2.1. Introduction

Charge-transfer processes between multi-charged ions and hydrogen atoms are of considerable interest and have recently received appreciable attention in connection with its practical applications in controlled thermonuclear fusion processes\(^1,2\), astrophysical plasmas\(^3\), and in the development of X-ray laser devices\(^4,5\). Most of the recent experimental measurements and theoretical works have been focused on the determination of total capture cross sections. Electron capture from hydrogen atoms by multi-charged ions \(Z_p^+\), leads to the production of excited projectile states

\[
Z_p^+ + H(1s) \rightarrow X^{(Z_p-1)^+} + H^+ \tag{1}
\]

If the incident ion is fully stripped so that \(Z_p\) is equal to the
nuclear charge, the ion $X^{(Z_p-1)+}$ is hydrogenic and characterized by a set of single-electron quantum numbers $n_l m$.

Recently, the experimental investigations$^5$–$^9$ have been undertaken with a view to studying the role played by the impurities in neutral beam heating of tokamak fusion plasmas and this requires a knowledge of the subshell populations. However, the theoretical investigations to study the distribution of excitation in projectile ions resulting from electron capture in collisions between fully stripped ions and atomic hydrogen are available only in a very few cases. This is because of the fact that with increasing projectile charge, the electrons are captured into increasingly higher principal shells of the projectile. Quantum mechanical calculations suffer from serious computational difficulties for the calculation of cross sections for such high quantum states.

As an alternative approach, the classical trajectory Monte Carlo method has been applied by Salop$^{10}$ to study the distribution of capture into the excited states resulting from collisions between fully stripped ions of $C^{6+}$, $O^{8+}$ and $B^{5+}$ and atomic hydrogen. The classical distributions in angular momentum and binding energy are converted into the distributions over $n, l$ states. However, such a procedure may not be fully justified for small values of $n$ and $l$.

Obviously, quantum mechanical calculations for electron capture into arbitrary states of $X^{(Z_p-1)+}$ ion formed by, fully
stripped projectiles passing through hydrogen atoms are motivated by these new experiments to study these cross sections. Some efforts have been made on this motivation in recent years. Among these are the calculations performed in the unitarized distorted-wave approximation (UDWA), eikonal approximation, two-state atomic expansion model and continuum-distorted-wave (CDW) approximation.

Electron capture into highly excited states of atomic hydrogen formed by fast protons passing through hydrogen atoms and some ionic targets has been investigated in the first Born approximation (FBA) and first order Coulomb-Born (CB) approximation. However, the FBA method though proved valuable in the study of direct collisional processes is open to serious theoretical objections when applied to rearrangement collisions. The partial cross sections for electron transfer from the ground state of hydrogen atom to the excited state of fully stripped ions of $^6$C$^+$, Ne$^{10+}$, and Si$^{14+}$ have been calculated by Ryufuku and Watanabe in the framework of the UDWA.

At high impact energies of the projectile, since the total cross sections in the UDWA approach are overestimated due to the neglect of ionization and excitation channels, the relative distribution of final-state population obtained by this method is not reliable. Cross sections for electron capture into the individual orbitals around the projectiles are also investigated by Bransden et al in the two-state atomic expansion method.
The overlap and exchange matrix elements for any arbitrary values of \( n, l \) and \( m \) required for the calculation of cross sections are obtained from a standard computer package. The cross sections obtained by using the two-state atomic expansion method agree well in shape with the experimental data but always overestimate the experimental findings throughout the energy range \((5-200 \text{ keV amu}^{-1})\) of the projectiles considered. Eichler and Chan\(^2\) have proposed a method for capture of \( 1s \) electrons into arbitrary principal shells \( n \) of energetic projectiles based on the eikonal approximation. This method has been extended\(^{12}\) to describe the capture of hydrogenic \( 1s \) electrons into arbitrary hydrogenic \( n, l \) excited states of fast projectiles. Recently, the eikonal theory has been applied\(^{13,14}\) to describe the charge exchange in fast collisions between arbitrary hydrogenic states of target and projectile. Although the agreement between the eikonal theory and experiment is quite satisfactory for \( H^+ - H \) and \( He^{2+} - H \) collisions even at low projectile energies, the theory overestimates the measured cross sections with increasing projectile charge in the intermediate and high energy region. This is due to the fact that the electron binding energies are kept fixed at their asymptotic values throughout the collision.

First-order methods consider only the direct reaction path, and take no account of couplings to other states which are important in rearrangement processes. It has become increasingly...
apparent in connection with electron capture processes\textsuperscript{29-31} that the first-order methods may be inadequate and it is now well established\textsuperscript{32-34} that one should incorporate the second-order terms to obtain the correct high-energy behaviour of charge-transfer cross sections. Various types of second-order methods, such as the impulse approximation (IA)\textsuperscript{35-37}, continuum intermediate state (CIS)\textsuperscript{38}, and continuum distorted-wave (CDW)\textsuperscript{39} methods have been proposed in connection with the calculation of charge transfer cross sections in the high-energy region.

In the CDW approximation, first introduced by Cheshire\textsuperscript{39}, the associated amplitude for electron capture contains transitions into and from the intermediate states of the continuum. The ambiguity concerning the part played by the internuclear potential is avoided as no term containing the internuclear interaction occurs through the perturbing potential. On the other hand, correct boundary conditions for the charge exchange problem are preserved by taking into account the distortion of the wave function due to the internuclear Coulomb potential. The energy dependence of the capture cross sections in the high-energy limit are in agreement with that predicted by the second-Born approximation\textsuperscript{40}. A full quantal version of this approximation is given by Gayet\textsuperscript{41}, where it is shown that the CDW approximation is the rigorous first-order term of a perturbation series\textsuperscript{42}. The calculation of cross sections for charge transfer in $H^+\text{-H}$, $He^{2+}\text{-H}$, and $H^+\text{-He}$ collisions\textsuperscript{43-45} by the CDW
method is in excellent agreement with experiment in the energy range greater than 100 keV amu\(^{-1}\). It is well known that excitation and ionization processes dominate over charge exchange at high impact-energies. Since all channels are open, the final state of the system can be reached in many ways through different elastic, inelastic, or break-up intermediate channels. It is quite expected that the charge-transfer processes will be significantly affected due to the inclusion of the intermediate channels describing excitation or ionization of two-body subsystems at high energies. The continuum intermediate states are properly taken into account in the CDW approximation and since the CDW method allows for the distortion of the bound electrons by the incident and scattered ion, it is expected to give reliable results in the calculation of the cross sections involving highly charged ions. Belkić and Gayet\(^4\) used the CDW method to calculate electron capture from atomic hydrogen and helium into specific subshells (n\(\leq 4\)) of fast H\(^+\) ion. Further, in their calculation for the capture cross sections of the higher excited states, they have used the repeated parametric differentiation with respect to suitable parameters. Although an extensive study has been performed for the collision of the projectiles, H\(^+\) and He\(^{2+}\) in atomic hydrogen, not much detailed calculations have so far been reported for heavy stripped ion-atom collisions in the CDW method.

As the charge of the incident projectile increases, the electrons are captured into increasingly higher principal shells
of the projectile. The customary procedure for the calculation of cross sections for such high quantum states involves the process of repeated parametric differentiation of the relevant generating function. The number of such differentiations increases with increasing values of \( n \) and \( l \). The generation of higher excited states by this procedure makes the problem almost untenable. An alternative procedure which avoids the use of successive parametric differentiation technique is necessary to deal with the calculation of cross sections for electron capture into arbitrary \( n, l \), and \( m \) states of the projectile.

The present chapter is aimed at developing a method for the calculation of cross sections for electron capture into arbitrary \( n, l \), and \( m \) states of fast projectiles in collisions of fully stripped projectiles with hydrogenic targets in the ground state using the CDW approximation. The present method reduces the scattering amplitudes to a one-dimensional integral in real space which is very convenient for numerical evaluation. The present method has been applied to calculate the charge transfer cross sections for Li\(^{3+}\)-H collisions and the results obtained are compared with the previously reported theoretical results\(^{13,15,46-49}\) and the recent experimental observation \(^{50}\). In a very recent calculation, Crothers\(^{51}\) has also proposed a method using parabolic coordinates for electron capture into arbitrary principal shells \( n \) of the fully stripped projectiles in the framework of the CDW approximation. However, the relative distributions of the final-state population are not available from their calculated results.
Belkić et al.\textsuperscript{52} have recently reviewed the CDW method of Cheshire in the context of electron capture in the intermediate and high energy region.

The present chapter is organized as follows. The development of the continuum distorted-wave approximation for collisions between a fully stripped projectile and an hydrogenic target is described in section 2.2. Our method for obtaining the cross sections for capture into an arbitrary $n|l|m$ state and the numerical procedures used in the present calculation are presented in sections 2.3, 2.4, 2.5, and 2.6. In section 2.7, we present our results followed by discussion. Finally, a concluding summary is given in section 2.8.

2.2. Development of the continuum distorted-wave approximation

In this section we derive the charge exchange amplitude in the continuum distorted-wave approximation for collisions between a fully stripped projectile and an hydrogenic target. To show a systematic development into this theory we start with the formal theory of rearrangement collisions. We also describe the distorted wave formalism for three body rearrangement series and finally we show the derivation of the continuum distorted-wave approximation.

2.2.1. Formal theory of rearrangement collisions

Let $\alpha$, $\beta$, $\gamma$ be three particles interacting through two body potential $V_{\alpha}$, $V_{\beta}$, $V_{\gamma}$ where $V_{\gamma}$ is the interaction between the two particles not labelled by $i$. We consider the process:

$$\alpha + (\beta + \gamma) \rightarrow (\alpha + \gamma) + \beta$$

(2)
with total Hamiltonian
\[ H = K + V_\alpha + V_\beta + V_\gamma \]  
where \( K \) is the kinetic energy operator for the relative motion of the three particles.

We introduce the channel potentials:
\[ v_\alpha = v_\beta + v_\gamma \]  
\[ v_\beta = v_\alpha + v_\gamma \]  
\[ v_\gamma = v_\alpha + v_\beta \]  
The Hamiltonian for the entrance channel is:
\[ H_\alpha = K + v_\alpha = H - v_\alpha \]  
and for the exit channel:
\[ H_\beta = K + v_\beta = H - v_\beta \]  
Let \( \phi_{i,\alpha}^+ \) and \( \phi_{j,\beta}^- \) be the respective eigenfunctions of \( H_\alpha \) and \( H_\beta \) with the same eigenvalue \( E \). The exact transition amplitude from the state \((i,\alpha)\) to the state \((j,\beta)\) may be written in either the 'post' or the 'prior' form respectively:
\[ T_{ij}^{\alpha_+} = \langle \phi_{j,\beta}^- | v_\beta | \psi_{i,\alpha}^+ \rangle \]  
\[ T_{ij}^{\alpha_-} = \langle \psi_{j,\beta}^- | v_\alpha | \phi_{i,\alpha}^+ \rangle \]  
Both forms are equal on the energy shell. \( \psi_{i,\alpha}^+ \) and \( \psi_{j,\beta}^- \) are eigenfunctions of the total Hamiltonian with eigenvalue \( E \) and are shown to satisfy the Lippmann-Schwinger equation:
\[ | \psi_{i,\alpha}^+ \rangle = (1 + G^+ v_\alpha) | \phi_{i,\alpha}^+ \rangle \]
The transition amplitude (9) may be written as:

\[ T_{ij}^{\alpha \beta} = \langle \psi_j^\beta | u_{\alpha \beta} | \phi_i^\alpha \rangle \quad (14) \]

The matrix form of the transition operator is

\[ u_{\alpha \beta} = v_{\beta}(1 + G_{\alpha}^+) \quad (15) \]

\[ v_{\alpha \beta} \] is shown to satisfy the integral equation

\[ v_{\alpha \beta}(1 + \mathcal{K}_1) = v_{\beta} \quad (16) \]

\[ \mathcal{K}_1 = G_{\alpha}^+ v_{\alpha} \quad (17) \]

where \( v_{\beta} \) is the inhomogeneous term and \( \mathcal{K}_1 \) is the Kernel (or homogeneous term) of the integral equation and

\[ G_{\alpha}^+ = (E - H_{\alpha} + ie)^{-1} \quad (18) \]

