CHAPTER 2

The Close-Coupling Method (CC)

The details of the close-coupling method (CC) which is based on the work by Mitroy and Ratnavelu (1994) are described in this chapter. The CC had been used in the study of hydrogenic atoms such as lithium, sodium and potassium. Here, the CC is used in the investigation of theoretical scattering of electrons and positrons by atomic Rb.

2.1 Terminology

Before moving on to the theoretical details of both methods, the following terminology must be understood:

1) Wavefunction, Ψ

In quantum mechanics, the wavefunction is a function in Hilbert space that describes the states of subatomic particles. The wavefunction is a probability amplitude (complex vector) and $|\Psi * \Psi|$ yields the probability of finding the particles at certain position and time. It is the solution of Schrodinger equation.

2) Schrodinger equation

In quantum mechanics, the Schrodinger equation is an equation that describes the behavior of particles in time, i.e. the changes of quantum state with time. There are 2 types of Schrodinger equation, the time-dependent Schrodinger equation and the time-independent Schrodinger equation.

3) Channel

Channel is the possible mode of fragmentation of the system during the collision. A channel is “open” if the particular collision is allowed by some known conservation laws, else the channel is “closed”. Initial channel and final channels are the possible fragmentation of system before and after the collision process. The incident channel is always “open” and elastic. Non-elastic channels are considered to be different channels and the channels are “closed” as long as the energy required to excite the system into inelastic states is insufficient. Once the energy is sufficient to excite the system to the excited states, the non-elastic channels will “open”. Once a non-elastic channels is opened, the incident flux will either be diverted into the elastic or the non-elastic channels. Fig. 2.1 illustrates the concept of channel.

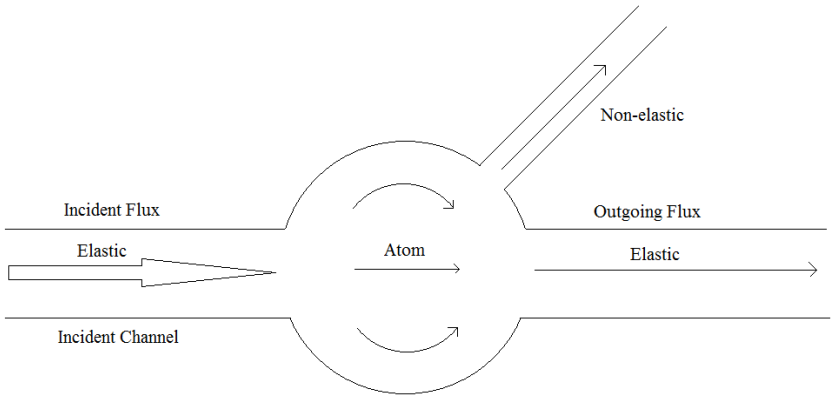

Fig. 2.1 : The concept of channel.

2.2 Type of Interaction

When an incident particle approaches an atom and eventually collides with the target atom, a few types of interaction may happen. If an electron collides with an atom, elastic scattering, inelastic scattering or ionization might happen. If a positron collides

with an atom, elastic and inelastic scattering, ionization and Ps formation might happen.

The following figures show the types of interactions.

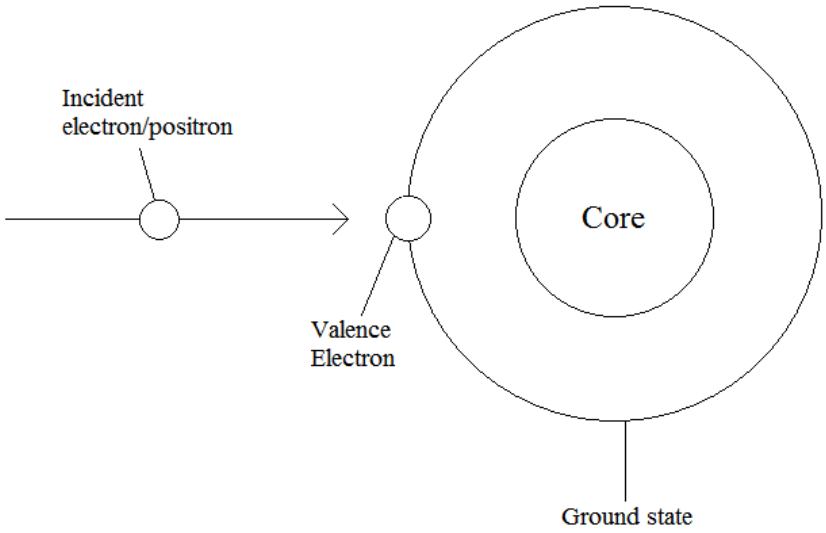

Fig. 2.2 : An incident particle is approaching an atom with a valence electron orbiting the core in the ground state. The core consists of the nucleus and all the other electrons of the atom except the valence electron.

2.2.1 Electron-atom Scattering

Elastic Scattering

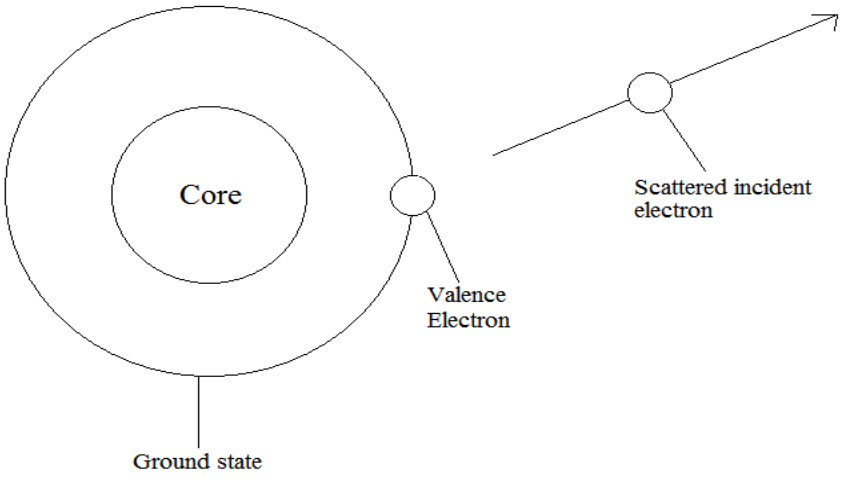

Fig. 2.3 : The elastic scattering of electron-atom scattering. The incident electron collides with the atom. The incident electron is scattered without changing the internal quantum state of the atom.

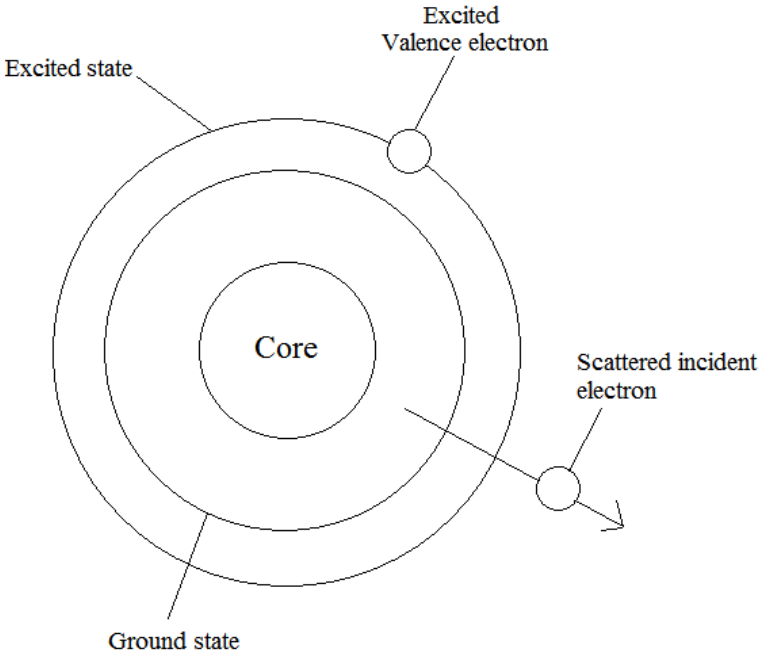

Fig. 2.4 : Part 1 of the inelastic scattering of electron-atom scattering. When the incident electron collides with the valence electron in the ground state, it changes the internal quantum state of the atom where the valence electron is excited into the excited state.

