CHAPTER 5

ELECTRON CAPTURE BY FULLY STRIPPED LITHIUM IONS
FROM ATOMIC HYDROGEN IN COULOMB-BORN
APPROXIMATION
Fig. 5.1. Co-ordinate system; A, B, and C denote the fully stripped Li\(^{3+}\) ion, proton, and electron.
Upon substitution of (2) or (3) into (4) and using the bound state wave functions satisfying

\[ -\frac{1}{2m} \nabla^2 r' - \frac{1}{r'} - \varepsilon_1 \psi_1(r') = 0 \]  

We obtain the coupled integro-differential equations

\[ (\nabla^2_{R_1} + k_1^2)\psi_1(R_1) = 2\mu_1 \left[ \int \psi_1^*(r') \left( \frac{3}{R} - \frac{1}{r} \right) \psi_1(r') \psi_1(R_1) dr' \right] + \left[ \int \psi_1^*(r') (H-E) \psi_1(r) \psi_1(R_1) dr' \right], \]  

or

\[ (\nabla^2_{R_f} - 2\frac{2u_f}{R_f} + k_f^2)\psi_n(R_f) = 2\mu_f \left[ \int \psi_n^*(r) \left( \frac{3}{R} - \frac{1}{r} - \frac{2}{R_f} \right) \right. \]

\[ \times \left. \psi_n(r) \psi_n(R_f) dr + \int \psi_n^*(r) (H-E) \psi_1(r') \psi_1(R_f) c_{rf} \right]. \]  

\( \varepsilon_1 \) and \( \varepsilon_f \) are the eigenenergies of the hydrogen atom and Li\(_{2+} \) ion, respectively. The term \( 2u_f/R_f \) occurring on the left-hand side of (9) represents the long-range Coulomb repulsion between the free proton and the screened positively charged Li\(_{2+} \) nucleus. \( k_1 \) and \( k_f \) are the momenta of the incident and scattered particle, respectively.

The function \( \psi_n(r') \) must represent the scattered waves only, and so have an asymptotic form as
where \( a \) and \( f(\omega, \lambda) \) represent the repulsive Coulomb parameter \((2\mu_{c}/k_{f})\) and the scattering amplitude, respectively. The solution of Eq. (9) with the correct asymptotic form (10) may be obtained by using the asymptotic Coulomb Green's function \( G_{C} \) of Hostler for the proton moving in the repulsive Coulomb field of the nucleus.

\[
G_{C}(R_{f}', R_{f}) \sim -\left(4\pi R_{f}\right)^{-1} \exp(i k_{f} R_{f}') \left(-2 i k_{f} R_{f}\right)^{-1} i \pi \Gamma(1+i\alpha) \left(\text{arc}(-2i k_{f} R_{f})\right)^{i\alpha} \exp(-i k_{f} R_{f}) \left[1+i G(R_{f}'/R_{f})+C(1/k_{f}) R_{f}'\right]^{-1}.
\]

In the two-state approximation, where only the coupling between the initial and the final states has been retained, we can neglect the self-coupling term in Eq. (9) and obtain

\[
\overrightarrow{F}_{n}(R_{f}') = 2\mu_{c} \int s_{n}(r) \left[\delta_{1}(r') - \delta_{1}(R_{f})\right] C_{C}(R_{f}', R_{f}) g_{C}(R_{f}') R_{f}'.
\]

In the CB approximation, we substitute in (12),

\[
\left(\frac{\hbar}{\mu_{c}}\right)^{2} + \kappa_{f}^{2} F_{1}(R_{f}) = 0,
\]

which is obtained by setting the right-hand side of (8) equal to zero. Using the asymptotic Coulomb-Green's function (11) in (12) and comparing it with (10), we find the scattering amplitude in the CB approximation to be
\[ F_{CB}^{\mathbf{k}_1 \rightarrow \mathbf{k}_f} = -\frac{\hbar}{2\alpha} \exp\left(\frac{-i\alpha}{2}\right) \Gamma(1+i\alpha) \int d\mathbf{r}d\mathbf{R}_f \exp(-i\mathbf{k}_f \cdot \mathbf{R}_f) \]
\[ \times \delta_n^{(r)}(r') \exp(\mathbf{i}k_1 \cdot \mathbf{R}_1) \, \mathbf{F}_1(-i\alpha, 1, i\mathbf{k}_f \cdot \mathbf{R}_f, i\mathbf{k}_1 \cdot \mathbf{R}_f). \]

The interaction potential \( V \) can be written in either prior- or post-collision form, i.e.,

\[ V_{\text{prior}} = \frac{3}{R} - \frac{3}{r}, \quad (14) \]
\[ V_{\text{post}} = \frac{3}{R} - \frac{1}{r'} - \frac{2}{R_f}. \quad (15) \]