The equations (16) and (17) are obtained by putting the following relation for \( G_{\alpha}^+ \) in (15)

\[ G_{\alpha}^+ = G_{\alpha}^+ + G_{\alpha}^+ v_{\alpha} G_{\alpha}^+ = G_{\alpha}^+ + G_{\alpha}^+ v_{\alpha} G_{\alpha}^+ \quad (19) \]

After \( N \) iterations, we obtain the following series of operators, wave functions and matrix elements as:

\[ G_{\alpha}^+ v_{\alpha} = \sum_{n=1}^{N-1} (G_{\alpha}^+ v_{\alpha})^n + (G_{\alpha}^+ v_{\alpha})^N (1 + G_{\alpha}^+ v_{\alpha}) \quad (20) \]

\[ \psi^+_{i,\alpha} = \phi_i^\alpha + \sum_{n=1}^{N-1} (G_{\alpha}^+ v_{\alpha})^n \phi_i^\alpha + (G_{\alpha}^+ v_{\alpha})^N \psi^+_{i,\alpha} \quad (21) \]

\[ T_{ij}^{\alpha \beta} = \langle \phi_j^\beta | v_{\beta} (G_{\alpha}^+ v_{\alpha})^N | \phi_i^\alpha \rangle \]

\[ + \langle \phi_j^\beta | v_{\beta} (G_{\alpha}^+ v_{\alpha})^N | \psi^+_{i,\alpha} \rangle \quad (22) \]
In the case of potential scattering, it has been found\textsuperscript{54} that the above three series (20), (21) and (22) are convergent and the first term gives the limit of the cross section for high velocities. However, in the case of rearrangement collision the situation is completely different. It may be shown that, $u_{\alpha \beta}^+$ can be expanded in a power series of $\mathcal{K}_1$ as

$$u_{\alpha \beta}^+ = v_{\beta}(1 + \sum_{n=1}^{\infty} \mathcal{K}_1^n) \quad (23)$$

Unfortunately, it has been shown\textsuperscript{55} that in the case of rearrangement collisions the series (23) is divergent. This is attributed to the existence of disconnected diagrams in which one particle does not interact with the other ones. In the case of three body collisions, $G_{\alpha}^+$ may be written as

$$G_{\alpha}^+ = G_{\alpha}^+ + G_{\alpha}^+ v_{\alpha} G_{\alpha}^+ \quad (24)$$

where

$$G_{\alpha}^+ = (E - K + i\epsilon)^{-1} \quad (25)$$

Equation (17) may be expressed as:

$$\mathcal{K}_1 = \mathcal{K}_0 + \mathcal{K}' \quad (26)$$

$$\mathcal{K}_0 = G_{\alpha}^+ v_{\alpha} \quad (27)$$

$$\mathcal{K}' = G_{\alpha}^+ v_{\alpha} G_{\alpha}^+ v_{\alpha} = G_{\alpha}^+ v_{\alpha} G_{\alpha}^+ v_{\alpha} + \cdots \quad (28)$$

$\mathcal{K}'$ contains only connected diagrams whereas $\mathcal{K}_0$ contains two disconnected diagrams and we obtain the following series of disconnected diagrams for $u_{\alpha \beta}^+$ as

$$u_{\alpha \beta}^{+(0)} = v_{\beta}(1 + \sum_{n=1}^{\infty} \mathcal{K}_0^n) \quad (29)$$
2.2.2. Distorted-wave formalism for three-body rearrangement series

The disconnected diagrams contained in $\mathcal{K}_o$ for rearrangement collisions can be avoided by using an approach in the distorted wave method. Let $w_\alpha(t_\alpha)$ and $w_\beta(t_\beta)$ are the distorting potentials which depend only on $t_\alpha$ and $t_\beta$ respectively. With these potentials are associated the Green's functions:

$$g^{\alpha\beta} = (E - H_{\alpha\beta} - w_\alpha + i\epsilon)^{-1}$$

$$g^{-\alpha\beta} = (E - H_{\beta\alpha} - w_\beta - i\epsilon)^{-1}$$

and the corresponding wave operators:

$$\omega^{\alpha} = 1 + g^{\alpha\beta} w_\alpha$$

$$\omega^{-\beta} = 1 + g^{-\beta\alpha} w_\beta$$

where

$$H_{\alpha\beta} = H_\alpha + W_{\alpha\beta}$$

$$\omega_\alpha = w_\alpha + W_{\alpha\beta}$$

$$\omega_\beta = w_\beta + W_{\beta\alpha}$$

$W_{\alpha\beta}$ and $W_{\beta\alpha}$ are Coulomb distorting potentials which occur when we consider two nuclei and one electron. When $v_\alpha$ and $v_\beta$ are short range potentials, we have $W_{\alpha\beta} = W_{\beta\alpha} = 0$.

The transition operator $U_{\alpha\beta}^+$ satisfies the integral equation:

$$U_{\alpha\beta}^+(1 - \mathcal{K}_2) = \omega_\beta^+ (v_\beta - W_{\beta\alpha}^+) \omega_\alpha^+$$
Greider and Dodd\textsuperscript{57} have found that in the case of short range potentials, the kernel $\mathcal{K}_2$ contains disconnected diagrams since only one potential $(v - w)$ appears in its expression. Later on Dodd and Green\textsuperscript{42} removed the disconnected part of the kernel by the introduction of a virtual intermediate channel $\chi$ corresponding to a potential $v_\chi$ associated with the Green function

$$g^+_\chi = (E - H + v_\chi + i\epsilon)^{-1}.$$  \hfill (39)

Using the identity:

$$g^+_\chi = (1 + g^+_\chi v_\chi g^+_\chi) g^+_\chi$$  \hfill (40)

$u^+_{\alpha\beta}$ is shown to satisfy the following integral equation\textsuperscript{52}:

$$u^+_{\alpha\beta}(1 - \mathcal{K}_3) = \omega^+_{\beta}(v_\beta - \bar{W}_\beta) [1 + g^+_\chi (v_\chi - \bar{W}_\chi)] \omega^+_{\alpha}$$  \hfill (41)

where

$$\mathcal{K}_3 = G^+_{\alpha\beta} v_\chi g^+_\chi (v_\chi - \bar{W}_\chi) \omega^+_{\alpha}.$$  \hfill (42)

By a suitable choice of $v_\chi$, the disconnected diagram in the kernel $\mathcal{K}_3$ may be avoided. Similarly one can also obtain $U^+_{\alpha\beta}$ as

$$u^+_{\alpha\beta}(1 - \mathcal{K}_4) = \omega^+_{\beta} [1 + g^+_\chi (v_\chi - \bar{W}_\chi)] (v_\alpha - \bar{W}_\alpha) \omega^+_{\alpha},$$  \hfill (43)

with

$$\mathcal{K}_4 = \omega^+_{\beta} (v_\beta - \bar{W}_\beta) g^+_\chi v_\chi G^-_{\beta\alpha},$$  \hfill (44)

and

$$G^-_{\beta\alpha} = (E - H_{\beta\alpha} - i\epsilon)^{-1}.$$  \hfill (45)
The scattering amplitude for the three body scattering process becomes

\[ a_{ij}^{\alpha \beta} = \langle \phi_j^{\beta} | \omega_\beta^+ (v_\beta - w_\beta) \left[ 1 + g_x (v_\alpha - w_\alpha) \right] \omega_\alpha^+ | \phi_i^{\alpha} \rangle, \] (46)

\[ a_{ij}^{\alpha \beta} = \langle \phi_j^{\beta} | \omega_\beta^+ \left[ 1 + g_x (v_\beta - w_\beta) \right] (v_\alpha - w_\alpha) \omega_\alpha^+ | \phi_i^{\alpha} \rangle. \] (47)

2.2.3. Derivation of the CDW approximation

In this section we are explicitly dealing with the rearrangement process of the type (2) and the coordinate system for such a process is shown in Fig. 2.1. For convenience, let us identify the particles \( \beta, \gamma, \) and \( \alpha \) by the target nucleus, electron and structureless projectile respectively. Let \( \vec{r}_T, \vec{r}_e, \) and \( \vec{r}_p \) be the respective position vectors of the target nucleus, electron and incident projectile, respectively, in an arbitrary galilean frame. We introduce the coordinates

\[ \vec{x} = \vec{r}_e - \vec{r}_T, \]

\[ \vec{s} = \vec{r}_e - \vec{r}_p \] (48)

and

\[ \vec{R} = \vec{r}_p - \vec{r}_T. \]

Let \( \vec{r}_\alpha \) is the position vector of the projectile relative to the centre of mass of the target, while \( \vec{r}_\beta \) is a similar vector with the target nucleus and projectile interchanged. Furthermore, \( \vec{r} \) is the position vector of the electron with respect to the centre of mass of the projectile and the target nucleus. These may be
Fig. 2.1. Coordinate system for the process (2); \(\alpha\), \(\beta\), and \(\gamma\) represent the fully stripped projectile, target nucleus, and electron.
expressed as
\[ \begin{align*}
\vec{r}_\alpha &= \vec{r}_p - \frac{M_T \vec{r}_T + M_e \vec{r}_e}{M_T + M_e}, \\
\vec{r}_\beta &= \vec{r}_T - \frac{M_p \vec{r}_p + M_e \vec{r}_e}{M_p + M_e}
\end{align*} \]
and
\[ \vec{r} = \vec{r}_e - \frac{M_T \vec{r}_T + M_p \vec{r}_p}{M_T + M_p} \]
where \( M_T, M_e, \) and \( M_p \) are the masses of the target nucleus, electron, and projectile respectively. We define \( \mu_\alpha \) and \( \mu_\beta \) as the reduced masses associated with the initial and final channels, respectively, and \( \mu \) is the reduced mass of the whole system. These reduced masses can be written as
\[ \begin{align*}
\mu_\alpha &= \frac{M_p (M_T + M_e)}{M_{cm}}, \\
\mu_\beta &= \frac{M_T (M_p + M_e)}{M_{cm}}, \\
\mu &= \frac{M_p M_T}{M_p + M_T}
\end{align*} \]
with
\[ M_{cm} = M_p + M_T + M_e. \]

In order to calculate \( T_{ij}^{\alpha \beta +} \) given by the expression (46), let us set:
\[ | \chi_{i}^{\alpha +} \rangle = \omega_{\alpha}^{+} | \phi_{i}^{\alpha +} \rangle \]
In the limit \( \epsilon = 0 \), \( \chi_{i}^{\alpha +} \) and \( \phi_{i}^{\alpha +} \) satisfy the equation:
\[ (E - H_{\alpha} - W_{\alpha}) | \chi_{i}^{\alpha +} \rangle = (E - H_{\alpha}) | \phi_{i}^{\alpha +} \rangle \]
Since $\phi_1^{\alpha+}$ and $\phi_2^{\beta-}$ contain the correct asymptotic Coulomb phases due to the Coulomb interaction between aggregates in the entrance and exit channels, respectively, we have

$$ (H_{\alpha d} - E) |\phi_1^{\alpha+}\rangle = (H_\alpha + W_{\alpha d} - E) |\phi_1^{\alpha+}\rangle = 0 \quad (53) $$

and

$$ (H_{\beta d} - E) |\phi_2^{\beta-}\rangle = (H_\beta + W_{\beta d} - E) |\phi_2^{\beta-}\rangle = 0 \quad (54) $$

Let us choose $w_\alpha$ to be a function of $r_\alpha$ which decreases more rapidly than $1/r_\alpha$ as $r_\alpha \to \infty$. We choose $W_\alpha$ in Eq. (52) in such a way that $|\chi_1^{\alpha+}\rangle$ has the form:

$$ |\chi_1^{\alpha+}\rangle = |\phi_1^{\alpha+} (x) f (r_\alpha)\rangle \quad (55) $$

Then the state vector $|\chi_1^{\alpha+}\rangle$ has the same asymptotic behaviour as that of $|\phi_1^{\alpha+}\rangle$.