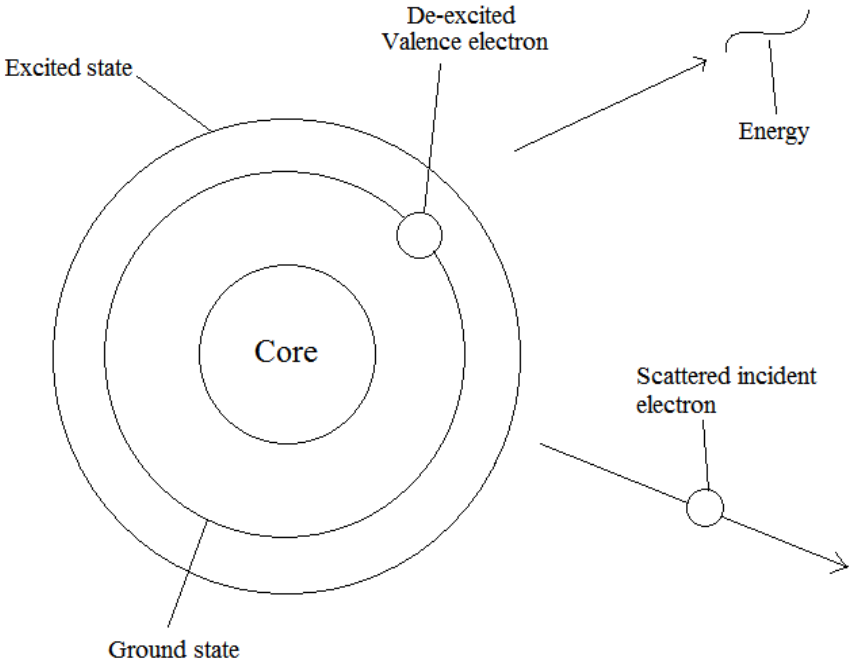

Fig. 2.5 : Part 2 of the inelastic scattering of the electron-atom scattering. The excited valence electron is de-excited into ground state by emitting energy in the form of a photon.

Ionization

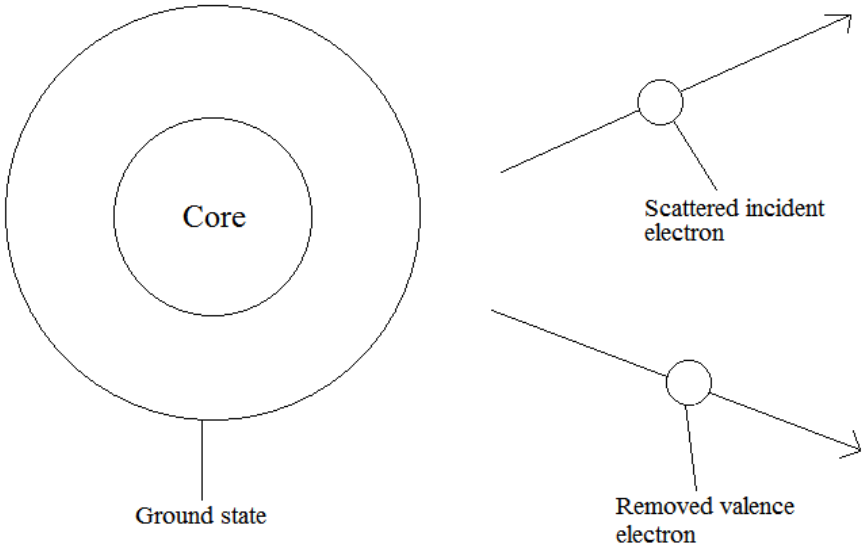

Fig. 2.6 : Ionization in electron-atom scattering. The valence electron is removed from the atom. The atom is ionized and becomes an ion.

2.2.2 Positron-atom Scattering

Elastic Scattering

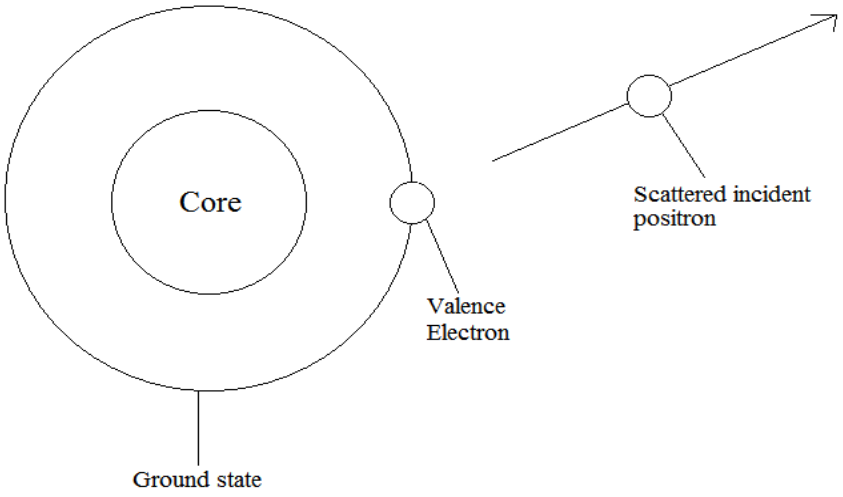

Fig. 2.7 : Elastic positron-atom scattering.

Inelastic Scattering

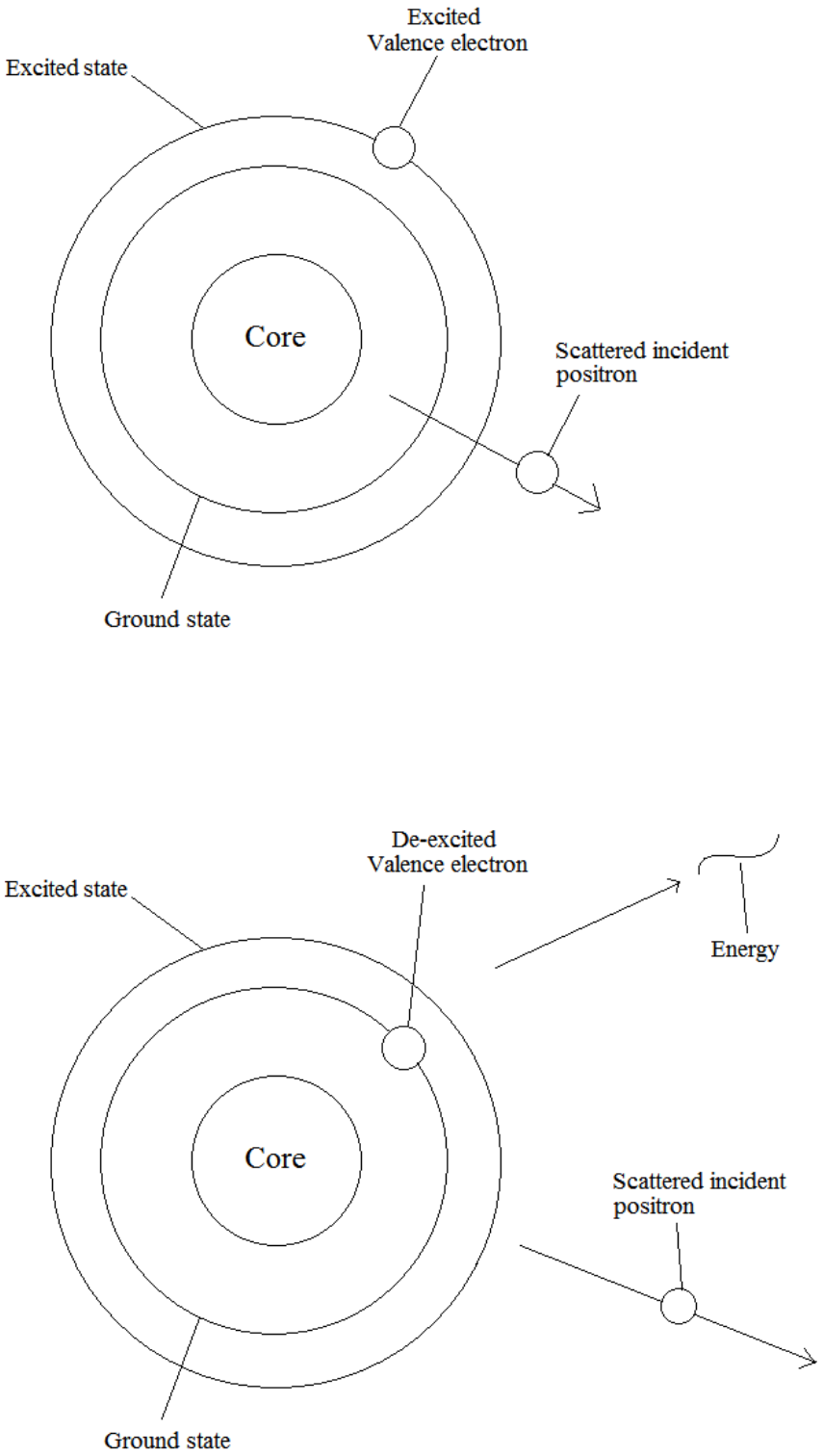

Fig. 2.8 : Inelastic scattering in positron-atom scattering.