It may be pointed out here that, if we use (2) for \( H \) in (12) and operate on the right-hand side, we obtain the prior form of the interaction; the post form of the interaction can be obtained if one uses (3) for \( H \) in (12) and then let it operate on the left-hand side, which is permissible owing to the Hermitian property of the \( H \) operator. Following Geltman's analysis

\[ \frac{1}{R} - \frac{1}{R_f} = \frac{1}{R} - \frac{1}{|R+e\mathbf{r}|} - \varepsilon \varepsilon \left(\frac{R+e\mathbf{r}}{R^2}\right) + O(\varepsilon^2), \quad (16) \]

where \( \varepsilon = M_e/(N_{\text{Li}^3+} + \lambda) \), \( M_e \) and \( M_{\text{Li}^3+} \) being the masses of the electron and the stripped lithium nucleus, respectively. As \( \varepsilon \) is very small (of the order of \( 10^{-4} \)), \( V_{\text{post}} \) may be written as

\[ V_{\text{post}} = \frac{1}{R} - \frac{1}{r'}, \quad (17) \]

In the present case, for convenience in the calculation, we adopt the post form of the interaction. It may be pointed out here that since we are dealing with exact bound-state wave
functions, there arises no post-prior discrepancy. The internuclear separation $\mathbf{R}$ is approximated by $\mathbf{R}_f$, the distance between the proton and the center of mass of the Li$^{2+}$ ion. This approximation introduces the neglect of a small quantity of order $10^{-4}$.

The final bound-state wave function can be written in the form
\[
\psi_n(r) = C_f D(u, r) \exp(-u \cdot r - i \cdot r) \bigg|_{r=0},
\]
where $C_f$ is the normalization constant and $D(u, r)$ is the appropriate differential operator (defined in Appendix A) which generates the required wave functions. The ground state wave function of the hydrogen atom is
\[
\psi_1(r') = \frac{1}{\sqrt{\pi}} \exp(-r').
\]

Evaluation of amplitudes and cross sections:

We first consider the $1/R$ term in the interaction potential $V_{\text{post}}$ in (17) and the evaluation of scattering amplitude (13) and follow a procedure similar to that of Geltman\textsuperscript{37} as used in the proton-hydrogen charge-transfer collision in the Coulomb-projected-Born approximation. Using the Fourier transform of $\psi_1(r')$ and integrating over $dr'$, we obtain
\[
\mathcal{F}^{\text{CB}}(k_1 \rightarrow k_2) = -\frac{4\pi^5}{5\sqrt{2}} \Gamma(1+i\omega) \exp\left(-\pi z/2\right) C_f D(u, r) \int \frac{d^3k \exp(i \cdot k \cdot r)}{(k^2 + 1)^2} \left\{ \int dR_f \frac{\exp\left[i(c \cdot \mathbf{k}_1 - c \cdot \mathbf{k}_2) \cdot \mathbf{R}_f\right]}{R_f} \right\} F_1(-i;1;ik_f \cdot k_1 \cdot k_2 \cdot k_2),
\]
(2C)
where
\[ C_1 = m_x = m \sqrt{(k_1 + 1)}; \quad C_2 = m_y = \frac{h}{13} \sqrt{\frac{3}{2}} (k_3 + 1), \]
\[ C_3 = m \left( \frac{1}{m_x} - \frac{m_p}{m} \right) ; \quad \Omega = c_2 \kappa - c_3 \kappa_1 \times t. \]

\( C_h^+ \) and \( Li_3^+ \) being the masses of proton and stripped lithium nucleus. Introducing Feynman's identity
\[ (a^2b^2)^{-1} = 6 \int_0^1 dx \ x(1-x) \left[ ax + b(1-x) \right]^{-4}, \quad (21) \]
we obtain
\[ \xi C_3 (k_1 \rightarrow k_f) = -\frac{24\pi}{\pi^2} \exp \left( \frac{-\pi x}{2} \right) \Gamma(1+i\epsilon) C_x D(i\epsilon, \gamma) \int_0^1 x(1-x) dx \int \frac{dk}{c^4} \exp \left( ik \cdot R_f \right) \int \frac{dk_f}{R_f} \exp \left[ i \left( c_3 \kappa_f - k_3 \kappa_1 \right) \times t_f \right] \]
\[ \times _1 F_1 (-i\omega; 1; ik \cdot R_f \times ik \cdot R_f) \quad (22) \]

where
\[ \omega^2 = \left[ 1 - x(\lambda^2 + (\lambda^2)^2 - 1) \right] / x; \quad \lambda = c_j \kappa_1 \]
\[ g = 1 + x(c_2^2 - 1); \quad K_0 = (c_2^2 x/g) \lambda. \]