Let us now set:

$$ |\xi_1^{\alpha+}\rangle = [1 + g_1^{\alpha+} (v_\alpha - w_\alpha)] |\chi_1^{\alpha+}\rangle \quad (56) $$

which is needed in Eq. (46).

In the limit $\epsilon = 0$, $|\xi_1^{\alpha+}\rangle$ and $|\chi_1^{\alpha+}\rangle$ satisfy the equation:

$$ (E - H + v_x) |\xi_1^{\alpha+}\rangle = (E - H + v_x + v_\alpha - w_\alpha) |\chi_1^{\alpha+}\rangle \quad (57) $$

Since $|\chi_1^{\alpha+}\rangle$ satisfies Eq. (52), the Eq. (57) reduces to

$$ (E - H + v_x) |\xi_1^{\alpha+}\rangle = v_x |\chi_1^{\alpha+}\rangle \quad (58) $$

Instead of choosing for $v_x$ a local two body potential which makes Eq. (58) too difficult to solve, Gayet has taken for $v_x$ an operator
such that
\[ v_{\chi} | \chi_{\alpha}^{+} \rangle = 0 \quad (59) \]
and for \( | \gamma_{\alpha}^{+} \rangle \) the form:
\[ | \gamma_{\alpha}^{+} \rangle = | \phi_{\alpha}^{+} (x) \rangle h^{+} \quad (60) \]
Eq. (58) may be written as
\[ \left( E - H_{0} + \frac{Z_{T}}{x} + \frac{Z_{P}}{s} - \frac{Z_{P} Z_{T}}{R} + v_{x} \right) | \chi_{\alpha}^{+} \rangle = 0 \quad (61) \]
where \( Z_{P} \) and \( Z_{T} \) are the nuclear charges of the projectile and target nucleus respectively. We look for a solution of (61) with the exact asymptotic behaviour as
\[ \chi_{\alpha}^{+} \rightarrow \phi_{\alpha, i}^{+} (x) \exp \left[ i \frac{Z_{P} (Z_{T} - 1)}{u_{\alpha}} \ln \left( k_{\alpha} r_{\alpha} - k_{\alpha} r_{\alpha} \right) \right] \quad (62) \]
where
\[ u_{\alpha} = k_{\alpha} / \mu_{\alpha} ; \quad k_{\alpha} \] represents the momentum of the incident particle in the initial channel. The kinetic energy operator \( H_{0} \) may be written in the following two forms:
\[ H_{0} = - \frac{1}{2 \mu_{\alpha}} \nabla_{\alpha}^{2} - \frac{1}{2 a} \nabla_{x}^{2} = - \frac{1}{2 \mu_{\beta}} \nabla_{\beta}^{2} - \frac{1}{2 b} \nabla_{s}^{2} \quad (63) \]
where
\[ a = \frac{M_{P} M_{T}}{(M_{T} + M_{P})} \quad (64) \]
\[ b = \frac{M_{P} M_{e}}{(M_{P} + M_{e})} \quad (65) \]
Since we have
\[ \nabla_{x}^{2} \phi_{\alpha, i}^{+} (x) = 0 \]
it implies
\[
(\epsilon_i - H_0 + \frac{\frac{\nu_T}{\epsilon_i}}{\alpha}) \phi_i^\alpha (\vec{x}) = 0 \quad (66)
\]
where $\epsilon_i$ is the energy of the bound state $\alpha$. Then putting (15)

\[
E = E - \epsilon_i, \quad \text{Eq.} (61) \text{ becomes:}
\]

\[
\phi_i^\alpha (\vec{x}) \left( E - H_0 + \frac{\nu_T}{s} - \frac{\frac{\nu_T}{R}}{s} \right) h^+ + \frac{1}{a} \nabla_x \phi_i^\alpha (\vec{x}) \cdot \nabla_x h^+ + v_x \phi_i^\alpha = 0 \quad (67)
\]

Here $v_x$ represents an operator such that applied to an arbitrary function $\psi$ of $\vec{x}$ and $\vec{r}_\alpha$ or $(\vec{s}$ and $\vec{r}_\beta)$ the following relationship holds:

\[
v_{x} \psi = - \frac{1}{a} \nabla_x \phi_i^\alpha (\vec{x}) \cdot \nabla_x \left[ \frac{\psi}{\phi_i^\alpha (\vec{x})} \right] \quad (68)
\]

With this form for $v_x$, Eq. (59) is satisfied since

\[
\frac{\psi}{\phi_i^\alpha (\vec{x})} = f(\vec{r}_\alpha) \equiv 0 \quad (69)
\]

and Eq. (67) reduces to:

\[
\left( E - H_0 + \frac{\nu_T}{s} - \frac{\frac{\nu_T}{R}}{s} \right) h^+ = 0 \quad (70)
\]

Eq. (70) becomes separable in the variables $\vec{s}$ and $\vec{r}_\beta$ if $\vec{n}$ is replaced by $\vec{r}_\beta$ which is justified in the limit $M_\beta \gg M_\gamma$ and $M_\gamma \gg M_\epsilon$. We thus obtain

\[
h^+ = \mu^{-\frac{\nu_T}{\alpha}} \phi_N (\psi_N) \exp(ik_{\alpha} \cdot \vec{n}) \sum_{\gamma} F_{\gamma} (i\nu_{\gamma}; I_v + i\nu_{\gamma}) \cdot F_{\gamma} (i\nu_{\gamma}; I_v + i\nu_{\gamma}) \quad (71)
\]
where

\[ N(\nu) = \Gamma(1 + i\nu) \exp(\pi\nu/2) \]  
\[ N(\nu_p) = \Gamma(1 - i\nu_p) \exp(\pi\nu_p/2) \]

\[ \nu_p = z_p/v \quad \text{and} \]  
\[ \nu = z_p^2 z_T / v \] (72)

and

\[ \mathbf{v} = \mathbf{v}_\alpha \] .

Let us now examine the exit channel problem. The state vector \(|\chi_j^-\rangle\) is written as

\[ |\chi_j^-\rangle = \omega^- \left| \psi_j^-\rangle \right. \] (73)

we require \(|\chi_j^-\rangle\) as

\[ |\chi_j^-\rangle = |\psi_j^-\rangle (\mathbf{r}) \mathbf{g}^- \] (74)

where \( \mathbf{g}^- \) is chosen to be a continuum wave. Let \( \epsilon_j \) be the energy of the final bound state. We set:

\[ \epsilon' = \epsilon - \epsilon_j \] (75)

and

\[ U_\beta = \nu_\beta - \omega_\beta \] .

In the limit \( \epsilon = 0 \), \(|\chi_j^-\rangle\) satisfies the equation:

\[ (E - H + U_\beta') |\chi_j^-\rangle = (E - H_\beta') |\psi_j^-\rangle \] (76)

or, since \( \psi_j^- \) is an eigenfunction of \( H_\beta \) for the eigenvalue \( E \):

\[ (E - H'_0 + \frac{z_p}{s} + \frac{z_r}{x} - \frac{z_p z_T}{R} + U_\beta) |\psi_j^-\rangle (\mathbf{g}^-) = 0 \] (77)
The appropriate boundary condition is:
\[ \chi_j^\beta \xrightarrow{r_\beta \to \infty} \phi_j^\beta(s) \exp \left[ -i k_\beta \cdot r_\beta - i \frac{Z_T(Z_T - 1)}{u_\beta} \ln \left( \frac{k_\beta}{u_\beta} \right) \right], \quad (78) \]

where
\[ \vec{u}_\beta = \frac{\vec{k}_\beta}{u_\beta}; \quad \vec{k}_\beta \]
is the momentum of the scattered particle in the final channel. Now in the same way as for \( \xi_1^x \), the Eq.(77) reduces to
\[ \Phi_i(E' - H_0 + \frac{Z_T}{x} - \frac{Z_T^2}{R}) g^- \cdot \frac{1}{\partial} \vec{V}_s \phi_j^\beta(s) \vec{V}_s g^- + U_\beta \chi_j^\beta = 0. \quad (79) \]

Gayet has chosen \( U_\beta \) as an operator, analogous to \( \vec{v}_x \):
\[ U_\beta^{\text{op}} = -\frac{1}{\partial} \vec{V}_s \phi_j^\beta(s) \vec{V}_s \left[ \frac{1}{\phi_j^\beta(s)} \right]. \quad (80) \]
The operator is such that applied to a function \( \psi \) the result is:
\[ U_\beta^{\text{op}} \psi = -\frac{1}{\partial} \vec{V}_s \phi_j^\beta(s) \vec{V}_s \left[ \frac{\psi}{\phi_j^\beta(s)} \right]. \quad (81) \]
The Eq.(79) reduces to:
\[ (E' - H_0 + \frac{Z_T}{x} - \frac{Z_T^2}{R}) g^- = 0. \quad (82) \]

We now replace \( \vec{r} \) by \( \vec{r}_{\alpha} \) which is justified in the limit \( M_{P,T} \gg M_e \) and we get
\[ g^- = \mu N^* (\psi_T) N^* (\psi') \exp (-i k_\beta \cdot \vec{x}) \frac{E_1 (-i \psi_T; l; -i \vec{v}_x - i \vec{v}_x', \vec{x})}{E_1 (i \psi'; l; -i k_{\beta} \cdot \vec{x} - i k_\beta' \cdot \vec{x}')}, \quad (83) \]

where
\[ \psi_T = \frac{Z_T}{\psi'}, \quad (84) \]
\[ \psi' = \frac{Z_T^2}{\psi'} \]
\[ \vec{v}' = \vec{u}_\beta \]
\[ N(\psi_T) = \exp \left( \pi \psi_T / 2 \right) \Gamma (1 + i \psi_T). \]
\[ N(\psi') = \exp \left( \pi \psi' / 2 \right) \Gamma (1 - i \psi'). \]
The post transition amplitude \( \langle 4|> \) in the limit \( M_P \rightarrow M_e \) becomes
\[
T_{ij}^\alpha = -\int d\bar{\beta} d\bar{s} \phi^\alpha_i (\bar{x}) h^+ (\bar{s}) V_\beta V_g^* (\bar{s}) V_s V_j^\beta \ . \tag{85}
\]
An analogous expression may be derived for the 'prior' form of the transition amplitude:
\[
T_{ij}^\alpha = -\int d\bar{\alpha} d\bar{x} \phi^\beta_j (\bar{x}) V_g^* V_\alpha \phi^\alpha_i (\bar{x}) \ . \tag{86}
\]
In that case, the transition amplitude is defined by:
\[
\langle \chi_i^{\alpha +} \rangle = \omega^+ |\phi_i^{\alpha +} \rangle = |\phi_i^{\alpha} (\bar{x}) h^+ \rangle , \tag{87}
\]
\[
(\psi_\alpha - \omega_\alpha) \psi = -\frac{1}{a} \frac{\psi}{\phi_i^{\alpha} (\bar{x})} \nabla \left[ \frac{\psi}{\phi_i^{\alpha} (\bar{x})} \right] , \tag{88}
\]
\[
| \xi_j^{\beta -} \rangle = [1 + g_\beta (v_\beta - \omega_\beta)] | \chi_j^{\beta -} \rangle = [1 + g_\beta (v_\beta - \omega_\beta)] \omega^- | \phi_j^{\beta -} \rangle = | \phi_j^{\beta} (\bar{s}) g^- \rangle , \tag{89}
\]
and
\[
\psi_\beta \psi = -\frac{1}{b} \frac{\psi}{\phi_j^{\beta} (\bar{s})} \nabla \left[ \frac{\psi}{\phi_j^{\beta} (\bar{s})} \right] . \tag{90}
\]
The wave functions (87) and (89) have the correct asymptotic behaviors and \( \psi_\beta \) contains no two-body potential that appears in \( v_\beta - \omega_\beta \), as required by the theory of Dodd and Greider. The potential \( \psi_\beta \) also satisfies the condition
\[
\psi_\beta | \chi_j^{\beta -} \rangle = 0 \ , \tag{91}
\]
imposed in the calculation of \( | \xi_j^{\beta -} \rangle \). In heavy particle collisions the scattering amplitudes are sharply peaked in the forward direction and scattering at small angles contributes to the total cross section.
In such a case, we have
\[ \mathbf{u}_u \approx \mathbf{u}_\beta = \mathbf{v}, \]
\[ \mathbf{v}' \approx \mathbf{v}, \]
\[ \mathbf{R} = \mathbf{p} + \mathbf{Z}, \]
\[ k_\beta - k = \eta + \left[ \frac{M_e}{2} \left( \frac{M_T - M_p}{M_{cm}} \right) + \frac{\epsilon_i - \epsilon_j}{v^2} \right] \mathbf{v}, \]
and
\[ \eta \cdot \mathbf{v} = \eta \cdot \mathbf{Z} = \mathbf{p} \cdot \mathbf{v} = \mathbf{p} \cdot \mathbf{Z} = 0, \]
where \( \eta \) is the transverse momentum transfer in the plane perpendicular to the incident velocity \( \mathbf{v} \) of the projectile. Then the following general relations may be obtained:
\[ k_u \cdot \mathbf{r}_u + k_\beta \cdot \mathbf{r}_\beta \approx \mathbf{p} \cdot \mathbf{x} + \mathbf{q} \cdot \mathbf{s} = \mathbf{r} \cdot \mathbf{R} - M_e \mathbf{v} \cdot \mathbf{R}, \quad (93) \]
where
\[ \mathbf{p} = -\eta - \left( \frac{\epsilon_i - \epsilon_j}{v^2} + \frac{M_e}{2} \right) \mathbf{v}, \]
\[ \mathbf{q} = \eta + \left( \frac{\epsilon_i - \epsilon_j}{v^2} - \frac{M_e}{2} \right) \mathbf{v}, \]
and
\[ \gamma = -\eta - \frac{\epsilon_i - \epsilon_j}{v^2} \mathbf{v} \equiv \eta - \mathbf{k}. \quad (94) \]

