CHAPTER 1

INTRODUCTION

This work will report on the theoretical investigation of elastic, inelastic, differential and total cross sections of electron and positron scattering by the rubidium atom. The positronium formation of the positron-Rb scattering will also be reported. The coupled-channel optical method (CCOM) is implemented in the study of the electron and positron scattering by the rubidium atom (McCarthy and Stelbovics 1983a, Ratnavelu and Rajagopal 1999).

1.1 General Introduction

Atomic collision theory is very important in many fields of sciences, for example, astrophysical sciences, laser physics, lighting industry, medical and material sciences. Due to the wide applications of atomic collision theory in other field of sciences, there has been always significant interest among experimental groups as well as theorists to measure and calculate the physical quantities to the best of the state of art.

Since the early 1960s', researchers have applied various methods in the study of electron and positron scattering on hydrogenic atoms such as hydrogen, sodium, lithium etc. There are various reviews that have described the progress of theories and experimental measurements in these scattering systems (Bransden and McDowell (1977, 1978), Walters 1984, Laricchia and Charlton 2000, Surko *et al.* 2005). Most of the studies involved the calculations of the total cross section (TCS) of the scattering as the TCS is the most basic and general information that describes the scattering. The differential cross section (DCS) also provides substantial information of each scattering channel, which gives in-depth analysis of the scattering process.

The electron (e^-) , a sub-atomic particle of negative charge, was discovered by Joseph John Thomson in 1897. An electron is bound to the nucleus of an atom and it orbits the nucleus. As an elementary particle, an electron is very tiny in size and the mass of an electron is about 1/1836 that of a proton. A positron is the antiparticle of an electron. The positron is identical to an electron but it contains positive charge, with the symbol of e^+ . It was discovered by Carl David Anderson in 1932.

Rubidium is an alkali-atom with the chemical symbol Rb. It has the atomic number 37 with the electron configuration of $[Kr]5s^1$ (electrons per shell : 2.8.18.8.1). It is categorized in group 1, period 5 and block s. In its ground state this atom has only 1 valence electron (5s electron) which is bound to the closed shell. The closed shell consists of the tightly bound inner electrons ($1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^{10}$, $4s^2$, $4p^6$ electrons). The first ionization energy of Rb is about 4.18eV, which indicates that the valence electron is loosely bound to the closed shell. The electron-Rb and positron-Rb scattering system can be reduced to a 3-body scattering system (1^{st} body = incident electron/positron, 2^{nd} body = valence electron, 3^{rd} body = closed shell). The dipole polarizability of the Rb atom is 9.076 au (Migdalek and Kim 1998).

The interactions of electron/positron-atom scattering are mainly governed by the Coulomb potential. The two crucial interactions in the electron/positron-atom scattering are the exchange interaction and the polarization interaction. The exchange interaction is a quantum effect which affects the energy of two identical particles when their wavefunctions overlap. Exchange effect arises as the consequences of 2 facts: electrons are indistinguishable and they obey the Pauli Exclusion Principle. In electron-atom scattering, this effect exists in between the incident and valence electron. The polarization interaction causes distortion of the electron cloud. The tendency of an electron cloud to be distorted from its normal shape is called polarizability. Polarization happens when an incident particle approaches an atom. The electric field of the incident particle will produce a potential on the scattering atom.

Since a positron contains positive charge, the physics of positron-atom scattering is different from the electron case. Exchange effect does not exist in the positron case because the positron has different sign of charge. In addition the positron is repulsed by the static potential of the atomic Coulomb field whereas for the electron the potential is attractive.

The main difference between electron-atom scattering and positron-atom scattering is the positronium (Ps) formation channel which exists only in positron-atom scattering. Ps is formed when an electron (valence electron) and a positron (incident positron) are bound together. It is unstable and the particles will annihilate each other to produce photons. Ps is much like a hydrogen atom but with a reduced mass equal to one-half the mass of the electron. It is possible that the Ps states can be formed at zero incident kinetic energy, provided that the first ionization energy of the target atom is lower than the binding energy of Ps, which is 6.8eV. Ps was experimentally discovered by Martin Deutsch at MIT in 1951.

The objective of this work is to implement the coupled-channel optical method (CCOM) in the study of electron and positron scattering from a large alkali atom such as the Rb atom. The results will include differential and total cross sections. The elastic, inelastic, and Ps formation cross section will also be reported. These results will be compared to the available experimental measurements and theoretical data.

The CCOM has been implemented in the study of some hydrogenic atoms such as hydrogen, sodium, lithium and potassium (McCarthy and Stelbovics (1983a), McCarthy et al. (1993) Natchimuthu and Ratnavelu (2001), Ratnavelu et al. (2002)). These works show that the CCOM is a good method in the study of quantum scattering. Thus, this motivated the present work to extend the CCOM into a larger alkali atom such as the Rb atom. Since the studies on electron-Rb and positron-Rb scattering, both experimental and theoretical, are relatively scarce, we hope that our results can provide impetus for future experimental and theoretical studies on this problem.

Besides this introductory chapter, there are other chapters:

1) Theory: There are 2 chapters for the theory, which are the theoretical parts of the close-coupling approximation (CC) (Chapter 2) and the coupled-channel optical method (CCOM) (Chapter 3).