Ionization

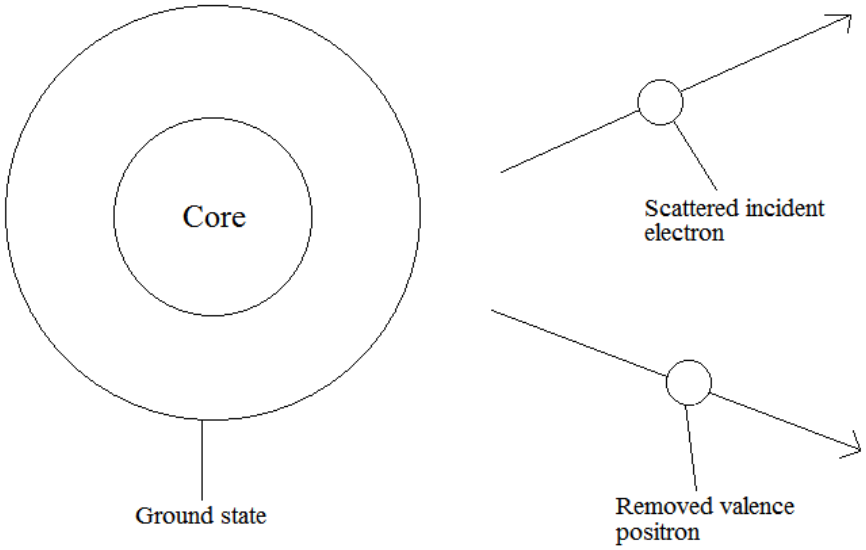

Fig. 2.9 : Ionization in positron-atom scattering.

Ps Formation

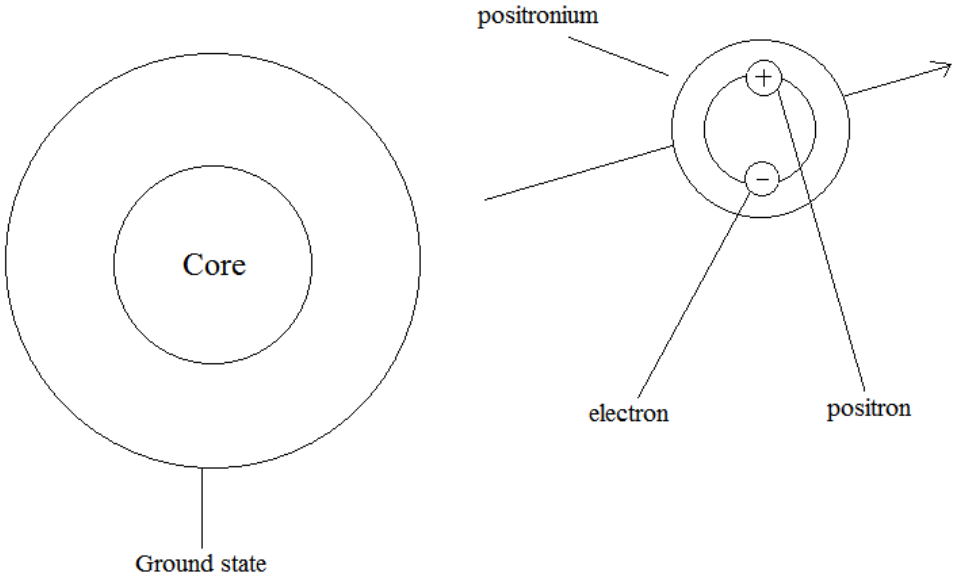

Fig. 2.10 : Ps formation in positron-atom scattering. The incident positron binds together with the valence electron and forms an unstable 'atom' which eventually annihilates and produces photons.

2.3 Theoretical Details

2.3.1 Electron-Rb Scattering

In general, the Schrodinger equation for a (*N*+1)-body system is defined as:

$$(H - E)\Psi(r_i, r_0) = 0 \tag{2.1}$$

where r_0 is the coordinate of the incident particle (electron) and r_i is the coordinates of the N electron where $i = \{1,2, \dots, N\}$ (r_1 represents the valence electron of the target atom). H denotes the total Hamiltonian of the system while *E* represents the total energy of the (*N*+1)-body system.

In the CC formalism, the wavefuntion, $\Psi(r_i, r_0)$ is expanded in an eigenfunction expansion of electron scattering states which are coupled to the atomic states:

$$\Psi(r_i, r_0) = \sum_\alpha \Psi_\alpha(r_i) F_\alpha(r_0) \tag{2.2}$$

By expanding equation (2.2), the following expression can be obtained:

$$\Psi(r_i, r_0) = \Psi_{11}(r_i) F_{11}(r_0) + \Psi_{12}(r_i) F_{12}(r_0) + \Psi_{13}(r_i) F_{13}(r_0) + \cdots \tag{2.3}$$

Following McCarthy and Stelbovics (1983a), it is possible to transform the Schrodinger equation into the momentum-space Lippmann-Schwinger (LS) equation for an incident electron with momentum k on a Rb atom. The LS equation in the operator form is given by:

$$T_{\alpha' \alpha} = V_{\alpha' \alpha} + \sum_{\alpha''} V_{\alpha' \alpha''} G_{\alpha''} T_{\alpha'' \alpha'} \tag{2.4}$$

The LS equation in the explicit T-matrix elements:

$$\langle k' \psi_{\alpha'} | T | k \psi_\alpha \rangle = \langle k' \psi_{\alpha'} | V | k \psi_\alpha \rangle + \sum_{\alpha''} \int d^3 k'' \, \frac{\langle k' \psi_{\alpha'} | V | k'' \psi_{\alpha''} \rangle \langle k'' \psi_{\alpha''} | T | k \psi_\alpha \rangle}{\left(E^{(+)} - \varepsilon_{\alpha''} - \frac{1}{2} k''^2 \right)} \tag{2.5}$$

(Refer to Appendix I for the crude illustration describing the T-Matrix (equation (2.5))

2.3.2 Positron-Rb Scattering

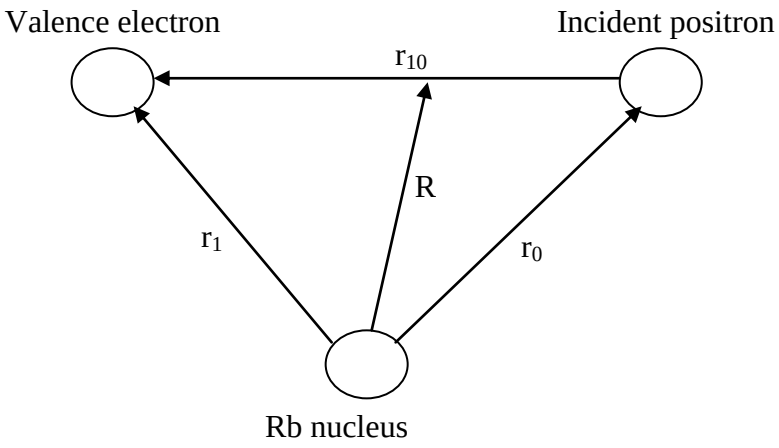

Fig. 2.11 : Positron-Rb scattering.

Figure 2.11 shows the illustration of the positron-Rb scattering. Similar to the electron-Rb scattering case, r_0 is defined in the coordinate system as the coordinate of the incident positron and r_i as the coordinates of the N electron where $i = \{1,2,\dots,N\}$ (r_1 represents the valence electron of the target atom). The distance between the valence electron and the incident particle (positron) is r_{10}, which is defined as $r_{10} = |r_1 - r_0|$.