The continuum distorted wave method (Cheshire) may be obtained from the expressions of \( T_{ij}^{\alpha \beta} \) in (85) and (86) when we replace the product:
\[ [N(\psi)]^2 \mathcal{F}_1(-i\psi;1;ik_\alpha r_\beta + ik_\beta r_\alpha) \mathcal{F}_1(-i\psi;1;ik_\alpha r_\beta + ik_\beta r_\alpha) \quad (95) \]
by its asymptotic limit when \( M_p, \tau \to \infty \). McCarrill and Salin have shown that the limit of (95) takes the form \((\mu v \rho)^{2i\psi}\). The tran-
Position amplitudes of the CDW approximation for forward capture is:

\[ T_{\alpha^+}^{\beta^+} = \bar{\chi} N(v) \int d^3p \, d^3s \, (\pi s)^{2i} \exp(i\mathbf{p} \cdot \mathbf{x} + i\mathbf{s} \cdot \mathbf{z}) \, L_{\alpha^+}^{\beta^+}(v) \]

where

\[ N(v) = \sqrt{(1 - i\gamma_{s})} \sqrt{(1 - i\gamma)} \, \exp \left[ \frac{\pi}{2} \left( (\gamma - \gamma_{s}) \right) \right] \]

\[ L_{\alpha^+}^{\beta^+} = \phi_{i}^{\alpha}(\mathbf{x}) \, \mathcal{F}_{\alpha}^{\beta} \left( \mathbf{p}, \mathbf{x} \right) \, \mathcal{F}_{\alpha}^{\beta} \left( \mathbf{p}, \mathbf{x} \right) \]

and

\[ L_{\alpha^+}^{\beta^+} = \phi_{j}^{\beta}(\mathbf{s}) \, \mathcal{F}_{\beta}^{\alpha} \left( \mathbf{p}, \mathbf{s} \right) \, \mathcal{F}_{\beta}^{\alpha} \left( \mathbf{p}, \mathbf{s} \right) \]

It is to be noted that the factor \( p^{2i} \) in Eq. (96) cannot be taken out from the integrals over \( s \) and \( \mathbf{p} \). Consequently, the differential cross sections calculated from (96) will be affected by the factor \( p^{2i} \), which is attributed to the inclusion of the internuclear potential exactly to first order in \( M_e / \mu \). On the other hand, if the total cross section is calculated with (96), the factor \( p^{2i} \) may be omitted, indicating that the internuclear potential does not contribute to the capture process. In the present investigation, since we are dealing with exact bound state wave functions, there arises no post-prior discrepancy. Then neglecting all unimportant phase factors which do not contribute in the total capture cross sections, the prior form of the transition amplitude becomes:

\[ T_{\alpha^+}^{\beta^-} = -\bar{N}(v) \tilde{\chi} \tilde{K} \]

where

\[ \tilde{\chi} = \int d^3x \exp(i\mathbf{p} \cdot \mathbf{x}) \left[ \mathcal{F}_{\alpha}^{\beta} \phi_{i}^{\alpha}(\mathbf{x}) \right] \mathcal{F}_{\beta}^{\alpha} \left( \mathbf{p}, \mathbf{x} \right) \]

\[ \tilde{K} = \int d^3s \exp(i\mathbf{q} \cdot \mathbf{s}) \phi_{j}^{\beta}(\mathbf{s}) \mathcal{F}_{\beta}^{\alpha} \left( \mathbf{p}, \mathbf{s} \right) \mathcal{F}_{\alpha}^{\beta} \left( \mathbf{p}, \mathbf{s} \right) \]

This form of transition amplitude (98) has been used by Belkic and
McCarroll\textsuperscript{59} to investigate the projectile charge dependence of electron-capture cross sections in the CDW approximation. The total capture cross section is obtained from the relation:

\[ Q_{ij}^{\alpha \beta \pm} = \left| \frac{\mathcal{T}_{ij}^{\alpha \beta \pm}(\eta)}{2\pi v} \right|^2 d\eta. \]  

(101)

2.3. Evaluation of the integral \( \mathcal{J} \)

The ground state wave function of the hydrogen atom is

\[ \psi_1(x) = \frac{1}{\sqrt{\pi}} (Z_T)^{3/2} \exp \left( -Z_T x \right), \]  

(102)

\( Z_T \) being the nuclear charge of the target. The \( \mathcal{J} \) integral in Eq. (99) can be expressed as

\[ \mathcal{J} = i \left( \frac{2\pi}{Z_T} \right)^{1/2} \int_{\mathcal{P}} \frac{\exp(i\mathcal{P} \cdot x - Z_T x)}{x} \mathcal{F}_1(i\mathcal{P}, 1; i\mathcal{P} + i\mathcal{P} \cdot x) \]  

(103)

Now, we use the integral representation\textsuperscript{60} of the confluent hypergeometric function occurring in the expression (103)

\[ \mathcal{F}_1(i\alpha, 1; 2) = \frac{1}{2\pi i} \oint_{\Gamma} dt \frac{\exp(\gamma t) \exp(\omega t)}{t} \]  

(104)

with

\[ \gamma(t) = t^{i\alpha - 1} (t - 1)^{-i\alpha}. \]  

(105)

\( \Gamma \) is a closed contour encircling the two points 0 and 1 once counter-clockwise. At the point where the contour crosses the real axis to the right hand side of 1, \( \arg(t) \) and \( \arg(t - 1) \) are both zero.

Substituting (104) in (103) the \( \mathcal{J} \) integral becomes

\[ \mathcal{J} = i \left( \frac{2\pi}{Z_T} \right)^{1/2} \int_{\mathcal{P}} \frac{1}{2\pi i} \oint_{\Gamma} dt \frac{\exp[i\mathcal{P} \cdot x + t(\mathcal{P} \cdot \mathcal{P} + \mathcal{P} \cdot x)]}{x}. \]  

(106)
We replace \( \frac{\exp(-\lambda x)}{x} \) in Eq. (106), by its Fourier transform integral representation, namely,

\[
\frac{1}{x} \exp (-\lambda x) = \frac{1}{2\pi^2} \int \frac{\exp(iKx)}{(K^2 + \lambda^2)} \, dK \quad (107)
\]

After performing the space integration in (106), the integral reduces to

\[
\overline{\rho} = 4\pi i \left( \frac{Z_T}{\pi} \right)^{1/2} \int_P \frac{1}{2\pi i} \int_{C_I} i \nu_T - 1 - i \nu_T \, V(t) \nu(t) \quad (108)
\]

with

\[
V(t) = 1/(A_1 - B_1 t),
\]

\[
A_1 = p^2 + Z_T^2,
\]

\[
B_1 = (2Z_T v - 2p v). \quad (109)
\]

The quantity \( V(t) \) has one singularity, a simple pole, at \( t = \gamma = A_1 / B_1 \). \( \gamma \) lies outside the \( t \) contour. We may expand the complete \( t \) contour to infinity, and by Cauchy's residue theorem we have

\[
\int_{C_H} i \nu_T - 1 - i \nu_T \, V(t) \nu(t) = \int_{\gamma = R, R \to \infty} i \nu_T - 1 - i \nu_T \, V(t) \nu(t) = 0 \quad (110)
\]

Since the right hand side vanishes, we find that

\[
\int_{\gamma = R, R \to \infty} i \nu_T - 1 - i \nu_T \, V(t) = -2\pi i (\text{residue at } \gamma) = \frac{1}{B_1} \left( \frac{\gamma - 1}{\gamma} \right) - i \nu_T \frac{1}{\gamma} \quad (111)
\]

Thus we get

\[
\overline{\rho} = 4\pi i \left( \frac{Z_T}{\pi} \right)^{1/2} \int_P \frac{1}{p^2 + Z_T^2} \left[ 1 + \frac{2(p \cdot v - iZ_T v)}{(p^2 + Z_T^2)} \right]^{-i \nu_T} \quad (112)
\]
2.4. Evaluation of the integral $K$

The $K$ integral in Eq. (100) may be expressed as

$$K = \mathbf{v}_v \int ds \, \exp \left( \frac{i \mathbf{v}_s \cdot \mathbf{s}}{s} \right) \phi_j^*(\mathbf{s}) \mathbf{F}_1 \left( i \mathbf{v}_p, l; i \mathbf{v}_s + i \mathbf{v}_s \right),$$

where in Eq. (100) we make use of the relation

$$\mathbf{v}_s \mathbf{F}_1 \left( i \mathbf{v}_p, l; i \mathbf{v}_s + i \mathbf{v}_s \right) = \frac{V}{s} \mathbf{v}_v \mathbf{F}_1 \left( i \mathbf{v}_p, l; i \mathbf{v}_s + i \mathbf{v}_s \right),$$

which may be easily verified using the relation

$$\mathbf{v}_s (\mathbf{v}_s + \mathbf{v}_s) = (\mathbf{v}/s) \mathbf{v}_v (\mathbf{v}_s + \mathbf{v}_s).$$