Using the identity
\[ \int dt \ \frac{\exp(\lambda t)}{(t^2 + \lambda^2)^4} = \frac{\pi^2}{24} \frac{d}{dt} \left[ \frac{1}{t} \frac{d}{dt} \exp(-\lambda t) \right], \quad (23) \]
and then applying the Mordisk's integral technique
\[ \int \frac{\exp(-\lambda^2 t - i\kappa \cdot R_f)}{t} \ _1 F_1 (-i\omega; 1; i\kappa \cdot R_f, t) dt \]
\[ = 2\pi \left[ \frac{1}{2} (q^2 + \lambda^2) \right]^{-\frac{1}{2} - 1} \left[ \exp(-i\omega \cdot \kappa_1) - \frac{1}{2} (c_2^2 \lambda^2) \right]^{-\omega}, \quad (24) \]
we obtain the scattering amplitude as
\[ F_R(k_i \rightarrow k_f) = - \frac{2\mu_f}{\pi} \exp \left( -\frac{\pi \alpha}{2} \right) \Gamma(1+i\alpha) C_D(\mu, \gamma) \mu \]
\[ \times \int_0^1 dx \frac{x(1-x)}{q^4} \frac{1}{\eta} \frac{d}{d\eta} \frac{1}{\eta} \frac{d}{d\eta} \left( \frac{\xi(\eta)}{\eta} \right) , \]
where
\[ \xi(\eta) = \left[ \frac{1}{2}(q^2+\eta^2) \right]^{-1/2} \left[ k_f^2 - q^2 - i\eta k_f + \frac{1}{2}(q^2+\eta^2) \right]^{i/2}, \]
\[ q = -K_0 + c_1 k_i - k_f . \]

Similarly, the $1/\eta'$ term in the interaction potential $V_{\text{post}}$ in (17), when we substitute it into (13) and proceed exactly as before, we obtain the scattering amplitude
\[ F_R(k_i \rightarrow k_f) = \frac{2\mu_f}{\pi} \exp \left( -\frac{\pi \alpha}{2} \right) \Gamma(1+i\alpha) C_D(\mu, \gamma) \mu \]
\[ \times \int_0^1 dx \frac{x(1-x)}{q^3} \frac{1}{\eta} \frac{d}{d\eta} \frac{1}{\eta} \frac{d}{d\eta} \xi(\eta) . \]

The integral for scattering amplitudes (25) and (26) and finally the necessary one-dimensional integral for the total capture cross sections are performed numerically by applying the Gauss-Legendre quadrature method.

5.3. RESULTS AND DISCUSSIONS

In Table 5.1 we have presented our results for the 1s, 2s, 2p, 3s, 3p and 3d excited-state capture cross sections
TABLE 5.1 The CB cross sections $\sigma_{nl}$ (in units of $10^{-16}$ cm$^2$) for charge transfer in Li$^{3+}$ + H(1s) $\rightarrow$ Li$^{2+}$(nl) + H$^+$ collisions. The numbers in parentheses denote the powers of ten by which the numbers are multiplied.

<table>
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<th>Energy (keV)</th>
<th>$\sigma_{1s}$</th>
<th>$\sigma_{2s}$</th>
<th>$\sigma_{2p}$</th>
<th>$\sigma_{3s}$</th>
<th>$\sigma_{3p}$</th>
<th>$\sigma_{3d}$</th>
<th>$Q_{tot}$</th>
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TABLE 5-II The Born cross section $\sigma_{nl}$ (in units of $10^{-16} \text{ cm}^2$) for charge transfer in Li$^3+$ + H(1s) $\rightarrow$ Li$^2+(nl)+H^+$ collisions. The numbers in parentheses denote the powers of ten by which the numbers are multiplied.

<table>
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<th>Energy $E$ (keV)</th>
<th>$\sigma_{1s}$</th>
<th>$\sigma_{2s}$</th>
<th>$\sigma_{2p}$</th>
<th>$\sigma_{3s}$</th>
<th>$\sigma_{3p}$</th>
<th>$\sigma_{3d}$</th>
<th>$Q_{\text{tot}}$</th>
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</table>

The internuclear potential is included in the first Born amplitude.
In Fig. 5.2 we present our theoretical values for the total cross section in the energy region 100 keV to 2 MeV and have compared them with the recent experimental results of Shah et al.\textsuperscript{84} and the theoretical results obtained by the use of UDWA by Ryufuku and Watanabe\textsuperscript{43}, and the results obtained by applying the classical Monte Carlo method to the low energy region by Olson and Salop\textsuperscript{41}. The present results obtained by the CB approximation are found to be in excellent agreement with the experimental results throughout the energy region considered except at the very low energy region $E < 275$ keV, whereas the present Born cross sections grossly overestimate the total cross section throughout the energy region considered.