Let ρ_i be the relative coordinate and R_i be the center of mass of the outgoing Ps, the following relation can be established:

$$r_i = R_i + \frac{1}{2}\rho_i \qquad r_0 = R_i - \frac{1}{2}\rho_i$$

$$\rho_i = r_i - r_0 \qquad R_i = \frac{1}{2}(r_i + r_0) \tag{2.6}$$

The Jacobian for the transformation between the 2 coordinate systems is:

$$\int d^3 r_i \int d^3 r_0 = \int d^3 \rho_i \int d^3 R_i \tag{2.7}$$

(Refer to Appendix II for the Jacobian transformation of equation (2.7))

With these definitions, the Schrodinger equation, equation (2.1) can now be rewritten as:

$$(H_{atom} + H_e - E)\Psi(r_i, r_0) = 0 \tag{2.8}$$

where H_{atom} is the *N*-electron Hamiltonian of the target Rb atom:

$$H_{atom} = \sum_{i=1}\left(-\frac{1}{2}\nabla_i^2 + \frac{Z}{r_i}\right) + \frac{1}{2}\sum_{\substack{i=1 \\ j\neq i}}\frac{1}{r_{ij}} \tag{2.9}$$

and H_e is the Hamiltonian consisting the coordinate of the incident positron:

$$H_e = -\frac{1}{2}\nabla_0^2 + \frac{Z}{r_0} - \sum_{i=1}\frac{1}{r_{i0}} \tag{2.10}$$

Following Mitroy and Ratnavelu (1994), Ps formation can be incorporated into the calculation. We can do so by partitioning the Hamiltonian in an alternative way:

$$(H_{Ps}(m) + H_{ion}(m) + H_{int}(m))\Psi(r_i, r_0) = 0 \qquad m \in \{1, \ldots, N\} \tag{2.11}$$

where H_{Ps} is the interaction of the Ps molecule which contain the valence electron, r_1, with the residual ion:

$$H_{Ps} = \left(-\frac{1}{4}\nabla_R^2 + \frac{Z}{r_0} - \frac{Z}{r_1}\right) - \sum_{i=2}\left(\frac{1}{r_{i0}} - \frac{1}{r_{i1}}\right) \tag{2.12}$$

H_{ion} is the Hamiltonian of the residual ion with the valence electron removed from the Rb atom:

$$H_{ion} = \sum_{i=2}\left(-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right) + \frac{1}{2}\sum_{\substack{i,j=2 \\ i\neq j}}\left(\frac{1}{r_{ij}}\right) \tag{2.13}$$

Finally, H_{int} is the internal Hamiltonian of the Ps molecule containing the removed valence electron from Rb atom:

$$H_{int} = -\nabla_{\rho_1}^2 + \frac{1}{r_{10}} \tag{2.14}$$

The wavefuntion, $\Psi(r_i, r_0)$ can now be expanded in an eigenfunction expansion of Ps and continuum positron state which are coupled to the ionic and atomic states:

$$\Psi(r_i, r_0) = \sum_\alpha \Psi_\alpha(r_i) F_\alpha(r_0) + \sum_{\beta\gamma} \Omega_\gamma(r_{i'}) \Phi_\beta(\rho) G_{\beta\gamma}(R) \tag{2.15}$$

where $r_{i'}$ is the *N*-1 electrons of the Rb residual ion. The notations $\Psi_\alpha(r_i)$, $\Omega_\gamma(r_{i'})$ and $\Phi_\beta(\rho)$ represent the bound atomic, ionic and Ps stationary states respectively. All these satisfy the following conditions:

$$\langle \Psi_\alpha(r_i) | H_{atom} - \epsilon_\alpha | \Psi_\alpha(r_i) \rangle = 0 \tag{2.16}$$

$$\langle \Phi_\beta(\rho) \left| H_{\text{int}} - \epsilon_\beta \right| \Phi_\beta(\rho) \rangle = 0 \tag{2.17}$$

$$\langle \Omega_\gamma(r_{i'}) | H_{ion} - \epsilon_{core} | \Omega_\gamma(r_{i'}) \rangle = 0 \tag{2.18}$$

Substituting equation (2.15) into equation (2.1), the Schrodinger equation is now:

$$(E - H)\left(\sum_\alpha \Psi_\alpha(r_i) F_\alpha(r_0) + \sum_{\beta\gamma} \Omega_\gamma(r_{i'}) \Phi_\beta(\rho) G_{\beta\gamma}(R)\right) = 0 \tag{2.19}$$

By multiplying the left hand side of equation (2.19) with $\Psi^*_{\alpha'}(r_i)$ and integrating the equation with respect to $d^3 r_i$, the following equation can be obtained:

$$\left(E + \frac{1}{2}\nabla_0^2 - \epsilon_{\alpha'} - \epsilon_{core}\right) F_{\alpha'}(r_0) = \sum_\alpha \langle \Psi_{\alpha'} \left| \frac{Z}{r_0} - \sum_{i=1} \frac{1}{r_{0i}} \right| \Psi_\alpha \rangle F_\alpha(r_0) + \sum_{\beta\gamma} \langle \Psi_{\alpha'} | H - E | \Omega_\gamma \Phi_\beta(\rho) \rangle G_{\beta\gamma}(R) \tag{2.20}$$

Similarly, by multiplying the left hand side of equation (2.19) with $\Omega^*_{\gamma'}(r_{i'}) \Phi^*_{\beta'}(\rho)$ and integrating with respect to $d^3 r_{i'}$ and $d^3 \rho$, we can obtain the following equation:

$$\left(E + \frac{1}{4}\nabla_R^2 - \epsilon_{\beta'} - \epsilon_{core}\right) G_{\beta'\gamma'}(R) = \sum_\alpha \langle \Phi_{\beta'} \Omega_{\gamma'} | H - E | \Psi_\alpha \rangle F_\alpha + \sum_{\beta\gamma} \langle \Phi_{\beta'} \Omega_{\gamma'} \left| \frac{Z}{r_0} - \frac{Z}{r_1} - \sum_{i=2} \left(\frac{1}{r_{i0}} - \frac{1}{r_{i1}}\right) \right| \Phi_\beta \Omega_\gamma \rangle G_{\beta\gamma}(R) \tag{2.21}$$

(Refer to Appendix III for the details of integration of equation (2.20) and (2.21))

Following Mitroy and Ratnavelu (1994), three approximations have been used to simplify the system:

a) The wavefunctions for the atomic and residual ionic state will be computed in a fixed-core model.

b) There is only one possible residual ionic state. Hence only the valence electron will be removed during the Ps formation.

c) The exchange in between the electron in the residual ion and the electron in the Ps is neglected.

Thus, equation (2.20) and equation (2.21) can be transformed into the momentum-space LS equations. The momentum-space LS equation for an incident positron with momentum *k* impacting on a Rb atom in atomic state Ψ_α are:

$$\langle k'\Psi_{\alpha'}|T|k\Psi_\alpha\rangle = \langle k'\Psi_{\alpha'}|V|k\Psi_\alpha\rangle + \sum_{\alpha''}\int d^3k'' \left(\frac{\langle k'\Psi_{\alpha'}|V|k''\Psi_{\alpha''}\rangle}{E^{(+)} - \frac{1}{2}k''^2 - \epsilon_{\alpha''} - \epsilon_{core}}\right)\langle k''\Psi_{\alpha''}|T|k\Psi_\alpha\rangle + \sum_{\beta''\gamma''}\int d^3k'' \left(\frac{\langle k'\Psi_{\alpha'}|V|k''\Phi_{\beta''}\Omega_{\gamma''}\rangle}{E^{(+)} - \frac{1}{4}k''^2 - \epsilon_{\beta''} - \epsilon_{core}}\right)\langle k''\Phi_{\beta''}\Omega_{\gamma''}|T|k\Psi_\alpha\rangle \quad (2.22a)$$

$$\langle k'\Phi_{\beta'}\Omega_{\gamma'}|T|k\Psi_\alpha\rangle = \langle k'\Phi_{\beta'}\Omega_{\gamma'}|V|k\Psi_\alpha\rangle + \sum_{\alpha''}\int d^3k'' \left(\frac{\langle k'\Phi_{\beta'}\Omega_{\gamma'}|V|k''\Psi_{\alpha''}\rangle}{E^{(+)} - \frac{1}{2}k''^2 - \epsilon_{\alpha''} - \epsilon_{core}}\right)\langle k''\Psi_{\alpha''}|T|k\Psi_\alpha\rangle + \sum_{\beta''\gamma''}\int d^3k'' \left(\frac{\langle k'\Phi_{\beta'}\Omega_{\gamma'}|V|k''\Phi_{\beta''}\Omega_{\gamma''}\rangle}{E^{(+)} - \frac{1}{4}k''^2 - \epsilon_{\beta''} - \epsilon_{core}}\right)\langle k''\Phi_{\beta''}\Omega_{\gamma''}|T|k\Psi_\alpha\rangle \quad (2.22b)$$

(Refer to Appendix IV for the transformation of the momentum-space LS equations (equation (2.22a) and equation (2.22b)))

2.3.3 The Interaction Matrix Elements

The term *V* in the T-matrices is in the matrix form representing the interaction between the different classes of channels. The 3 different classes are the interaction between different positron channels, the interaction between Ps and the residual ion, and the rearrangement matrix elements.

