PART - I

Charge Transfer in Ion-ion Collisions
CHAPTER - I

1. General Introduction: Past work and Present study:

In recent years the study of the charge transfer phenomenon has immense importance in the field of plasma physics, thermonuclear fusion and astrophysical problems. So the study of the charge transfer phenomena is not only to have an understanding of basic mechanism of rearrangement collision, it has practical importance too. The charge exchange also takes place in laboratory and astrophysical plasma's decay and formation. The state selective nature of this phenomenon can be applied in the diagnostic systems for laboratory plasmas, in pumping atomic levels that exhibit laser action and other application too.

Charge exchange reaction in atomic physics is one in which an electron or several electrons are transferred from one atomic system to the other as a result of collision between ions or atoms. Our interest is in the study of the charge exchange in two-body ion-ion collision with subsequent neutralization of one of the ions. The charge exchange reaction under consideration is of the form

\[ A^+ + B^{1+} \rightarrow A^0 + B^{2+} \]

In 1923, Henderson [1] was doing experiments on \( \alpha \) -particles passing them through absorbing screens of mica—, as a result of his observations, he discovered the phenomena of charge exchange. Later it was studied by Rutherford [2] in 1924 and Jacobson [3] in 1926. After the discovery of charge transfer, Thomas [4] in 1927 constructed a theoretical model of charge transfer based on classical mechanics. Classically, the target atom has uniform spherical electron distribution on the surface of it and all electrons are stated to be stationary. Firstly, ion A strikes on an electron of B. And this electron comes out after colliding with the nucleus of B-the target, with the same velocity and direction as that of A. This outgoing
electrons are considered to be captured. Thomas [4] found the capture cross section decreasing with $v^{-11}$ where $v$ is velocity of projectile. This asymptotic decrease of non-relativistic cross section is also achieved by the quantum mechanical approach.

First application of quantum mechanics to describe charge transfer was done by Oppenheimer [5] in 1928 by using perturbation treatment. But Brinkman and Kramer [6] in 1928 gave first explanation of perturbation theorem to describe charge transfer phenomena and usefully applied the fact that except in very low energy, the wavelength associated with the relative motion of the heavy particle is very small compared to the distance over which the interaction has taken place. As a consequence, heavy particles follow a classical Newtonian trajectory, while electronic motion follows quantum mechanical rules. At low energies, the charge exchange cross section is large and a perturbation treatment is non-adequate. When the velocity of heavy particle is small, the interaction time is long compared with the characteristic time of electrons in bound state orbits. Under this circumstances the electron to be captured is shared between the two ions during the collision, forming a quasi molecule. As the ions separate, the probabilities of capture by the projectile or of remaining associated with the target ion are comparable. Later, Massey and Smith [7] in 1933 developed a theory on charge transfer based on the expansion of electronic wave function in series of molecular orbital. This model had some serious difficulties, which was corrected and presented in modern forms by McCarrrell [8] (1968). But, it is only after the development of ion accelerators; quantitative measurements of cross-section of inelastic scattering could be done. Systematic measurements of total cross section over wide range of energies and processes were carried out first in 1960. Then slightly later, followed measurements of angular distribution of the scattered particles. Very recently, experiments on angular distribution of charged particles in charge exchange reaction are being carried on in Geissen, Germany [9].

We shall give below some basic mathematical preliminaries used in quantum mechanical calculation of charge transfer and Lippman and Schwinger Integral equation on post-prior discrepancy.
2. The Schrödinger equation:

The time independent non-relativistic Schrödinger equation [10] for the three body system \(A^+, B^+\) and \(e^-\) is

\[
H\psi = E\psi
\]

where \(H = T + V\)

and \(T\) and \(V\) are kinetic and potential energy operators respectively, \(E\) being the total energy.

It is convenient to work in the position representation and in the center-of-mass (CM) frame. Two independent position vectors are required to describe the relative motion of the particles in center-of-mass frame and these can be chosen as in defined as follows and illustrated in fig. 1 [10].

The kinetic energy operator \(T\) takes a simple form in Jacobi coordinates.