The final bound-state wave function characterized by the set of quantum numbers $n, l, m$ may be written as

$$\psi_j^0(\mathbf{s}) = N_{nlm} \mathbf{R}_n(\mathbf{s}) \mathbf{Y}_l^m(\mathbf{s}),$$

where $N_{nlm}$ is the normalization constant given by

$$N_{nlm} = \frac{(2Y_n)^{l+1}}{n+1} \frac{\left[ Y_n(n-l-1) \right]^{1/2}}{n(n+1)!},$$

and $Z_p$ being the charge of the incident projectile. The radial wave function $\mathbf{R}_n(\mathbf{s})$ and the spherical harmonics $\mathbf{Y}_l^m(\mathbf{s})$ are expressed as

$$\mathbf{R}_n(\mathbf{s}) = s \exp(-Y_n) \mathbf{I}^{2l+1}_{n+1} \left( 2Y_n \right),$$

$$\mathbf{Y}_l^m(\mathbf{s}) = (-1)^m \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2}} \frac{1}{\sqrt{(2l+1)(l-m)!}} \exp(i\mathbf{m} \cdot \mathbf{s}) \mathbf{L}^m_l(\cos \theta_s),$$

where $\mathbf{I}^\mu_l(x)$ is the associated Laguerre polynomial of degree $\mu$ and order $l$, and $\mathbf{L}^m_l(\cos \theta_s)$ is the associated Legendre polynomial of degree $l$ and order $m$. $\theta_s$ and $\phi_s$ are the polar coordinates of the unit vector $\mathbf{s}$. We use the integral representation of the

$$\frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2}} \frac{1}{\sqrt{(2l+1)(l-m)!}} \exp(i\mathbf{m} \cdot \mathbf{s}) \mathbf{L}^m_l(\cos \theta_s),$$

where $\mathbf{L}^m_l(x)$ is the associated Legendre polynomial of degree $l$ and order $m$. $\theta_s$ and $\phi_s$ are the polar coordinates of the unit vector $\mathbf{s}$. We use the integral representation of the
confluent hypergeometric function occurring in (113) as
\[ \Gamma_1(i\psi_p,1;\tau) = \frac{1}{2\pi i} \int_{\gamma} dZ \exp(2Z) \left( \psi_p(Z) \right) \cdot \frac{1}{\Gamma(0+1+1)} \]
with
\[ p''(\psi_p,Z) = Z^{i\psi_p-1} (Z-1)^{-i\psi_p} \cdot \] \[ \gamma \] is a closed contour encircling the two points 0 and 1 once counter-clockwise. At the point where the contour crosses the real axis to the right hand side of 1, \( \arg() \) and \( \arg(1-t) \) are both zero. Making use of (120) in (113) we obtain the \( K \) integral as
\[ K = \frac{1}{2\pi i} \int_{\gamma} dZ p''(\psi_p,Z) \cdot \] where
\[ I = \int_{C} d\tau \exp(i\Omega \cdot s+ivZ) \cdot \] where the contour \( C \) encloses the origin only, the integral \( I \) in Eq.
\[ I = -\frac{(n+l)!}{2\pi i} \int_{C} \frac{d\tau}{(1-l)^{2l+2} + 2t^{n-l}} \cdot \] where
\[ I_1 = \int_{C} d\tau \exp(-i\mu s+i\nu \tau) \cdot \] where
\[ \mu = \frac{1}{2} \left( \frac{1+\tau}{1-\tau} \right) ^{-ivZ} \cdot \] To evaluate \( I_1 \) in Eq.
\[ I_1 = \int_{C} d\tau \exp(-i\mu s+i\nu \tau) \cdot \] where
the spherical harmonics
\[ \exp(i\mathbf{q} \cdot \mathbf{s}) = 4\pi \sum_{L M} i^L j_L(Qs) Y_{LM}^*(\hat{\mathbf{q}}) Y_{LM}(\hat{\mathbf{s}}). \tag{129} \]

The integration over the entire solid angle in (127) yields
\[ I_1 = 4\pi i L_{LM}(\hat{\mathbf{q}}) \int_0^\infty j_L(Qs) s^{l+1} \exp(-\mu s) ds, \tag{130} \]
where we have used the orthogonality relation,
\[ \int Y_{LM}(\hat{\mathbf{r}}) Y_{LM}^*(\hat{\mathbf{r}}) d\hat{\mathbf{r}} = \delta_{LL} \delta_{MM}. \tag{131} \]

In view of the relation,
\[ j_L(Qs) = \sqrt{\frac{\pi}{2Qs}} J_{l+\frac{1}{2}}(Qs), \tag{132} \]
the radial integration in (130) can be easily performed using the following relation,\(^62\)
\[ \int_0^\infty \exp(-ax) J_\nu(\beta x) x^\nu dx = \frac{(2\beta)^\nu \Gamma(\nu + \frac{1}{2})}{\sqrt{\pi} (\alpha^2 + \beta^2)^{\nu + 1/2}}. \tag{133} \]

The integral \( I_1 \) in (130) reduces to
\[ I_1 = 4\pi i L_{LM}(\hat{\mathbf{q}}) (2\Omega)^l / (\mu^2 + \Omega^2)^{l+1}. \tag{134} \]

Substituting (134) in Eq. (126), we get
\[ I = -(n+1)! 4\pi i L_{LM}(\hat{\mathbf{q}}) (2\Omega)^l / (\mu^2 + \Omega^2)^{l+1}. \tag{135} \]

The function \( F(t) \) is given by
\[ F(t) = \left[ A(1 - 2Bt + Dt^2) \right]^{-(l+1)}, \tag{136} \]
We use the following expansion
\[
(1 - 2uz + u^2)^{-\nu} = \sum_{\mu=0}^{\infty} C_\mu^\nu (z) u^\mu,
\]
where the coefficients $C_\mu^\nu(z)$ of the above series are the Gegenbauer polynomials of degree $\mu$ and order $\nu$. Thus $F(t)$ can be expressed as,
\[
F(t) = A^{-(l+1)} \sum_{\nu=0}^{\infty} C_\nu^{l+1}(\lambda) (\xi t)^\nu,
\]
with
\[
\lambda^2 = \frac{B^2}{D},
\]
\[
\xi^2 = D.
\]
Substituting (139) in Eq. (135), one obtains
\[
I = -(n+l)! 4\pi i \int_{\gamma_{\text{Im}}} Y^*_l(\hat{\lambda}) (2\Omega)^l A^{-(l+1)} \frac{1}{2\pi i} \int_{t-\infty}^{t+\infty} \sum_{\nu=0}^{\infty} C_\nu^{l+1}(\lambda)(\xi t)^\nu.
\]
Since the contour integral is equal to $2\pi i$ times the sum of the residues at the singularities within the contour (here the singularity lies at the origin only), we can easily find the result by collecting the coefficients of $t^{-1}$ from the expansion of the integrand in terms of $t$. On substitution of the result of contour integration we obtain
\[
I = -(n+l)! 4\pi i \int_{\gamma_{\text{Im}}} Y^*_l(\hat{\lambda}) (2\Omega)^l A^{-(l+1)} C_{n-l-1}^{l+1}(\lambda) \xi^{n-l-1}.
\]
where we have put
\[ \Delta^2 = \left[ (\gamma_n + ivz)^2 + v^2 \right]^{n-l-1} \left( -v^2 \right)^{(n+l+1)} \]  
(143)

Substituting the value of I given by (142) in Eq. (122) for the K integral, we get

\[ K = -(n+1)! \ 4\pi! (2i)^n \text{nlim}_v \frac{1}{2\pi i} \oint_{\Gamma} dZ \ Z^{-i\nu} (Z-1)^{-i\nu} f(z) \]  
(144)

2.5. Evaluation of the transition amplitude \( T_{ij}^{\alpha\beta} \)

After performing the dot product between the two integrals \( J \) and \( K \) (shown in the appendix B), one obtains the transition amplitude \( T_{ij}^{\alpha\beta} \) as

\[ T_{ij}^{\alpha\beta} = N(v) N_{JK} \ \frac{1}{2\pi i} \oint_{\Gamma} dZ \ Z^{-i\nu} (Z-1)^{-i\nu} f(z) \]  
(145)

with

\[ N_{JK} = (n+1)! \ 4\pi! (2i)^n \text{nlim}_v \]  
(146)

The scattering amplitude in (145) may be equivalently written as,

\[ T_{ij}^{\alpha\beta} = N_{ij} \ \exp(-\pi i\nu) \ \frac{1}{2\pi i} \oint_{\Gamma} dZ \ Z^{-i\nu} (Z-1)^{-i\nu} f(z) \]  
(147)

where

\[ N_{ij} = N(v) N_{JK} \]  
(148)

\( \Gamma \) being a closed contour surrounding the points \( Z=0 \) and \( Z=1 \) once counter-clockwise and the lower part of \( \Gamma \) is located on the real axis. We choose this form for convenience of numerical evaluation of the integral. To evaluate this one-dimensional complex integral (147) we adopt the procedure of Mukherjee et al. with some modified...
fications. The function $f(z)$ is free from singularity in the region $0 < z < l$. For the evaluation of $T_{ij}^{\alpha\beta}$, we introduce a function $g(z) = z[f(1)-f(0)] + f(0)$ in the integrand by virtue of which the integrand vanishes at $z=0$ and $z=1$. We may thus write Eq. (147) as

$$T_{ij}^{\alpha\beta} = N_{ij} \exp(-\pi \nu P) \frac{1}{2\pi i} \oint_{\gamma} dz \, z^P (1-z)^{-i\nu P} \left[ f(z) - g(z) + g(z) \right] ,$$

(149)

and

$$F(z) = f(z) - g(z) .$$

Now on the contour $\gamma$ for the integral in Eq. (150), we have on the real axis between 0 and 1,

$$\arg(z) - \arg(1-z) = 0 ,$$

(151)

and on the proton on $\gamma$ above the real axis between 0 and 1

$$\arg(z) - \arg(1-z) = -2\pi .$$

(152)

Further, on the contour $\gamma$ we do not have any contribution in the integral from the infinitesimal circles surrounding 0 and 1, since $F(z)$ has no singularities at these points. Thus, following Mukherjee et al., we convert (149) into a real one-dimensional integral
\[
T_{ij}^{\alpha\beta} = N_{ij} \left[ \exp(-\pi\nu_p) \cdot \exp(\pi\nu_p) \right] \frac{1}{2\pi i} \int d\nu P(1-\nu) \exp(-\nu f) 
\]
\[
+ N_{ij} \exp(-\pi\nu_p) \frac{1}{2\pi i} \int d\nu P(1-\nu) \left[ f(1)-f(0) \right] 
\]
\[
+ N_{ij} \exp(-\pi\nu_p) \frac{1}{2\pi i} \int d\nu P(1-\nu) \left[ f(1)-f(0) \right] 
\]
\[
\text{Since} 
\]
\[
\exp(-\pi\nu_p) \frac{1}{2\pi i} \int d\nu P(1-\nu) \left[ f(1)-f(0) \right] 
\]
we equate the coefficients of \( t \) and \( t^2 \) after the expansions of \( \exp(Zt) \) and \( \frac{F_1(i\nu_p;1,t)}{\nu_p} \), in Eq. (154), and obtain
\[
\left( \frac{1}{2\pi i} \right) \exp(-\pi\nu_p) \int d\nu P(1-\nu) \left[ f(1)-f(0) \right] = i\nu_p 
\]
Substituting Eqs (155) and (156) in (153), we obtain the transition amplitude as
\[
T_{ij}^{\alpha\beta} = N_{ij} \left[ \exp(-\pi\nu_p) \cdot \exp(\pi\nu_p) \right] \frac{1}{2\pi i} \int d\nu P(1-\nu) \exp(-\nu f) 
\]
\[
+ N_{ij} \exp(-\pi\nu_p) \frac{1}{2\pi i} \int d\nu P(1-\nu) \left[ f(1)-f(0) \right] 
\]
2.6. Numerical procedure

To evaluate the one-dimensional integral in real space occurring in the transition amplitude, we change the variable of integration from \( Z \) to \( y \), using the transformation

\[
\exp(y) = \frac{1-Z}{Z},
\]

so that the integral

\[
\int_0^\infty dZ Z (1-Z) F(2) \text{ in (157) reduces to}
\]

the form

\[
T = \int_0^\infty \frac{\exp(-i\phi y)}{[1+\exp(y)]^2} \exp(y) F(y) dy + \int_{-\infty}^{0} \frac{\exp(-i\phi y)}{[1+\exp(y)]^2} \exp(y) F(y) dy.
\]

In the second term of (159) we put \( y = -y \), arriving at

\[
T = \int_0^\infty \frac{\exp(-i\phi y)}{[1+\exp(y)]^2} \exp(y) F(y) dy + \int_0^\infty \frac{\exp(-i\phi y)}{[1+\exp(-y)]^2} \exp(-y) F(-y) dy.
\]

Multiplying the numerator and denominator by \( \exp(ay) \) and replacing \( (a+1)y \) by \( y' \), Eq. (160) reduces to

\[
T = \frac{1}{a+1} \int_0^\infty \frac{\exp(-i\phi y'/a+1)}{[1+\exp(-y'/a+1)]^2} \exp(a\phi y'/a+1) \exp(-y') dy' + \frac{1}{a+1} \int_0^\infty \frac{\exp(i\phi y'/a+1)}{[1+\exp(-y'/a+1)]^2} \exp(-y'/a+1) \exp(-y') dy'.
\]

The integrals in (161) are of the type

\[
\int_0^\infty e^{-x} f(x) dx
\]
which may be approximated to the summation
\[ \sum_{r=1}^{n} \omega_r f(x_r) \]

Here the \( x_r \)'s are those values of \( x \) for which the \( n \)-th order Laguerre polynomial \( L_n(x) \) is zero. The weight coefficients \( \omega_r \) are given by
\[ \omega_r = \frac{1}{x_r} \left[ \frac{n!}{n_r(x_r)} \right]^2 \]

(162)

\( x_r \) and \( \omega_r \) are supplied as the input. The convergence of the result is tested by increasing the number of Gauss-Laguerre points for a suitable value of the parameter \( a \). To calculate the total capture cross sections \( q_{ij}^{\beta^-} \), the gauss-Legendre quadrature method has been used for the integration over the transverse momentum transfer \( \eta \). The value of \( \eta \) has been increased step-wise until the desired accuracy of \( .05\% \) in the total capture cross sections is obtained.