a) Interaction Between Different Positron Channels

This interaction is defined as:

$$\langle k'\Psi_{\alpha'}|V|k\Psi_{\alpha}\rangle = (2\pi)^{-3}\int d^3r_0 \int d^3r_i \Psi^*_{\alpha'}(r_i) exp(-ik'.r_0) \times \left[\frac{Z}{r_0} - \sum_i^N \frac{1}{r_{i0}}\right]\Psi_{\alpha}(r_i) exp(ik.r_0) \quad (2.23)$$

Following these relations:

$$\Psi_{\alpha}(r_i) \approx \Psi_{\alpha}(r_1)\Omega(r_{i'}) \qquad \int d^3r_i \approx \int d^3r_{i'} \int d^3\, r_1 \quad (2.24)$$

Equation (2.23) can be written as:

$$\langle k'\Psi_{\alpha'}|V|k\Psi_{\alpha}\rangle = (2\pi)^{-3}\int d^3r_0 \int d^3r_{i'} \int d^3\, r_1 \Psi^*_{\alpha'}(\mathrm{r}_1)\Omega^*(r_{i'}) exp(-ik'.r_0) \times \left[\frac{Z-1}{r_0} - \sum_{i\neq 1}\frac{1}{r_{i0}} + \frac{1}{r_0} - \frac{1}{r_{01}}\right]\Psi_{\alpha}(r_1)\Omega(r_{i'})\, exp(ik.r_0) \quad (2.25)$$

Defining the core potential, υ_{core} as:

$$\upsilon_{core}\,(r_0) = \left[\frac{Z-1}{r_0} - \sum_{i\neq 1}\frac{1}{r_{i0}}\right] \quad (2.26)$$

and V_{core} as:

$$V_{core} = \langle \Omega | v_{core}(r_0) | \Omega \rangle = \sum_{\gamma} (4l_{\gamma} + 2) \int d^3 r_{i'} \, \omega_{\gamma}^*(r_{i'}) \omega_{\gamma}(r_{i'}) \left(\frac{1}{r_0} - \frac{1}{r_{0i'}} \right) \quad (2.27)$$

where $\omega_{\gamma}(r_{i'})$ represents the wavefunction of the frozen core. The sum over γ covers all the fully occupied orbitals in the frozen core.

After substituting equation (2.26) into equation (2.25), we have:

$$\langle k' \Psi_{\alpha'} | V | k \Psi_{\alpha} \rangle = (2\pi)^{-3} \int d^3 r_0 \int d^3 r_{i'} \int d^3 r_1 \Psi_{\alpha'}^*(\mathrm{r}_1) \Omega^*(r_{i'}) exp(-ik'.r_0)$$
$$\times \left[v_{core}(r_0) + \frac{1}{r_0} - \frac{1}{r_{01}} \right] \Psi_{\alpha}(r_1) \Omega(r_{i'}) \, exp(ik.r_0) \quad (2.28)$$

By using equation (2.27), equation (2.28) can be simplified as:

$$\langle k' \Psi_{\alpha'} | V | k \Psi_{\alpha} \rangle = (2\pi)^{-3} \int d^3 r_0 \int d^3 r_1 \Psi_{\alpha'}^*(r_1) \, exp(-ik'.r_0)$$
$$\times \left[V_{core} + \frac{1}{r_0} - \frac{1}{r_{01}} \right] \Psi_{\alpha}(r_1) \, exp(ik.r_0) \quad (2.29)$$

b) Interaction Between Ps and the Residual Ion

Generally, there are 2 types of interactions between Ps and residual ion: the direct-type and the exchange-type interactions. As mentioned previously in the 3 approximations that simplify the system, the exchange-type interaction will be neglected in the calculation. The direct-type interaction is given as:

$$\langle k' \Omega_{\gamma'} \Phi_{\beta'} | V | k \Omega_{\gamma} \Phi_{\beta} \rangle = (2\pi)^{-3} \int d^3 \rho \int d^3 R \int d^3 r_{i'} \, \Omega_{\gamma'}^*(r_{i'}) \Phi_{\beta'}^*(\rho) exp(-ik'.R)$$
$$\times \left[\frac{Z}{r_0} - \frac{Z}{r_1} - \sum_{i \neq 1} \left(\frac{1}{r_{i0}} - \frac{1}{r_{i1}} \right) \right] \Omega_{\gamma}(r_{i'}) \Phi_{\beta}(\rho) \, exp(ik.R) \quad (2.30)$$

Equation (2.30) can be expanded into:

$$\langle k' \Omega_{\gamma'} \Phi_{\beta'} | V | k \Omega_{\gamma} \Phi_{\beta} \rangle = (2\pi)^{-3} \int d^3 \rho \int d^3 R \int d^3 r_{i'} \, \Omega_{\gamma'}^*(r_{i'}) \Phi_{\beta'}^*(\rho) exp(-ik'.R)$$
$$\times \left[\left(\frac{Z-1}{r_0} - \sum_{i \neq 1} \frac{1}{r_{i0}} \right) - \left(\frac{Z-1}{r_1} - \sum_{i \neq 1} \frac{1}{r_{i1}} \right) + \frac{1}{r_0} - \frac{1}{r_1} \right]$$

$$\times \Omega_{\gamma}(r_{i'})\Phi_{\beta}(\rho)\, exp(ik.R) \tag{2.31}$$

We define the v_{core} and V_{core} as:

$$v_{core}(r_0) = \left[\frac{Z-1}{r_0} - \sum_{i\neq 1}\frac{1}{r_{i0}}\right] \qquad v_{core}(r_1) = \left[\frac{Z-1}{r_1} - \sum_{i\neq 1}\frac{1}{r_{i1}}\right] \tag{2.32a}$$

$$V_{core}(r_0) = \langle\Omega|v_{core}(r_0)|\Omega\rangle \qquad V_{core}(r_1) = \langle\Omega|v_{core}(r_1)|\Omega\rangle \tag{2.32b}$$

By using the similar procedure of substitution and simplification as in section (a), equation (2.30) can be written as:

$$\begin{aligned}\left\langle k'\Omega_{\gamma'}\Phi_{\beta'}\middle|V\middle|k\Omega_{\gamma}\Phi_{\beta}\right\rangle = (2\pi)^{-3}\int d^3\rho \int d^3R\, \Phi^*_{\beta'}(\rho) exp(-ik'.R) \\ \times\left[V_{core}(r_0) - V_{core}(r_1) + \frac{1}{r_0} - \frac{1}{r_1}\right] \\ \times \Phi_{\beta}(\rho)\, exp(ik.R)\end{aligned} \tag{2.33}$$

c) Rearrangement Matrix Element

The rearrangement matrix element of the Ps formation is:

$$\begin{aligned}\left\langle k'\Omega_{\gamma'}\Phi_{\beta'}\middle|V\middle|k\Omega_{\gamma}\Phi_{\beta}\right\rangle = (2\pi)^{-3}\int d^3r_0 \int d^3\, r_1 \int d^3r_{i'}\, \Omega^*(r_{i'})\Phi^*_{\beta'}(\rho)\, exp(-ik'.R) \\ \times [H-E]\Psi_{\alpha}(r_i)\, exp(ik.r_0)\end{aligned} \tag{2.34}$$

Defining $H = H_{atom} + H_e$ and following equation (2.10) and (2.16), equation (2.34) is written as:

$$\begin{aligned}\left\langle k'\Omega_{\gamma'}\Phi_{\beta'}\middle|V\middle|k\Psi_{\alpha}\right\rangle = (2\pi)^{-3}\int d^3r_0 \int d^3\, r_1 \int d^3r_{i'}\, \Omega^*(r_{i'})\Phi^*_{\beta'}(\rho)\, exp(-ik'.R) \\ \times\left[-\frac{1}{2}\nabla_0^2 + \frac{Z}{r_0} - \sum_i\frac{1}{r_{i0}} + \varepsilon_{core} + \varepsilon_{\alpha} - E\right]\Psi_{\alpha}(r_i)\, exp(ik.r_0)\end{aligned}$$

(2.35)

It was shown in section (a) that $\frac{Z}{r_0} - \sum_i \frac{1}{r_{i0}} = \upsilon_{core}(r_0) + \frac{1}{r_0} - \frac{1}{r_{01}}$, so by using equation (2.27) and some algebraic manipulation, equation (2.35) can be written as:

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Psi_\alpha\rangle = (2\pi)^{-3}\int d^3r_0 \int d^3 r_1 \Phi^*_{\beta'}(\rho)\, exp(-ik'.R) \times \left[\frac{1}{2}\kappa^2 + V_{core}(r_0) + \frac{1}{r_0} - \frac{1}{r_{01}} + \varepsilon_{core} + \varepsilon_\alpha - E\right] \times \Psi_\alpha(r_i)\, exp(ik.r_0) \quad (2.36)$$