Fig. 1: Relative coordinates for a one electron system. \(A\) and \(B\) are nuclei, or ionic cores, with masses \(M_A\) and \(M_B\) respectively. \(C\) is the centre of mass of \(A\) and \(B\), \(C_1\) is the CM of \(A\) and the electron \(e\), and \(C_2\) is the CM of \(B\) and the electron. \(O\) is an arbitrary point on the line \(AB\) with \(AO = pR\) and \(BO = qR\) with \((p+q) = 1\).
2.1. Co-ordinate set:

In the fig. 1 coordinates \((x, \rho)\), \(x\) is defined as the position vector of \(e'\) relative to \(A^+\), while \((\rho)\) is the position vector of \(B^+\), relative to the CM of the sub-system \((A^+ + e')\). This set of coordinates provides the simplest description of the arrangement \(B^+ + (A^+ + e')\) in the charge exchange channel. The kinetic energy operator is expressed as

\[
T = -\frac{1}{2m_A} \nabla^2 x - \frac{1}{2\mu_B} \nabla^2 \rho, \tag{2.2}
\]

Where the reduced masses are

\[
m_A = \frac{M_A}{M_A + 1}, \quad \mu_B = \frac{M_B(M_A + 1)}{M_A + M_B + 1} \tag{2.3}
\]

2.2. The potential energy:

The potential energy operator is the sum of the inter-particle interaction energies:

\[
V = V_{Ae}(x) + V_{Be}(r) + V_{AB}(R) \tag{2.4}
\]

Where, \(x, r, R\) are to be expressed in the form of independent variables given above. In the case of proton scattering by atomic hydrogen, both \(A^+\) and \(B^+\) are protons, and the interactions are Coulombic (spin-orbit coupling being neglected) with

\[
V_{Ae} = -\frac{1}{x}, \quad V_{Be} = -\frac{1}{r}, \quad V_{AB} = -\frac{1}{R} \tag{2.5}
\]

More generally, \(V_{Ae}, V_{Be}\) and \(V_{AB}\) are effective potentials chosen to represent the interaction between the 'active' electron and the ion cores A and B, and the interaction between the cores. It will be assumed that these effective potentials are central. For example, if \(A^+\) and \(B^+\) represent \(H^+\) and \(He^+\) ions, \(V_{Ae}\) and \(V_{Be}\) represent effective central potentials between the electron and \(H^+\) and \(He^+\) ions.
respectively, and $V_{ab}$ represents an effective $H^+ - He^+$ interaction. Usually, a specific form is chosen for a potential such as $V_{ab}(x)$ depending on parameters which are adjusted so that on diagonalizing the Hamiltonian $H_A$ of the atom $(A^+e^-)$, where

$$H_A = -\frac{1}{2}\nabla^2_x + V_{ae}(x),$$

the energy spectrum obtained represents the observed energy spectrum of the atom as accurately as possible. The problems that arise in constructing effective potentials have been discussed by, among others, Bardsley [11], Daniele [12], Peach [13], and Ermolaev [14].

2.3. Exchange scattering:

To determine the asymptotic form of the wave function in the charge exchange channels, above coordinate set is used. At large separations of the atom $(A^+e^-)$ and the residual ion $B^+e^-$, $\rho \gg x$, and $\psi \rightarrow \psi_B$, where the asymptotic wave function satisfies the equation

$$\left[ -\frac{1}{2}\nabla^2_x - 1/2\nabla^2_x + V_{ae}(x) - E \right] \psi_B = 0 \quad (2.6)$$

The wave function $\chi_{\eta}(x)$ and eigen energies $\eta_\eta$ of the atom $(A^+e^-)$, are introduced where $n$ labels all necessary quantum numbers, satisfying

$$\left[ -1/2\nabla_x^2 + V_{ae}(x) - \eta_\eta \right] \chi_n(x) = 0 \quad (2.7)$$

with

$$\langle \chi_n | \chi_{\eta} \rangle = \int \chi_n^* (x) \chi_{\eta}(x) dx = \delta_{n\eta} \quad (2.8)$$

Solutions of (2.6) are of the form $G_\eta(p)\chi_{\eta}(x)$ and the general solution is

$$\psi_B = \sum_n G_\eta(x) \chi_n(x), \quad (2.9)$$
where the sum is over the whole set of functions $\chi_a(x)$ and where $G_n(p)$ is a solution of the free particle equation

$$\left[-\frac{1}{2\mu} \nabla^2_p - \frac{1}{2\mu} k^2 \right] G_a(p) = 0$$

(2.10)

with

$$-\frac{1}{2\mu} k^2 = (E - \eta_a)$$

(2.11)