In the intermediate- and high energy region for the incident-ion energy of 275 to 1500 keV, the present CB results almost coincide with the experimental results. Unfortunately, no experimental results are available beyond the incident energy of 1500 keV. The UDWA results of Ryufuku and Watanabe\textsuperscript{43} on the other hand, give quite good agreement in the low-energy region up to the incident energy of 400 keV, but beyond this incident energy the UDWA results grossly overestimate the observed values. The values of the cross section estimated by the Monte Carlo approach of Olson and Salop\textsuperscript{41} gives good agreement with the observed values for the lower energy range up to 300 keV, but beyond that it grossly overestimates the observed findings.
Fig. 5.2. Total capture cross section $Q_{tot}$ for the projectile $^{7}\text{Li}^{3+}$ ion incident on ground state atomic hydrogen.

Theory: ———, UDWA calculation of Ryufuku and Watanabe (1979) (Ref. 43); ————, Monte Carlo calculation of Olson and Salop (Ref. 41); ———, Present CB calculation; ———, present Born calculation.

Experiment: †, Shah et al (Ref. 84).
Upon comparison with the present Born calculation, the CB results are found to give much lower values for the cross sections for all the individual excited states throughout the energy region considered. However, the Born cross sections for all the individual excited states show the same trend as the CB cross sections. The reduction in the values of the cross sections in the CB approximation may be attributed to the appreciable long-range Coulomb repulsive force present in the final product of the charge transfer reaction which is completely neglected in the Born approximation. Further it has been pointed out by Halpern and Law\textsuperscript{143} that although the Born approximation yields reasonable results for the charge transfer of lighter ions such as H\textsuperscript{+}+H collisions it leads to unphysical results for more highly charged species. Unfortunately neither any theoretical results nor any experimental findings are available for comparison with the individual excited-state cross sections. In the UDWA approximation of Ryufuku and Watanabe\textsuperscript{43} all interactions among the product channels are ignored, and thus the results obtained by this method are largely overestimated, especially in the high energy region where the direct excitation channels and the ionization channels contribute significantly in the cross section calculations.
A rigorous close-coupling approximation based only on the atomic- and molecular-state expansion can give accurate results for the cross sections, but it is rather difficult and tedious to handle such a large number of excitation and charge transfer channels involved in the case of highly charged heavy ions, for which contributions from the large values of the principal quantum number \( n \) in the capture state should be considered in the calculations. Thus the present CB method, though essentially a first-order high energy approximation, may be useful to give an estimate for the capture cross sections for such highly charged species as a projectile on the ground-state atomic hydrogen, at least in the intermediate and high energy region.

5.4. CONCLUDING REMARKS

Good agreement between the experimental and the theoretical results obtained by the CB approximation makes one optimistic to calculate charge transfer cross sections by highly charged ions from atoms or ions. Further, to test the theory more critically, it may be necessary to apply the CB approximation in heavier ion-atom collision cases. In the usual method for the evaluation of the scattering amplitude, we are to adopt the technique of parametric differentiations to calculate charge transfer cross sections into excited states.
This procedure may not be so suitable for the application of the CB approximation to heavier ion-atom collision systems. So a new straightforward technique which should be devoid of parametric differentiations, is needed for the evaluation of the transition amplitude in the CB approximation.
Capture into the $3d_0$ state:

$$D(\mu, \gamma) = -z_p^2 \left[ 3 \frac{\partial^2}{\partial r^2} + \frac{x^2}{\partial \mu^2} \right], \quad c_f = \frac{1}{81 \sqrt{\pi}} z_p^{3/2}, \quad \mu = \frac{1}{3} z_p. \quad \text{(A8)}$$

Capture into the $3d_{\pm 1}$ state:

$$D(\mu, \gamma) = z_p^2 \left[ \frac{\partial^2}{\partial \gamma_z \partial \gamma_z} \pm i \frac{\partial^2}{\partial \gamma_z \partial \gamma_y} \right], \quad c_f = -\frac{1}{81 \sqrt{\pi}} z_p^{3/2},$$

$$\mu = \frac{1}{3} z_p. \quad \text{(A9)}$$

Capture into the $3d_{\pm 2}$ state:

$$D(\mu, \gamma) = z_p^2 \left[ \frac{\partial^2}{\partial \gamma_x \partial \gamma_x} - \frac{\partial^2}{\partial \gamma_y \partial \gamma_y} \pm 2i \frac{\partial^2}{\partial \gamma_x \partial \gamma_y} \right], \quad c_f = -\frac{1}{162 \sqrt{\pi}} z_p^{3/2},$$

$$\mu = \frac{1}{3} z_p. \quad \text{(A10)}$$