In order to check the numerical program developed for the present calculation, some known results for the total capture cross sections into a few low-lying states have been reproduced.

2.7. Results and discussions
2.7.1 Charge transfer cross sections in \( \text{Li}^{3+}-\text{H}(1s) \) collisions

Calculations have been carried out at incident energies between 100 keV and 1500 keV for capture into all final states with \( n \leq 4 \) for the projectile \( \text{Li}^{3+} \) ion in ground state atomic hydrogen target. In table 2.1 we have presented our results for the \( n, l \)-dependent cross sections \( q_{nl} = \sum_m q_{nlm} \) as well as the capture

\[ \sum_{nl} q_{nl} \]
Table 2.1. The present CDW cross sections (in $\pi a_0^2$ unit) for charge transfer in
$^7\text{Li}^3^+ + \text{H}(1s) \rightarrow ^7\text{Li}^2^+ (n\ell) + \text{H}^+$ collisions. $Q_{1s}$, $Q_{2s}$, $Q_{2p}$, $Q_{3s}$, $Q_{3p}$, $Q_{3d}$, $Q_{4s}$, $Q_{4p}$, $Q_{4d}$, and
$Q_{4f}$ represent, respectively, the cross sections for capture into the 1s, 2s, 2p, 3s, 3p, 3d,
4s, 4p, 4d, and 4f states of Li$^2^+$ ion. $Q(n)$ denotes the cross sections for capture into
each complete shell of Li$^2^+$ ion for $n \leq 4$, $Q$(total) being the total capture cross sections.
The numbers in bracket denote the powers of ten by which the numbers are multiplied.

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>$Q_{1s}$</th>
<th>$Q_{2s}$</th>
<th>$Q_{2p}$</th>
<th>$Q_{3s}$</th>
<th>$Q_{3p}$</th>
<th>$Q_{3d}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.08(-1)</td>
<td>9.26(0)</td>
<td>1.28(1)</td>
<td>4.48(0)</td>
<td>2.81(1)</td>
<td>7.98(1)</td>
</tr>
<tr>
<td>200</td>
<td>1.43(-1)</td>
<td>1.56(0)</td>
<td>7.41(0)</td>
<td>6.72(-1)</td>
<td>7.07(0)</td>
<td>1.37(1)</td>
</tr>
<tr>
<td>400</td>
<td>3.67(-2)</td>
<td>2.76(-1)</td>
<td>1.43(-1)</td>
<td>1.30(0)</td>
<td>1.59(0)</td>
<td></td>
</tr>
<tr>
<td>800</td>
<td>2.01(-2)</td>
<td>4.62(-2)</td>
<td>2.65(-1)</td>
<td>3.21(-2)</td>
<td>1.44(-1)</td>
<td>1.04(-1)</td>
</tr>
<tr>
<td>1250</td>
<td>1.33(-2)</td>
<td>1.60(-2)</td>
<td>5.08(-2)</td>
<td>6.68(-2)</td>
<td>8.93(-3)</td>
<td>2.54(-2)</td>
</tr>
<tr>
<td>1500</td>
<td>9.81(-3)</td>
<td>9.46(-3)</td>
<td>2.39(-2)</td>
<td>3.34(-2)</td>
<td>4.87(-3)</td>
<td>1.16(-2)</td>
</tr>
</tbody>
</table>
### Table 2.1 (continued)

<table>
<thead>
<tr>
<th>Energy keV</th>
<th>Q(3)</th>
<th>Q_{4s}</th>
<th>Q_{4p}</th>
<th>Q_{4d}</th>
<th>Q_{4f}</th>
<th>Q(4)</th>
<th>Q(total)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.12(2)</td>
<td>2.79(0)</td>
<td>2.57(1)</td>
<td>3.11(1)</td>
<td>1.82(1)</td>
<td>7.78(1)</td>
<td>3.33(2)</td>
</tr>
<tr>
<td>200</td>
<td>2.14(1)</td>
<td>5.03(-1)</td>
<td>5.08(0)</td>
<td>6.87(0)</td>
<td>3.51(0)</td>
<td>1.59(1)</td>
<td>7.15(1)</td>
</tr>
<tr>
<td>400</td>
<td>3.03(0)</td>
<td>1.03(-1)</td>
<td>7.99(-1)</td>
<td>9.19(-1)</td>
<td>3.64(-1)</td>
<td>2.18(0)</td>
<td>1.08(1)</td>
</tr>
<tr>
<td>800</td>
<td>2.81(-1)</td>
<td>1.89(-2)</td>
<td>7.99(-2)</td>
<td>6.47(-2)</td>
<td>1.77(-2)</td>
<td>1.81(-1)</td>
<td>1.07(0)</td>
</tr>
<tr>
<td>1250</td>
<td>4.73(-2)</td>
<td>4.78(-3)</td>
<td>1.32(-2)</td>
<td>8.13(-3)</td>
<td>1.71(-3)</td>
<td>2.78(-2)</td>
<td>1.98(-1)</td>
</tr>
<tr>
<td>1500</td>
<td>2.16(-2)</td>
<td>2.52(-3)</td>
<td>5.95(-3)</td>
<td>3.22(-3)</td>
<td>6.16(-4)</td>
<td>1.23(-2)</td>
<td>9.63(-2)</td>
</tr>
</tbody>
</table>
cross sections into each complete shell \( Q(n) = \sum_{l,m} Q_{l,m} \), where the axis of quantization is taken to be in the direction of the projectile and \( Q_{l,m} \) is the partial cross sections for charge transfer into the \( n,l,m \) orbitals around the projectile. To compare the observed data for the total capture cross sections, \( Q(\text{total}) = \sum_n Q(n) \); a correction term must be made for capture into higher excited levels with \( n \geq 5 \). In estimating \( Q(\text{total}) \), we may assume that the cross sections \( Q(n) \) is proportional to \( n^{-3} \) for \( n \geq 5 \) as in the Brinkman-Kramers (BK) approximation at high energies. This yields

\[
Q(\text{total}) = \sum_n Q(n) = Q(1) + Q(2) + Q(3) + \frac{Q(4)}{Q^{\text{BK}}(4)} \sum_{n=4}^\infty Q^{\text{BK}}(n) = Q(1) + Q(2) + Q(3) + 2.561Q(4).
\]

(163)

\( Q^{\text{BK}}(n) \) represent the cross sections for capture into the arbitrary principal shells \( n \) of \( \text{Li}^{2+} \) ion obtained by using the BK approximation. Using the values of \( Q(1) \), \( Q(2) \), \( Q(3) \) and \( Q(4) \) obtained by the present CDW approximation, the total capture cross sections are calculated for each individual energy and are included in table 2.1. From the table, it appears that throughout the energy region considered the capture into the ground state is almost negligible except at the highest energy of 1500 keV where it amounts to 10% of the total capture cross sections. The small values of ground state capture are also predicted by Bransden et al.\(^{15} \) in their calculation for the charge-transfer cross sections in the multi-charged ion-atom collision processes in the atomic state expansion method and also
by Mandal et al.\textsuperscript{49} in their calculation of the CB approximation. From the present calculation it follows that the maximum contribution in the capture cross sections arises from the $n = 3$ level of Li\textsuperscript{2+} ion in the intermediate-energy region and this is quite expected since the third-energy level of Li\textsuperscript{2+} ion is in resonance with H(1s) in the capture process, and as the $n$ value increases the capture probability decreases. This may be explained as the energy difference between the ground state of atomic hydrogen and Li\textsuperscript{2+} ion increases with the increase of $n$ (for $n \geq 3$), the capture cross sections for the levels specified by $n > 3$ are expected to be small compared to the resonating level ($n=3$). At higher energies of the projectile, the capture probability is found to be maximum at the second quantum level of Li\textsuperscript{2+} ion instead of the resonating level. This is attributed to the fact that at high energy, the capture probability is maximum at small values of impact parameter and, consequently, the electron transfer into the inner shells is more dominant. Thus the $n$-dependent cross sections in the intermediate- and high-energy region can be understood.

At intermediate impact energies, the $l$-dependent cross sections $Q_{nl}$ indicate a maximum at $l < n-1$ for $n = 4$, whereas the results for $n = 3$ indicate a maximum at $l = n-1$. In the low- and intermediate-energy region the effect of level crossing is responsible for the electron transfer and, consequently, the electron is mostly transferred into a state that has a wave function indicating a large amplitude at the crossing point, which usually has a smaller value
of \( l \) than \( n-1 \). At the higher energy, the distributions are completely free from the influence of level crossing, but are strongly affected by momentum-transfer effects and the cross sections are gradually reduced with the increase of \( l \). A similar trend is also observed in the BK approximation\(^{13} \), eikonal approximation\(^{66} \), UDWA\(^{11} \), and two-state atomic expansion method\(^{15} \).

Though we have not shown in the table, the \( m \)-dependent cross sections, it has been found that the distributions over \( m \) for given \( l \) and \( n \) indicate a maximum at \( m = 0 \) in the intermediate-and high-energy region. This behaviour is also in conformity with the previous calculations\(^{11,49} \). The high probabilities of electron transfer into \( m = 0 \) state correspond to the classical picture that the electron is mostly captured into the orbitals on the collision plane.

Belkić et al.\(^{52} \) gave an estimate for the total capture cross sections of the collision process \( \text{Li}^{3+} - \text{H}(1s) \), using the relation

\[
Q(\text{total}) = Q(1) + Q(2) + 2.081 \times Q(3),
\]

which is obtained by assuming the validity of the \( n^{-3} \) scaling law from the level \( n \gg 4 \). Further, they have not calculated the contribution from the 3d excited state of \( \text{Li}^{2+} \) ion for total capture cross sections. In the present investigation we propose to calculate the values of the total-capture cross section \( Q(\text{total}) \) by using the relation (163) instead of (164). Bransden et al.\(^{15} \) have also used the relation (163) to give an estimate for the total-capture cross sections for \( \text{Li}^{3+} - \text{H}(1s) \) collision process.
projectile, the use of the expression (163) seems to be more justified since in Li\(^{3+}\)-H(1s) charge exchange, the n=3 level is in energy resonance and the effect of resonant behaviour of the cross sections for capture into the third quantum level of Li\(^{2+}\) ion is manifested in the present calculation even below 800 keV. The values of the total cross section obtained by the use of (163) is found to be about 9% higher than that obtained by the use of (164) at the incident energy of 1500 keV. At 100 keV, this discrepancy amounts to 24%. The origin for such a difference in the values of the cross section may be due to the resonant behaviour of the electron-capture cross sections for the third quantum level of Li\(^{2+}\) ion.