Since there is no incident plane wave in any arranged channel, for $k^2 > 0$,

$$G_n(p) = \rho^{-1} g_{nl}(\theta, \phi) \exp i k_{nl} p$$

(2.12a)

and in closed channels with $k^2 < 0$,

$$G_n(p) \rightarrow 0 \quad \text{as} \quad p \rightarrow \infty$$

(2.12b)

where $(\theta, \phi)$ are the polar angles of $p$. The differential cross sections for charge exchange from the incident channel $n$ are determined by the scattering amplitudes $g_{nl}$ by

$$\frac{d\sigma^C_n}{d\Omega} = k_n \left| g_{nl}(\theta, \phi) \right|^2$$

(2.13)

The total charge exchange cross section for capture into the final state $n$ is

$$\sigma^C_n = \frac{k_n}{k_l} \int_{(\theta_n)} \left| g_{nl}(\theta, \phi) \right|^2 d\Omega$$

(2.14)
3. **Lippman and Schwinger Integral equation**:

Let A and B be two complete systems such as atoms or molecules. In absence of interaction these may be described by wave functions $\varphi_A$ and $\varphi_B$; which are Eigen states of some Hamiltonian $H_1$ and $H_2$ respectively. These states are

$$|A;B\rangle = \langle \varphi_A | \varphi_B \rangle$$

(3.1)

form a complete set of eigen states of the Hamiltonian

$$H_0 = H_1 + H_2$$

(3.2)

Where,

$$H_1 | \varphi_A \rangle = E_A | \varphi_A \rangle$$

(3.3a)

$$H_2 | \varphi_B \rangle = E_B | \varphi_B \rangle$$

(3.3b)

Let, $H_I$ be the interaction between the two complete states A and B. When these are left to interact and let

$$H = H_0 + H_I$$

(The total Hamiltonian $H$ may have bound states, but we assume that energies of such eigen states are less than minimum $(E_A + E_B)$), then the incoming and outgoing scattering states $| \varphi_{AB} \rangle$ may be defined by the Lippman-Schwinger integral equation

$$| \varphi_{AB} \rangle = |A;B\rangle + \frac{1}{E_{AB} - H_0 + i\varepsilon} H_I | \varphi_{AB} \rangle$$

(3.4)

$$E_{AB} = E_A + E_B$$

These states are however eigen states of total Hamiltonian $H$, i.e.
The state $|\Phi_{AB}\rangle$ has an incoming plane wave corresponding to the second term. Similarly, $|\Phi_{-AB}\rangle$ represents an outgoing plane wave together with an incoming scattered wave.

Let us consider the scattering process

$$A+B \leftrightarrow C+D \quad (3.6)$$

Where, states $A$ and $B$ are eigenstates of Hamiltonian as $H_1$ and $H_2$ (direct scattering) or some different Hamiltonians $H'_1$ and $H'_2$ (re-arrangement scattering) such that

$$H = H_1 + H_2 = H'_1 + H'_2 \quad (3.7)$$

$H_1$ and $H'_1$ being the pre and post interactions. Initial and final scattering states satisfy the equations

$$|\Phi^+_{A,B}\rangle = |A; B\rangle + \frac{1}{E_{AB} - H + i\eta} (H - E_{AB}) |A; B\rangle \quad (3.8)$$

$$|\Phi^-_{C,D}\rangle = |C; D\rangle + \frac{1}{E_{CD} - H - i\eta} (H - E_{CD}) |C; D\rangle \quad (3.9)$$

We may write the last outgoing scattering states in terms of incoming scattering states as

$$|\Phi_{CD}\rangle = |\Phi^*_{CD}\rangle + \left( \frac{1}{E_{CD} - H + i\eta} - \frac{1}{E_{CD} - H - i\eta} \right) (H - E_{CD}) |C; D\rangle \quad (3.10)$$