Since there is an optional way of partitioning the Hamiltonian, H ($H = H_{ion} + H_{Ps} + H_{int}$), so there is an alternative way to obtain the matrix element. Thus, equation (2.34) can also be expressed as:

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Psi_\alpha\rangle = (2\pi)^{-3}\int d^3r_0 \int d^3 r_1 \int d^3r_{i'}\, \Omega^*(r_{i'})\Phi^*_{\beta'}(\rho)\, exp(-ik'.R) \times [H_{ion} + H_{Ps} + H_{int} - E]\Psi_\alpha(r_i)\, exp(ik.r_0) \quad (2.37)$$

Following equation (2.17) and equation (2.18), equation (2.37) can be written as:

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Psi_\alpha\rangle = (2\pi)^{-3}\int d^3r_0 \int d^3 r_1 \int d^3r_{i'}\, \Omega^*(r_{i'})\Phi^*_{\beta'}(\rho)\, exp(-ik'.R) \times \left[H_{Ps} + \varepsilon_\beta + \varepsilon_{core} - E\right]\Psi_\alpha(r_i)\, exp(ik.r_0) \quad (2.38)$$

By using equation (2.16), equation (2.17) and equation (2.18), equation (2.38) can be rewritten as:

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Psi_\alpha\rangle = (2\pi)^{-3}\int d^3\rho \int d^3R \int d^3 r_{i'}\, \Omega^*(r_{i'})\Phi^*_{\beta'}(\rho)\, exp(-ik'.R) \times \left[\frac{1}{4}\kappa'^2 + \frac{1}{2}\nabla^2_{r_1} + V_{core}(r_0) + \frac{1}{r_0} + \varepsilon_\beta + \varepsilon_{core} + \varepsilon_\alpha - E\right] \times \Psi_\alpha(r_i)\, exp(ik.r_0) \quad (2.39)$$

Both equation (2.36) and equation (2.39) are the matrix elements in different forms. Equation (2.36) is the post form while equation (2.37) is the prior form. Since the

interaction Hamiltonian is sandwiched between the plane waves, so essentially both matrix elements are equivalent.

2.3.4 Matrix Elements in Momentum Space

For computational purpose, the matrix elements are best expressed in the momentum space forms. For the interaction between positron channels, equation (2.29) in the momentum space form is written as:

$$\langle k'\Psi_{\alpha'}|V|k\Psi_{\alpha}\rangle = \left[\frac{1}{2\pi^2|k-k'|^2}\right]\{\delta_{\alpha'\alpha} - \int d^3r\,\Psi^*_{\alpha'}(r)\Psi_{\alpha}(r)exp[i(k-k')r]\}$$

$$+\delta_{\alpha'\alpha}\sum_{\gamma}\left[\frac{4l_{\gamma}+2}{2\pi^2|k-k'|^2}\right]\left\{1 - \int d^3\omega^*_{\gamma'}(r)\omega_{\gamma}(r)exp[i(k-k')r]\right\} \quad (2.40)$$

Defining $K = |k-k'|$, equation (2.40) can be written in details as:

$$\langle k'\Psi_{\alpha'}|V|k\Psi_{\alpha}\rangle = \left[\frac{1}{2\pi^2K^2}\right]\left[\delta_{\alpha'\alpha}\delta_{\lambda_0} - \sum_{\lambda\mu} i^{\lambda}(-1)^{m_{\alpha'}+\mu}\right.$$

$$\left.\times\chi^{\lambda}_{\alpha'\alpha}(K)C^{\lambda}_{-\mu}(k-k')\hat{l}_{\alpha}\hat{l}_{\alpha'}\hat{\lambda}^2\begin{pmatrix} l_{\alpha} & \lambda & l_{\alpha'} \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & l_{\alpha} & l_{\alpha'} \\ \mu & m_{\alpha} & -m_{\alpha}\end{pmatrix}\right]$$

$$+\delta_{\alpha'\alpha}\delta_{\lambda_0}V_{core}(K) \quad (2.41)$$

where:

$$\chi^{\lambda}_{\alpha'\alpha}(K) = \int_0^{\infty} dr\ r^2\Psi^*_{\alpha'}(r)\Psi_{\alpha}(r)j_{\lambda}(K_r) \quad (2.42a)$$

$$C^{\lambda}_{-\mu}(k-k') = \text{spherical tensor} \quad (2.42b)$$

$$\hat{\lambda}^2 = \sqrt{2\lambda-1} \quad (2.42c)$$

$$V_{core}(K) = \sum_{\gamma}\left[\frac{4l_{\gamma}+2}{2\pi^2K^2}\right]\left[1 - \int_0^{\infty} dr\ r^2\omega^*_{\gamma'}(r)\omega_{\gamma}(r)j_0(K_r)\right] \quad (2.42d)$$

For the interaction between Ps and the residual ion, equation (2.33) in the momentum space form is:

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Omega_{\gamma}\Phi_{\beta}\rangle = \left[V_{core}(K) + \frac{1}{2\pi^2K^2}\right]\int d^3\rho\,\Phi^*_{\beta'}(\rho)\Phi_{\beta}(\rho)$$
$$\times\left\{exp\left[\frac{1}{2}i(k-k').\rho\right] - exp\left[-\frac{1}{2}i(k-k').\rho\right]\right\} \quad (2.43)$$

In details,

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Omega_{\gamma}\Phi_{\beta}\rangle = \left[V_{core}(K) + \frac{1}{2\pi^2K^2}\right]$$
$$\times\left\{\left[1-(-1)^{\lambda}\right]\sum_{\lambda\mu} i^{\lambda}(-1)^{m_{\beta'}}Y^{\lambda}_{\beta'\beta}(K)C^{\lambda}_{-\mu}(k-k')\hat{l}_{\beta}\hat{l}_{\beta'}\hat{\lambda}^2\right\}$$
$$\times\begin{pmatrix} l_{\beta} & \lambda & l_{\beta'} \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & l_{\beta} & l_{\beta'} \\ \mu & m_{\beta} & -m_{\beta}\end{pmatrix} \quad (2.44)$$

where:

$$Y^{\lambda}_{\beta'\beta}(K) = \int_0^{\infty} d\rho\ \rho^2\Phi^*_{\beta'}(\rho)\Phi_{\beta}(\rho)j_{\lambda}\left(\frac{1}{2}K_{\rho}\right) \quad (2.45)$$

Referring to the term $\left[1-(-1)^{\lambda}\right]$ in equation (2.44), it is clear that equation (2.44) will be non-zero provided that λ is an odd number. This property forces the interaction between Ps and the residual ion core to only connect the states with different parity.

For the rearrangement matrix element, the Ps and alkali-atom wavefunctions are defined as:

$$\text{Alkali-atom}: \ (2\pi)^{-\frac{3}{2}}\int d^3r\Psi_{\alpha}(r)exp(-ip.r) \quad (2.46a)$$

$$\text{Ps}: \ (2\pi)^{-\frac{3}{2}}\int d^3\rho\Psi_{\alpha}(\rho)exp(-ip.\rho) \quad (2.46b)$$

The inverse Fourier transforms of equation (2.46) are:

$$\text{Alkali-atom}: \ (2\pi)^{-\frac{3}{2}}\int d^3p\Psi_{\alpha}(pr)exp(-ip.r) \quad (2.47a)$$

$$\text{Ps}: \ (2\pi)^{-\frac{3}{2}}\int d^3p\Psi_{\alpha}(p)exp(-ip.\rho) \quad (2.47b)$$

Following Mitroy and Ratnavelu (1994), after obtaining equation (2.46) and equation (2.47), we can reduce equation (2.36) and equation (2.39) to:

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Psi_{\alpha}\rangle = \left[\frac{1}{2}\kappa'^2 - \left|k - \frac{1}{2}k'\right|^2 + \varepsilon_{\beta} + \varepsilon_{core} + \varepsilon_{\alpha} - E\right]\Psi_{\alpha}(k' - k)\Phi_{\beta}^{*}\left(\frac{1}{2}k' - k\right) + \int d^3q\Psi_{\alpha}(k' - q)\,\Phi_{\beta}^{*}\left(\frac{1}{2}k' - q\right)\left[V_{core}(|q - k|) + \frac{1}{2\pi^2|q-k|^2}\right] \quad (2.48a)$$

$$\langle k'\Omega_{\gamma'}\Phi_{\beta'}|V|k\Psi_{\alpha}\rangle = \left[\frac{1}{4}\kappa'^2 - \frac{1}{2}|k - k'|^2 + \varepsilon_{\beta} + \varepsilon_{core} + \varepsilon_{\alpha} - E\right]\Psi_{\alpha}(k' - k)\Phi_{\beta}^{*}\left(\frac{1}{2}k' - k\right) + \int d^3q\Psi_{\alpha}(k' - q)\,\Phi_{\beta}^{*}\left(\frac{1}{2}k' - q\right)\left[V_{core}(|q - k|) + \frac{1}{2\pi^2|q-k|^2}\right] \quad (2.48b)$$

The terms $\Psi_{\alpha}(k' - q)\Phi_{\beta}^{*}\left(\frac{1}{2}k' - q\right)$ and $V_{core}(|q - k|) + \frac{1}{2\pi^2|q-k|^2}$ are the functions for k' & q and k & q, respectively. So, the integrands can be factorized into 2 parts and the partial wave expansion of each part can be solved separately. Although the term $V_{core}(|q - k|)$ will slow down the calculations of the matrix elements but this will not cause any major changes in the results of the calculation.

2.3.5 Partial Wave Analysis

Following Mitroy and Ratnavelu (1994), the matrix elements can be reduced to the partial wave form. For the interaction between different Rb channels:

$$V^{(J)}_{\alpha' L' \alpha L}(k', k) = \sum_{m_{\alpha'} m_{\alpha} M M'} \int d\hat{k} \int d\hat{k}'\, Y^{*}_{L' M'}(\hat{k}')\langle L'M' l_{\alpha'} m_{\alpha'}|JM_J\rangle \times \langle k'\alpha'|V|\alpha k\rangle\langle LM l_{\alpha} m_{\alpha}|JM\rangle Y_{LM}(\hat{k}) \quad (2.49)$$

where $\langle L'M' l_{\alpha'} m_{\alpha'}|JM_J\rangle$ is a Clebsch-Gordan coefficient.

Since there is no exchange interaction in equation (2.49), the singlet and triplet partial wave T-matrices are identical and thus all considerations of spin coupling can be ignored. Equation (2.49) can be further reduced to:

$$V^{(J)}_{\alpha' L' \alpha L}(k', k) = \sum_{\lambda' r} i^{\lambda} (-1)^{\tau+\lambda'+\lambda+J} \hat{\lambda}^3 \hat{\lambda}'^2 \hat{l}_{\alpha} \hat{l}_{\alpha'} \hat{L} \hat{L}'$$

$$\times \left[\frac{(2\lambda)!}{(2\tau)!(2\lambda-2\tau)!}\right]^{\frac{1}{2}} k^{\lambda-\tau} k'^{\tau} \mathrm{X}^{\lambda' \lambda}_{\alpha' \alpha}(\mathrm{k}', \mathrm{k})$$

$$\times \begin{pmatrix} L' & \lambda' & \lambda-\tau \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \tau & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_{\alpha'} & \lambda & l_{\alpha} \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{Bmatrix} \lambda & L' & L \\ \lambda' & \lambda-\tau & \tau \end{Bmatrix} \begin{Bmatrix} l_{\alpha'} & L' & J \\ L & l_{\alpha} & \lambda \end{Bmatrix} \quad (2.50)$$

where $\mathrm{X}^{\lambda' \lambda}_{\alpha' \alpha}(\mathrm{k}', \mathrm{k})$ is the angular integral defined as:

$$\mathrm{X}^{\lambda' \lambda}_{\alpha' \alpha}(\mathrm{k}', \mathrm{k}) = 2\pi \int_{-1}^{1} du\, P_{\lambda'}(u) \left[\delta_{\lambda_0} \delta_{\alpha\alpha'} - \mathrm{X}^{\lambda \lambda'}_{\alpha' \alpha}(K)\right] \frac{1}{2\pi^2 K^{\lambda+2}}$$

$$+\delta_{\lambda 0} \delta_{\alpha\alpha'} 2\pi \int_{-1}^{1} du\, P_{\lambda'}(u) V_{core}(K) \quad (2.51)$$

where $P_{\lambda'}(u)$ is a Legendre Polynomial, $u = \hat{k}'.\hat{k}$, $K = |k - k'|$

The interaction between different Ps channels is quite similar to the Rb channels case because of the similarity of having a non-zero interaction when there are different parities exist between the states:

$$V^{(J)}_{\beta' L' \beta L}(k', k) = \sum_{\lambda\lambda' \tau} i^{\lambda} (-1)^{\tau+\lambda+\lambda'+J} \hat{\lambda}^3 \hat{\lambda}'^2 \hat{l}_{\beta} \hat{l}_{\beta'} \hat{L} \hat{L}'$$

$$\times \left[\frac{(2\lambda)!}{(2\tau)!(2\lambda-2\tau)!}\right]^{\frac{1}{2}} k^{\lambda-\tau} k'^{\tau} \mathrm{Y}^{\lambda' \lambda}_{\beta' \beta}(\mathrm{k}', \mathrm{k}) \left[1 - (-1)^{\lambda}\right]$$

$$\times \begin{pmatrix} L' & \lambda' & \lambda-\tau \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \tau & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_{\beta'} & \lambda & l_{\beta} \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{Bmatrix} \lambda & L' & L \\ \lambda' & \lambda-\tau & \tau \end{Bmatrix} \begin{Bmatrix} l_{\beta'} & l_{\beta} & J \\ L & L' & \lambda \end{Bmatrix} \quad (2.52)$$

where $\mathrm{Y}^{\lambda' \lambda}_{\beta' \beta}(\mathrm{k}', \mathrm{k})$ is an angular integral defined as:

$$\mathrm{Y}^{\lambda' \lambda}_{\beta' \beta}(\mathrm{k}', \mathrm{k}) = \int_{-1}^{1} du \left(\frac{2\pi}{K^{\lambda}}\right) \left(V_{core}(K) + \frac{1}{2\pi^2 K^2}\right) P_{\lambda'}(u) \mathrm{Y}^{\lambda}_{\beta' \beta}(K) \quad (2.53)$$

Equation (2.51) and (2.53) can be solved numerically by using the composite Gauss-Legendre quadrature mesh. Since this method was widely used in the electron-atom scattering calculations, so it was proved to be a very reliable method to handle these calculations.

Among the 3 interactions, the matrix element for Ps formation is the most complicated. The matrix element of this interaction is defined as:

$$V^{(J)}_{\beta' L\alpha' L}(k',k) = \sum_{\lambda\tau_\beta\tau_\alpha cjk} i^{l_\alpha+l_\beta}(-1)^{L+J+c+l_\alpha}\hat{\lambda}^2\hat{\lambda}'^2\hat{l}_\alpha\hat{l}_\beta\hat{L}\hat{L}'$$
$$\times\left[\frac{(2l_\alpha)!(2l_\beta)!}{(2\tau_\alpha)!(2\tau_\beta)!(2l_\alpha-2\tau_\alpha)!(2l_\beta-2\tau_\beta)!}\right]^{\frac{1}{2}}\left(\frac{1}{2}\right)^{l_\beta-\tau_\beta}k'^{l_\alpha+l_\beta-\tau_\alpha}$$
$$\times\begin{pmatrix} j & \lambda & L' \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} k & \lambda & L \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \lambda_\alpha-\tau_\alpha & j & \lambda_\beta-\tau_\beta \\ 0 & 0 & 0\end{pmatrix}$$
$$\times\begin{pmatrix} \tau_\alpha & k & \tau_\beta \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} L & c & L' \\ j & \lambda & k\end{Bmatrix}$$
$$\times\begin{Bmatrix} l_\beta & L' & J \\ L & l_\alpha & c\end{Bmatrix}\begin{Bmatrix} k & c & j \\ \tau_\alpha & l_\alpha & l_\alpha-\tau_\alpha \\ \tau_\alpha & l_\beta & l_\beta-\tau_\alpha\end{Bmatrix}\left[Z^{\lambda,r}_{1,\beta\alpha}(k',k)+Z^{\lambda,\tau L}_{2,\beta\alpha}(k',k)\right] \quad (2.54)$$

where $\tau=\tau_\alpha+\tau_\beta$. Equation (2.54) consists of 2 separate integrals, $Z^{\lambda,r}_{1,\beta\alpha}(k',k)$ and $Z^{\lambda,\tau L}_{2,\beta\alpha}(k',k)$. The first integral is defined as:

$$Z^{\lambda,r}_{1,\beta\alpha}(k',k) = \frac{1}{2}k^\tau\int_{-1}^{1}du\left(\frac{1}{2}k^2+\frac{1}{2}K_1^2+\epsilon_{core}+\epsilon_\alpha+\epsilon_\beta-E\right)$$
$$\times\Psi_\alpha(K_1)\phi_\beta(K_2)P_\lambda(u) \quad (2.55a)$$

$$Z^{\lambda,r}_{1,\beta\alpha}(k',k) = \frac{1}{2}k^\tau\int_{-1}^{1}du\left(\frac{1}{4}k'^2+\frac{1}{2}K_2^2+\epsilon_{core}+\epsilon_\alpha+\epsilon_\beta-E\right)$$
$$\times\Psi_\alpha(K_1)\phi_\beta(K_2)P_\lambda(u) \quad (2.55b)$$

where $K_1=|k-k'|$ and $K_2=\left|k-\frac{1}{2}k'\right|$.

The numerical calculations of equations (2.55) are similar to equation (2.51) and equation (2.53). Thus, the second integral is defined as:

$$Z_{2,\beta\alpha}^{\lambda,\tau L}(k^{'},k)=\frac{1}{8\pi^3}\int_0^\infty dq\, q^{2+\tau}H_{\beta\alpha}^{\lambda}(k^{'},q)\left[V_{core,L}(k,q)+V_L(k,q)\right] \tag{2.56}$$

where $V_{core,L}(k,q)$ represents the Legendre coefficient of $V_{core}(|q-k|)$, defined as:

$$V_{core,L}(k,q)=2\pi\int_{-1}^{1}du\,2\pi^2V_{core}(|q-k|)P_L(u);\qquad u=\hat{q}.\hat{k} \tag{2.57}$$

and $V_L(k,q)$ is the partial wave component of the momentum-space form of the Coulomb potential:

$$V_L(k,q)=2\pi\int_{-1}^{1}du\,|q-k|^2P_L(u);\qquad u=\hat{q}.\hat{k} \tag{2.58a}$$

$$=\frac{2\pi}{qk}Q_L\left[\frac{1}{2}\left(\frac{q}{k}+\frac{k}{q}\right)\right] \tag{2.58b}$$

The term $Q_L\left[\frac{1}{2}\left(\frac{q}{k}+\frac{k}{q}\right)\right]$ is a Legendre function of the second kind.

The term $H_{\beta\alpha}^{\lambda}(k^{'},q)$ consists of the projections of the product of the spherically symmetric part of the momentum-space wavefunctions:

$$H_{\beta\alpha}^{\lambda}(k^{'},q)=2\pi\int_{-1}^{1}du\,\phi_\beta\left(\left|\frac{1}{2}k^{'}-q\right|\right)\Psi_\alpha\left(\left|k^{'}-q\right|\right)P_\lambda(u) \tag{2.59}$$

with $u=\hat{q}.\hat{k}'$. $H_{\beta\alpha}^{\lambda}(k^{'},q)$ is a function of k'.

Finally, the kernel matrix is converted into purely real numbers by dividing each individual matrix element by $i^{L-L^{'}}$ so that the matrices are ready for the numerical calculations. Thus, the partial wave forms of the LS equations are:

$$\begin{aligned}T_{\alpha'L'\alpha L}^{(J)}(\mathbf{k}',\mathbf{k})=V_{\alpha'L'\alpha L}^{(J)}(\mathbf{k}',\mathbf{k})&+\sum_{\alpha''}\int d^3k''\frac{V_{\alpha'L'\alpha''L''}^{(J)}(\mathbf{k}',\mathbf{k}'')T_{\alpha''L''\alpha L}^{(J)}(\mathbf{k}'',\mathbf{k})}{E^{(+)}-\varepsilon_{core}-\varepsilon_{\alpha''}-\frac{1}{2}k''^2}\\&+\sum_{\beta''}\int d^3k''\frac{V_{\alpha'L'\beta''L''}^{(J)}(\mathbf{k}',\mathbf{k}'')T_{\beta''L''\alpha L}^{(J)}(\mathbf{k}'',\mathbf{k})}{E^{(+)}-\varepsilon_{core}-\varepsilon_{\beta''}-\frac{1}{4}k''^2}\end{aligned} \tag{2.60a}$$

$$T^{(J)}_{\beta'L'\alpha L}(\mathbf{k}',\mathbf{k}) = V^{(J)}_{\beta'L'\alpha L}(\mathbf{k}',\mathbf{k}) + \sum_{\alpha''}\int d^3k'' \frac{V^{(J)}_{\beta'L'\alpha''L''}(\mathbf{k}',\mathbf{k}'')T^{(J)}_{\alpha''L''\alpha L}(\mathbf{k}'',\mathbf{k})}{E^{(+)} - \varepsilon_{core} - \varepsilon_{\alpha''} - \frac{1}{2}k''^2} + \sum_{\beta''}\int d^3k'' \frac{V^{(J)}_{\beta'L'\beta''L''}(\mathbf{k}',\mathbf{k}'')T^{(J)}_{\beta''L''\alpha L}(\mathbf{k}'',\mathbf{k})}{E^{(+)} - \varepsilon_{core} - \varepsilon_{\beta''} - \frac{1}{4}k''^2} \quad (2.60b)$$

2.3.6 Experimental Quantities

a) Differential Cross Section (DCS) and Total Cross Section (TCS)

The DCS for scattering from channel α to α' at angle θ is:

$$\frac{d\sigma_{\alpha'\alpha}}{d\Omega} = (2\pi)^4 \frac{k_{\alpha'}}{k_\alpha}\frac{\hat{S}^2}{\hat{l}^2}\sum_{m,m'}|\langle k';n',l',m'|T|n,l,m;k\rangle|^2 \quad (2.61)$$

where $\langle k';n',l',m'|T|n,l,m;k\rangle$ is the partial wave expansion of T-matrix.

The TCS is defined as:

$$\sigma_{\alpha'\alpha} = (2\pi)^4 \frac{k_{\alpha'}}{k_\alpha}\frac{\hat{S}^2}{\hat{l}^2}\frac{1}{4\pi}\sum_{L,L'J}(2J+1)\left|T^{n'L'l'(J)}_{nLl}\right|^2 \quad (2.62)$$

where J is the total angular momentum number.

Note that at intermediate energies, the differential cross section converges slowly with *J*. In order to solve this problem, the Born approximation is used beyond certain value of J_0 where:

$$T^{n'L'l'(J)}_{nLl} = V^{n'L'l'(J)}_{nLl} \quad (2.63)$$

The Born approximation is sufficiently accurate to substitute the close-coupling approximation beyond J_0. The T-matrix can be rewritten as:

$$\langle \vec{k}_i;n',l',m'|T|n,l,m;\vec{k}_j\rangle = \langle \vec{k}_i;n',l',m'|T-V|n,l,m;\vec{k}_j\rangle + \langle \vec{k}_i;n',l',m'|V|n,l,m;\vec{k}_j\rangle \quad (2.64)$$

For the first term on the right hand side of equation (2.46), the partial wave expansion is used up to J_0. For the second term, the closed-form expression for the Born approximation is being used where:

$$V = v_1 - (U + iW) + v_3 \tag{2.65}$$

b) Total Reaction Cross Section

The total reaction cross section is an essential part for the entrance channel. The total reaction cross section is defined as:

$$\sigma_R = \left(\frac{\pi}{k_0^2}\right) \sum_S (2S+1) \sum_J (2J+1) \left(1 - \left|S_J\right|^2\right) \tag{2.66}$$

where S_J is the *S*-matrix element defined as:

$$S_J = exp\left(2i\delta_J\right) = 1 - 2\pi i k_0 T_{nJ\,0}^{nJ\,0(J)} \tag{2.67}$$

δ_J is the phase shift and $T_{nJ\,0}^{nJ\,0(J)}$ is the elastic *T*-matrix.

Similar to the differential cross section, the total reaction cross section will converge quite slowly with *J*. Since the Born approximation is valid when $J > J_0$, the total reaction cross section can be rewritten as:

$$\sigma_R = \left(\frac{\pi}{k_0^2}\right) \sum_S (2S+1) \sum_J (2J+1) \left(\left|S_J^{Born}\right|^2 - \left|S_J\right|^2\right) + \sigma_R^{Born} \tag{2.68}$$

where S_J^{Born} is the *S*-matrix element of the Born approximation and σ_R^{Born} is the Born approximation to σ_R:

$$\sigma_R^{Born} = \left(\frac{2}{k_0}\right) (2\pi)^3 W(0) \tag{2.69}$$

$W(0)$ is the imaginary part of $V^{(Q)}$ with $K = 0$.