In figure 2.2, we present our theoretical values for the total capture cross sections in the energy range 100 keV to 1500 keV and have compared them with the recent experimental results of Shah et al.\(^5\) and the previously reported theoretical calculations.\(^{13,15,46,47,48,49}\) The present results obtained by the CDW approximation are found to be in excellent agreement with the experimental results in the energy range E > 700 keV, whereas it grossly overestimates the experimental findings at the lower energy side (E < 700 keV). However, at 100 keV the calculated results show some discrepancy with the experimental results which is not unlikely because the CDW approximation is a high-energy approximation and is not expected to be valid at low energy.

The values of the cross section estimated by the classical Monte Carlo approach\(^47\) overestimate the observed findings through-
Fig. 2.2. Total capture cross section for the projectile $^7$Li$^{3+}$ ion incident on a ground-state atomic hydrogen.

Theory: (---), Present CDW calculation; (-----), CB calculation of Mandal et al. (Ref.49); (------), FBA calculation of Mandal et al. (Ref.49); (-----), CDW calculation of Crothers and Todd (Ref.48); (-------), CIS calculation of Crothers and Todd (Ref.48); (-----), eikonal calculation of Eichler (Ref.13); (---), two-state-atomic expansion model calculation of Bransden et al. (Ref.15); (-----), UDWA calculation of Ryufuku and Watanabe (Ref.46); (---), classical Monte Carlo calculation of Olson and Salop (Ref.47).

Experiment: ○, Shah et al. (Ref.50).
out the energy region considered. Moreover, the shape of the cross section as a function of energy appears rather different; the cross sections decrease with the increase of energy more rapidly, showing complete disagreement with the observed trend. This may be attributed to the large statistical errors involved in their calculation.

The UDWA results, on the other hand, give quite good agreement in the intermediate energy region up to the incident energy of 400 keV, but beyond this energy it grossly overestimates the observed values. This is due to the fact that all interactions among the product channels are ignored in this method and the results thus obtained are large compared to the data specially in the high-energy region where the direct excitation channels and the ionization channels influence significantly in the cross section results.

The capture cross sections obtained by using the two-state atomic expansion method agree rather well in shape with the experimental data but always overestimate the data in the intermediate- and high-energy region. The UDWA cross sections, though agree well with the two-state cross sections of Bransden et al. at the higher energies, are considerably smaller at the lower energies. The cross sections obtained by the CB approximation are found to be in quite good agreement with the experimental results throughout the energy region considered except at the intermediate-energy region E < 275 keV, whereas the FBA cross sections grossly overestimate the experimental findings. Upon comparison with the FBA calculation, the CB results are found to give
much lower values for the cross sections for all the individual excited states and this is attributed to the appreciable long range Coulomb repulsive force present in the final channel of the charge transfer reaction which is completely neglected in the FBA calculation.

The present calculated results almost coincide with the CDW cross sections obtained by Crothers and Todd who have assumed the validity of the $n^{-3}$ law from the principal quantum number $n > 8$. Though we have given an estimate for the total capture cross sections using the $n^{-3}$ law from $n^5$, the close agreement between these two results indicate that the application of $n^{-3}$ law from $n^5$ is quite reasonable in the present investigation. The cross sections obtained by using the CIS and eikonal approximations are found to overestimate the present calculated results and also the experimental findings throughout the energy range of the projectile considered. Among the existing second-order calculations in the high energy region, the present CDW approximation is in close agreement with the experimental data whereas over the intermediate energy range reasonable agreement is obtained with the observed findings.

One of the drawbacks of the CDW theory is that it is particularly suitable for small impact parameters, at which the projectile may experience the bare nucleus of the target atom. In an ideal case one should calculate variationally the effective charge experienced at arbitrary impact parameter. Some efforts have recently been made by Shakeshaft in the light of variational approach.
2.7.2. Scaling law

Recently, Shah et al.\(^50\) measured total cross sections for electron capture by fully stripped ions of lithium from atomic hydrogen and empirically found an approximate \(Z_p^3\) scaling law for impact velocities greater than one atomic unit. Goffe et al.\(^68\) have further confirmed this scaling law experimentally for impact of fully stripped ions of boron, carbon and nitrogen in atomic hydrogen. To study the behaviour of the cross section as a function of incident charge of the projectile, we have plotted in fig. 2.3, the calculated capture cross sections divided by the cube of the projectile charge \(Q/\left(Z_p^3\right)\) against the equivalent proton energy obtained by using the present CDW approximation\(^16\) in \(\text{Li}^{3+}-\text{H}(1s)\) collision process and the previously reported CDW calculations\(^44,45\) of \(\text{He}^{2+}-\text{H}(1s)\) system. It appears from the fig. 2.3 that over an energy range 25 - 200 keV amu\(^{-1}\), \(Q/\left(Z_p^3\right)\) is the same for both the projectiles, \(\text{He}^{2+}\) and \(\text{Li}^{3+}\), indicating a \(Z_p^3\) variation of the cross section. In a very recent calculation, Crothers and Todd\(^48\) have also shown that high-energy approximations, such as the Oppenheimer-Brinkman-Kramers, eikonal, CIS, CDW, and Bohr-Lindhard theories give a good account of \(Z_p^3\) variation of cross sections. The CB approximation\(^49\) also exhibit \(Z_p^3\) variation of cross sections over the energy range 25 - 250 keV amu\(^{-1}\). It may be pointed out that, \(Z_p^2\) scaling law has been observed by Presnyakov and Ulantsev\(^69\) at lower energies and by Bransden et al.\(^15\) over the energy range 10 - 100 keV amu\(^{-1}\).
Fig. 2.3. Cross sections $Q_{(total)}/Z_p^3$ for electron capture by He$^{2+}$ and Li$^{3+}$ ions from the ground state of atomic hydrogen in the continuum distorted-wave (CDW) approximation.

Theory: (---), present calculation for Li$^{3+}$-H collisions;

(-----), calculation of Belkic and Gayet (Ref. 45) for He$^{2+}$-H collisions.
2.8. Conclusions

The present method of calculation provides an alternative way for the evaluation of the CDW scattering amplitude. It does not require the imposition of any restrictions on the values of the quantum numbers n, l, m and also the charge Zp of the incident projectile. In this proposed method the charge exchange scattering amplitude has been reduced to a one-dimensional integral in real space which can be very easily evaluated numerically with convenience for any values of n, l, m and Zp. As a result, we obtain more detailed theoretical predictions, which in turn might be checked with the experimental observations on radiative transitions and radiative cascades following electron capture.

The present method has been applied in Li$^3^+$-H(1s) collision process and calculations have been carried out at incident energies between 100 keV and 1500 keV for electron capture into all final states of Li$^2^+$ ion with principal quantum numbers n ≤ 4. Comparison with available experimental findings for total capture-cross sections shows that the present CDW approximation indicates an excellent agreement for incident energies of the projectile E > 700 keV. In the intermediate-energy region, the present CDW results always overestimate the observed data, whereas the existing theoretical results obtained by employing the UDWA, CB, two-state atomic expansion method and the classical Monte Carlo approach are in much better agreement with the observed values. However, with the increase of impact energy the earlier calculated
results\textsuperscript{15,46,47} show poor agreement with the observed findings. The present CDW approximation appears to follow a $Z_p^3$ variation of cross sections over an energy range 25 - 200 keV amu$^{-1}$. This is in conformity with the predictions\textsuperscript{48} of the semiclassical Oppenheimer-Brinkman-Kramers, eikonal, CIS theories as well as the semiclassical continuum theory of Bohr and Lindhard.

The influence of inelastic intermediate channels describing excitation and ionization on the charge transfer processes is expected to be considerable at high impact energies. At high incident velocities all intermediate channels are open and it is likely that the charge exchange process should be significantly affected by the inclusion of these intermediate states. The success of the CDW approximation may be attributed to the fact that the CDW method takes proper account of the continuum intermediate states in the charge exchange process ensuring the correct initial and final state boundary conditions of the problem. The present method for obtaining the cross sections for capture into n,l,m states may be helpful for the diagnostic techniques currently being developed for studying the role played by the impurities in neutral-beam heating of fusion-plasmas.
To show that $T_{ij}^{a\beta-}$ in Eq. (145) can be expressed as $\langle 0^+, l^+ \rangle$

$$T_{ij}^{a\beta-} = N(v)N_{JK} \frac{1}{2\pi i} \oint_{\Gamma} dz \frac{1}{z} \left( \begin{array}{c} i^\varphi - 1 \\ -i^\varphi \end{array} \right) z f(z)$$  \hspace{1cm} (B1)

The integral in Eq. (112) can be written as

$$\mathcal{J} = C_1 \mathbf{v} - C_2 \mathbf{p}$$  \hspace{1cm} (B2)

where

$$C_1 = 8\pi i \left( \frac{Z_T}{\pi} \right)^{1/2} (-i)^{\frac{T+1}{2}} \left[ 1 + \frac{(\mathbf{p} \cdot \mathbf{v} - iz_T v)}{(p^2 + z_T^2)} \right]^{-i^\varphi - 1}$$  \hspace{1cm} (B3)

$$C_2 = 8\pi i \left( \frac{Z_T}{\pi} \right)^{1/2} \left\{ \frac{1}{(p^2 + z_T^2)} \left[ 1 + 2 \frac{(\mathbf{p} \cdot \mathbf{v} - iz_T v)}{(p^2 + z_T^2)} \right]^{-i^\varphi_T - 1} \right\}$$  \hspace{1cm} (B4)

To calculate the $K$ integral in Eq. (144), we have to evaluate

$$\mathbf{V}_v \left[ Q \gamma_4 (\mathbf{q}) N \gamma_\lambda \mathbf{c}_{n-l-1} \mathbf{c}_{n-l-1}^\dagger \right]$$  \hspace{1cm} (B5)

It follows from (143) that

$$\mathbf{V}_v \Delta = (H_1 \mathbf{v} - D_1 \mathbf{q}) \mathbf{z}$$  \hspace{1cm} (B6)

with

$$H_1 = P_1^{(n-l-3)/2} A^{-(n+l+3)/2} H$$  \hspace{1cm} (B7)

$$D_1 = P_1^{(n-l-3)/2} A^{-(n+l+3)/2} D$$  \hspace{1cm} (B8)

$$D = 2 \left[ 2i \gamma_n v \mathbf{z} n + (l+1) (\gamma_n^2 + \gamma_n^2 - \mathbf{v}^2 z^2) \right]$$  \hspace{1cm} (B9)
\[ H = [n(Q^2 + Y^2 + v^2) + (l+1)2iY_nvZ] \frac{2iY_n}{\nu}, \]  
\[ P_1 = [(Y_n + ivZ)^2 + \varrho^2]. \]  
\[ A = [(Y_n - ivZ)^2 + \varrho^2]. \]  

We also obtain
\[ \mathcal{V}_v [c_{n-l-1}^{\mu} (\lambda)] = 2(l+1)(s_1^2 - s_2^2) \varrho c_{n-l-2}^{\mu} (\lambda), \]  
\[ S_1 = \frac{4\gamma_n^2 (\varrho^2 + Y_n^2 + v^2^2)}{[(Y_n - ivZ)^2 + \varrho^2][(Y_n + ivZ)^2 + \varrho^2]}^{3/2}. \]  
\[ S_2 = \frac{4\gamma_n^2 2(\varrho^2 - v^2^2 - \varpi^2)}{[(Y_n - ivZ)^2 + \varrho^2][(Y_n + ivZ)^2 + \varrho^2]}^{3/2}. \]  

The Gegenbauer polynomial \( C_n^\mu(t) \) in (B5) can be expressed as
\[ C_n^\mu(t) = \left[ \frac{(2\mu + n)}{(2n+1)\Gamma(2\mu)} \right] {}_2F_1 \left( 2\mu+n, -n; \mu + \frac{1}{2}; \frac{1}{2}(1-t) \right). \]  

To calculate \( \mathcal{V}_v (Q Y_{l,m} (\hat{\mathbf{Q}})) \) we express \( Y_{l,m} (\hat{\mathbf{Q}}) \) as
\[ Y_{l,m} (\hat{\mathbf{Q}}) = (-1)^m \sqrt{\frac{1}{2\pi}} \left\{ \frac{(2l+1)(l-m)!}{2(l+m)!} \right\}^{1/2} \exp(i\mathbf{m}_Q \cdot \mathbf{Q}) P_l^m (C_Q S_\mathbf{Q}). \]  