Now, we may define the scattering amplitude as the scalar product
\[ S_{fi} = \left< \Psi_{CD} \left| \Psi_{AB}^+ \right> \right. \]  
\[ = \left( \Psi_{CD}^+ \left| \Psi_{AB}^+ \right> + \langle C; D \mid (H - E_{CD}) \right) \]  
\[ \left( \frac{1}{E_{CD} - H + i\eta} - \frac{1}{E_{CD} - H - i\eta} \right) \left| \Psi_{AB}^+ \right> \]  
\[ = \lim_{\eta \to 0} \left[ \frac{i\eta}{E_{AB} - E_{CD} + i\eta} \langle C; D \mid A; B \rangle - \frac{2i\eta}{(E_{AB} - E_{CD})^2 + \eta^2} \langle C; D \mid (H - E_{CD}) \mid \Psi_{AB}^+ \rangle \right] \]  

(3.12)

In deducing the final step, one uses the fact \( \mid \Psi_{AB}^+ \rangle \) is an eigenfunction of \( H \). It is interesting to note that \( S_{fi} \) is zero unless \( E_{AB} = E_{CD} \) (i.e., if transition energy remains conserved). Next we see that in direct scattering \( \langle A; B \rangle \) and \( \langle C; D \rangle \) are eigenstates of the same Hamiltonian and hence \( \langle A; B \mid C; D \rangle = \delta_{fi} \). In rearrangement collisions this scalar product is in general non-zero but is always small. Consequently one put \( \delta_{fi} \) for the first term of Eqn.(3.12). This is subject to the criticism [15]– (Goldberger and Watson, 1964). Thus one finally have

\[ S_{fi} = \delta_{fi} - 2\pi i \delta(E_{AB} - E_{CD}) \left< C; D \left| (H - E_{CD}) \right| \Psi_{AB}^+ \right> \]  

(3.13)

Alternatively, one may express \( \mid \Psi_{AB}^+ \rangle \) in terms of \( \mid \Psi_{AB}^- \rangle \), proceeding as before and finally

\[ S_{fi} = \delta_{fi} - 2\pi i \delta(E_{AB} - E_{CD}) \left< \Psi_{CD}^- \left| (H - E_{CD}) \right| A; B \right> \]  

(3.14)

and we write,

\[ S_{fi} = \delta_{fi} - 2\pi i \delta(E_{AB} - E_{CD}) R_{fi} \]  

(3.15)
S is known as S-matrix or scattering matrix and R is known as R matrix or reaction matrix. Finally, differential cross section for the transition is

\[
d\sigma = \frac{(2\pi\hbar)^2 \delta(E_{AB} - E_{CD})}{R_{jj}^2 / \text{flux}}
\]  

(3.16)

Actually, one is always interested in transition to a group of final states, with energy between \(E_{CD}\) and \(E_{CD} + \delta E_{CD}\) and density of state \(\rho_{CD}\). The cross section for such transition is

\[
d\sigma = \frac{(2\pi\hbar)^2 R_{jj}^2 \rho_{CD}}{\text{flux}}
\]  

(3.17)

In practice, one determines \(R_{jj}\) through approximation. If one approximates \(\langle \phi^+_{AB} \rangle\) in Eqn. (3.13) by \(\langle A, B \rangle\) then one gets the first Born result

\[
R_{jj} = \langle C, D \rangle (H - E_{CD}) \langle A, B \rangle
\]  

(post-interaction form)  

(3.18)

or alternatively one may get from Eqn.(3.14) the result

\[
R_{jj} = \langle C, D \rangle (H - E_{AB}) \langle A, B \rangle
\]  

(pre-interaction form)  

(3.19)

Finally one may proceed to higher order of approximation [16], by an iterative procedure. The post -prior discrepancy in the present calculation of CT cross section is shown in chapter II, Part-I.

4. An Observation:

There are two respects in which the calculation of cross section is based on first-order perturbation theory (Born Approximation : Schiff [17]). First, the matrix element should be regarded as small, so that the interaction between the interacting particles is treated to first order. Second, the charged projectile wave
function is treated as a plane wave in the initial state. It is very difficult to improve on the calculation from the first point of view, and it is hardly worthwhile because of the smallness of the interaction term. On the other hand, an improvement with regard to the second point is feasible, and can be accomplished by making use of the distorted wave Coulomb-Born approximation.

5. Hypotheses:

The following hypotheses stated in full form were tested.

The study of the angular differential cross section (ADCS) for charge neutralization in ion-ion collision in QM approach needs attention to the following important points:

i. Inclusion of total interaction potential both in the post and in the prior reaction channels.

ii. Coulomb boundary conditions [12].

iii. Translational factors.

iv. Coulomb Distorted wave functions.
6. References: