbon, nitrogen, and oxygen in atomic and molecular hydrogen. *Physical Review A*. 1978; 17, 534-545. DOI:https://doi.org/10.1103/PhysRevA.17.534.
10. Eichler J, Suji AT, Ishihara J. Electron capture into partially stripped projectile ions. *Physical Review A*. 1981; 23, 2833-2840. DOI:https://doi.org/10.1103/PhysRevA.23.2833.
11. Olson RE, Salop A. Charge-transfer and impact-ionization cross sections for fully and partially stripped positive ions colliding with atomic hydrogen. *Physical Review A*. 1977; 16, 531-541. DOI:https://doi.org/10.1103/PhysRevA.16.531.
12. Kim HJ, Hvelplund P, Mayer FW, Phaneuf RA, Stelson PH, Bottcher C. Observation of Oscillations in the Charge Dependence of Total Electron-Capture Cross Sections. *Physical Review Letters.* 1978; 40, 1635-1638. DOI:https://doi.org/10.1103/PhysRevLett.40.1635.
13. Kim HJ, Phaneuf RA, Mayer FW, Stelson PH. Single electron capture by multiply charged ^{28}Si ions in atomic and molecular hydrogen. *Physical Review A*. 1978; 17, 854-858. DOI: https://doi.org/10.1103/PhysRevA.17.854.
14. Lewis RR. Potential Scattering of High-Energy Electrons in Second Born Approximation. *Physical Review*. 1956; 102, 537-543. DOI:https://doi.org/10.1103/PhysRev.102.537.
15. Sinha C, Sil NC. Electron Impact Excitation of hydrogenic ions to arbitrary states including exchange effects. *Journal of Physics B: Atomic and Molecular Physics*. 1978; 11, L333-L335. https://iopscience.iop.org/article/10.1088/0022-3700/11/10/005.
16. Mukherjee SC, Roy K, Sil N C. *Evaluation of the Coulomb integral for scattering problems*. *Physical Review A.* 1975; 12, 1719-1721. DOI:https://doi.org/10.1103/PhysRevA.12.1719.
17. Sinha C, Tripathi S. Electron impact ionization of atomic hydrogen. *Journal of Physics B: Atomic and Molecular Physics*. 1991; 24, 3659-3668. https://iopscience.iop.org/article/10.1088/0953-4075/24/16/018