Using the relations
\[ R_l^m (x) = (1 - x^2)^{m/2} \frac{d^m}{dx^m} R_l (x), \]  
and
\[ P_l (x) = \sum_{K=0}^{L} (-1)^K \frac{(2l - 2K)!}{2^l(l-K)!(l-2K)!K!} x^{l-2K}. \]  
where
\[ L = \begin{cases} \frac{l}{2} & \text{when } l \text{ is even}, \\ \frac{1}{2} (l-1) & \text{when } l \text{ is odd}, \end{cases} \]
we get

\[ r_{l}^{m}(x) = \sum_{K=0}^{L'} (-1)^{K} \frac{(2l - 2K)!}{2^{l} (l-K)! (l-m-2K)! K!} x^{l-m-2K} (1-x^2)^{m/2}, \quad (B21) \]

with

\[ L' = \begin{cases} \frac{1}{2} (l-m) & \text{when (l-m) is even,} \\ \frac{1}{2} (l-m-1) & \text{when (l-m) is odd.} \end{cases} \quad (B22) \]

Substituting (B21) in (B17), we obtain

\[ Q_{l} Y_{m}^{\ell} (\hat{\Omega}) = N_{y} y_{m}^{\ell} \exp(i\phi_{\Omega}) \sin^{\ell} \Theta_{\Omega} \sum_{K=0}^{L'} (-1)^{K} \frac{(2l-2K)!}{2^{l} (l-K)! (l-m-2K)! K!} \]

\[ \times (\cos \Theta_{\Omega})^{l-m-2K}, \quad (B23) \]

where

\[ N_{y} y_{m}^{\ell} = (-1)^{m} \frac{1}{\sqrt{2\pi}} \left\{ \frac{(2l+1)!(l-m)!}{2(l+m)} \right\}^{1/2} \quad (B24) \]

After proper rearrangement, we get

\[ Q_{l} Y_{m}^{\ell} (\hat{\Omega}) = N_{y} y_{m}^{\ell} \sum_{K=0}^{l} (-1)^{K} \frac{(2l-2K)!}{2^{l} (l-K)! (l-m-2K)! K!} \]

\[ \times (\cos \Theta_{\Omega})^{l-m-2K} \quad (B25) \]

\[ = N_{y} y_{m}^{\ell} \left[ Q_{x} + i Q_{y} \right]^{m} \sum_{K=0}^{l} (-1)^{K} \frac{(2l-2K)!}{2^{l} (l-K)! (l-m-2K)! K!} \]

\[ \times (\Omega \cos \Theta_{\Omega})^{l-m-2K} Q_{z}^{2K}, \quad (B26) \]

\[ = N_{y} y_{m}^{\ell} \left[ Q_{x} + i Q_{y} \right]^{m} \sum_{K=0}^{l} (-1)^{K} \frac{(2l-2K)!}{2^{l} (l-K)! (l-m-2K)! K!} \]

\[ \times \frac{Q_{x}^{2K} Q_{z}^{2K}}{Q_{z}^{2K}}, \quad (B27) \]
with

\[ Q_x = Q \sin \theta Q \cos \phi Q \]
\[ Q_y = Q \sin \theta Q \sin \phi Q \]
\[ Q_z = Q \cos \theta Q \]

Since

\[ Y_{lm}(\hat{Q}) = (-1)^m Y_{l,-m}(\hat{Q}), \]

we obtain

\[ Q Y_{lm}^*(\hat{Q}) = \sum_{K=0}^{L'} \frac{(-1)^K (2l-2K)!}{2^l (l-K)! (l-m-2K)! K! Q_Z^{l-m-2K} Q^2 K} \]

and

\[ Q Y_{l,-m}^*(\hat{Q}) = (-1)^{-m} \sum_{K=0}^{L'} \frac{(-1)^K (2l-2K)!}{2^l (l-K)! (l-m-2K)! K! Q_Z^{l-m-2K} Q^2 K} \]

We obtain from Eqs. (B29) and (B30)

\[ \vec{v}_v \left[ Q Y_{lm}^*(\hat{Q}) \right] = 2 \left[ \sqrt{v} (R_1^+ + R_2^+ Z) + \sqrt{q} R_2^+ (\hat{a}_x + i \hat{a}_y) R_3^+ \right] \]

and

\[ \vec{v}_v \left[ Q Y_{l,-m}^*(\hat{Q}) \right] = 2 \left[ \sqrt{v} (\bar{R}_1^+ + \bar{R}_2^+ Z) + \sqrt{q} R_2^+ (\hat{a}_x + i \hat{a}_y) R_3^+ \right] \]

where

\[ R_1^+ = N m \sum_{K=0}^{L'} (-1)^K \frac{(2l-2K)!}{(l-K)! (l-m-2K)! K!} Q_Z^{l-m-2K} (Q_x - i Q_y)^{l-m}, \]

\[ L' = \begin{cases} \frac{1}{2} (l-m-1), & \text{when } (l-m) \text{ is odd} \\ \frac{1}{2} (l-m-2), & \text{when } (l-m) \text{ is even} \end{cases} \]
\[ R_2' = 2^{-l} \sum_{K=1}^{L} \frac{(-1)^K (2l-2K)!}{(l-K)! (l-m-2K)! (K-1)!} Q_x^{l-m-2K} Q_z^2 (Q_x - iQ_y)^m \]  

\[ \iff \begin{array}{ll}
\frac{1}{2} (l-m) \text{, when } (l-m) \text{ is even} \\
\frac{1}{2} (l-m-1) \text{, when } (l-m) \text{ is odd}
\end{array} \]  

\[ R_3 = N \sum_{l=0}^{m} \frac{(-1)^l}{2^l} \sum_{K=0}^{l'} \frac{(2l-2K)!}{(l-K)! (l-m-2K)! K!} Q_x^{l-m-2K} Q_z^2 (Q_x - iQ_y)^m \]  

\[ \iff \begin{array}{ll}
\frac{1}{2} (l-m) \text{, when } (l-m) \text{ is even} \\
\frac{1}{2} (l-m-1) \text{, when } (l-m) \text{ is odd}
\end{array} \]  

\[ R_1 = N \sum_{l=0}^{m} (-1)^m \frac{1}{2^l} \sum_{K=0}^{l} \frac{(-1)^K (2l-2K)!}{(l-K)! (l-m-2K)! K!} Q_x^{l-m-2K} Q_z^2 (Q_x + iQ_y)^m \]  

\[ \iff \begin{array}{ll}
\frac{1}{2} (l-m) \text{, when } (l-m) \text{ is even} \\
\frac{1}{2} (l-m-1) \text{, when } (l-m) \text{ is odd}
\end{array} \]  

\[ M = \begin{cases} 
\frac{1}{2} (l-m), & \text{when } (l-m) \text{ is even} \\
\frac{1}{2} (l-m-1), & \text{when } (l-m) \text{ is odd} 
\end{cases} \]  

\[ M' = \begin{cases} 
\frac{1}{2} (l-m), & \text{when } (l-m) \text{ is even} \\
\frac{1}{2} (l-m-1), & \text{when } (l-m) \text{ is odd} 
\end{cases} \]
and

\[ R_3^- = N_y \left[ \frac{(-1)^{m}}{2} \sum_{K=0}^{m} \frac{(lK)!}{(l-K)! (l-m-2K)! K!} Q_z^{-2K} \Omega_x \Omega_y^{l-m-2K} (\Omega_x \Omega_y)^n \right] \]

\[ M = \begin{cases} \frac{1}{2} (l-m), & \text{when (l-m) is even} \\ \frac{1}{2} (l-m-1), & \text{when (l-m) is odd} \end{cases} \]

\( \Omega_x \) and \( \Omega_y \) are the x- and y components of \( \Omega \) and \( \hat{a}_x \) and \( \hat{a}_y \) are the unit vectors along the X- and Y-axis respectively.

Using the Eqs. (B43), (B44), we get

\[ \nabla_y \left[ \Omega^l \Omega^*(\Omega) \right] C_{n-l-1}^{l+1} (\Lambda) \Delta = 2 \left[ A^+ \Omega^+ + B^+ \Omega^+ + C^+ (\hat{a}_x - i\hat{a}_y) \right] \]

Similarly, we obtain by combining Eqs. (B43), (B44), and (B45)

\[ \nabla_y \left[ \Omega^l \Omega^*(\Omega) \right] C_{n-l-1}^{l+1} (\Lambda) \Delta = 2 \left[ A^- \Omega^- + B^- \Omega^- + C^- (\hat{a}_x + i\hat{a}_y) \right] \]

where

\[ A^+ = a_1^+ R_1^+ + a_2^+ R_2^+ S \Omega_2^+ + a_3^+ H_1 \]

\[ B^+ = a_1^+ R_2^+ + a_2^+ S_1 \Omega_2^+ - a_3^+ D_1 \]

\[ C^+ = R_3^+ \]

\[ a_1^+ = C_{n-l-1}^{l+1} (\Lambda) \Delta \]

\[ A^- = a_1^- R_1^- + a_2^- R_2^- S \Omega_2^- + a_3^- H_1 \]

\[ a_2^+ = C_{n-l-1}^{l+1} (\Lambda) \Delta \]

\[ a_3^+ = C_{n-l-1}^{l+1} (\Lambda) \Delta \]

\[ B^- = a_1^- R_2^- + a_2^- S_1 \Omega_2^- - a_3^- D_1 \]

\[ C^- = R_3^- \]

\[ s_1^+ = \Delta (l+1) C_{n-l-2}^{l+2} (\Lambda) S_1 \]

\[ s_2^+ = \Delta (l+1) C_{n-l-2}^{l+2} (\Lambda) S_2 \]
The $K$ integral in Eq (144) can be expressed as

$$K = \frac{1}{2\pi i} \oint \frac{dZ}{Z} Z^{l-1} \left( Z^{-1} \right) P \left[ A^+ \frac{\psi}{v} + B^+ \frac{\bar{\psi}}{q} \right] + C \left( a_x^+ + i a_y^+ \right)$$  \hspace{1cm} (B59)

The transition amplitude in (98) becomes

$$T_{ij}^{\beta -} = N(v)N_{JK} \frac{1}{2\pi i} \oint \frac{dZ}{Z} Z^{l-1} \left( Z^{-1} \right) f^+(z)$$  \hspace{1cm} (B60)

with

$$f^+(z) = C_1 A^+ \frac{\psi}{v} - C_2 A^+ \left( \frac{\bar{\psi}}{q} \right) + C_1 B^+ \left( \frac{\psi}{q} \right) - C_2 B^+ \left( \frac{\bar{\psi}}{p} \right) + C \left( \eta_x^+ + i \eta_y^+ \right)$$  \hspace{1cm} (B61)

$$\eta_x = \eta_x^+ \hspace{1cm} \eta_y = \eta_y^+$$  \hspace{1cm} (B62)

$\eta_x$ and $\eta_y$ are the $x$- and $y$ components of $\hat{\eta}$. In the present investigation, we have used $f(z) = f^+(z)$. However, both the forms of $f^+(z)$ in (B61) will give the same values for the cross section.
REFERENCES


60 A.Nordsieck, Phys. Rev. 93, 785 (1954).
61 H.Margenau and G.M.Murphy, The Mathematics of Physics and
"Chemistry (Van Nostrand Inc. Princeton, New Jersey, 1956)
P. 126.
62 I.S.Gradshteyn and I.M.Ryzhik, Tables of Integrals Series and
63 W.Magnus, F.Oberhetinger, and R.P.Soni, Formulas and Theorems
for the Special Functions of Mathematical Physics (Springer-
Verlag, New York, 1966), P. 222.
33, 937 (1930).
69 L.P.Presnyakov and A.D.Ulantsev, Sov. J. Quantum Electron,
4, 1320 (1975).