2) Computational and Numerical Details: Chapter 4 includes the methodology of the work, the discussion on the computational difficulties encountered and also the numerical convergence tests of the calculations.

3) Results and Discussion: Chapter 5 consists of the results of the calculation as well as the comparison and analysis on the results.

4) Conclusion: Finally, we will conclude our work on electron/positron-Rb scattering in this chapter. We will also discuss the possibility of further investigation on this topic.

1.2 Literature Review

In this section, we will review the other theoretical as well as experimental works on electron-Rb and positron-Rb scattering systems. Various theoretical methods have been implemented in the study of positron scattering on Rb, but not all these methods include the Ps formation in the calculations.

1.2.1 Close-Coupling Approximation (CC)

The earliest implementation of the CC in the study of the scattering system was done by Massey and Mohr (1932). The fundamental concept of CC is to expand the total wavefunction into an infinite number of orthogonal eigenstates of the target atom. The eigenstates have unknown scattering coefficient which can be obtained by solving a set of coupled integro-differential equations.

The CC is widely used in the study of electron/positron scattering on hydrogenic atoms. For the electron case, Burke *et al.* (1967) has done the 6-state CC calculations of electron-hydrogen scattering in the low-energy region. Burke and Mitchell (1973) also applied the CC method in the calculation of the TCS of electron-Cs scattering at low energy (from ionization energy to 5 eV). The studies of electron scattered by potassium atom by using the CC method were done by some researchers such as Moores (1976), Phelps *et al.* (1979) and Msezane *et al.* (1992).

For the positron case, Sarkar *et al.* (1988) implemented the CC method in the study of elastic and excitation scattering for the positron-lithium and positron-sodium scattering system. By using the CC method, Ward *et al.* (1988) calculated the TCS of the positron-potassium scattering. Subsequently, Ward *et al.* (1989a) extended the CC method in the investigation of the positron scattering on other alkali atoms such as lithium and sodium. Ward *et al.* (1989b) also showed the existence of resonances in some of the partial waves in the positron-alkali atoms scattering.

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All these CC calculations reported above are "incomplete" as the calculations do not include the Ps channels in their calculations. Mitroy and Ratnavelu (1994) performed the CC calculations which explicitly include the Ps channels. The formalism of their CC method can be found in Mitroy (1993a, b) and Mitroy and Ratnavelu (1994). Throughout the whole thesis, the label CC(m,n) will represent the closecoupling calculation in which 'm' Rb target states and 'n' Ps states are explicitly coupled together. Hewitt *et al.* (1990) pioneered the CC calculation for Ps(n=2) formation of positron-hydrogen scattering. Furthermore, Hewitt *et al.* (1993) is among the first theoretical group that realistically investigated the Ps formation of positronpotassium scattering by using the CC method.

Feng *et al.* (1998) have studied the positron scattering on Rb and Cs using the relativistic CC. The wavefunction is calculated by using a frozen-core Dirac-Fock method which is obtained using the MDCF program of Grant *et al.* (1980). By projecting the Dirac equations onto the target atomic states, the scattering equations for the incident positron can be obtained. After solving the equations, the scattering *K*-matrix can be extracted and the partial-wave scattering amplitudes can be found. Finally the cross sections for elastic and inelastic processes can be calculated. For positron-Rb scattering, the calculations include 5s, 5p and $5\vec{p}$ states. 5s is the ground state of Rb atom while 5p and $5\vec{p}$ are the excited states. The p represents an electron with l = 1 and j = 3/2 while \vec{p} is the relativistic notation of an electron with l = 1 and j = 1/2. Feng *et al.* (1998) conclude that the relativistic effect is important and it will improve the results of the positron-Rb scattering. They also state that the use of more accurate bound state function such as polarized Dirac-Fock wavefunction can further improve the results.

In general, the CC method (Burke *et al.* 1969) shows slow convergence in the study of electron scattering from atoms. This is due to the neglect of higher excited states as well as the continuum states. In order to overcome this slow convergence

problem, the higher eigen states as well as the continuum effect must be included into the calculation. There are 2 different ways of including the continuum effect into the calculation, which are the pseudostate method (Damburg and Karule 1967, Perkins 1968, Burke *et al.* 1969, Burke and Webb 1970, Fon and Gallaher 1972) and the optical potential method (McCarthy and Stelbovics 1983a).

In the positron scattering problem, besides this neglect of higher discrete and continuum states, the Ps channel are also needed in the calculation. Burke et al (1990), Hewitt *et al.* (1990), Mitroy (1993a) and Kernoghan *et al.* (1995) have demonstrated the realism of incorporating the Ps channels in positron scattering from hydrogen and other light atoms. Further, Mitroy (1996) and Kernoghan *et al.* (1996a) have used large L2 (pseudostate) expansions (28-state and 33-state) to incorporate the continuum effects in the positron scattering from H. Campbell *et al.* (1998) and Kernoghan *et al.* (1994) have also used the large L2 expansions for studying positron scattering from alkali atoms.

Another approach used in positron scattering by H and alkali atoms is the CCOM of McCarthy and Stelbovics (1983a) that was implemented by Ratnavelu and co-workers (Ratnavelu and Rajagopal 1999, Natchimuthu and Ratnavelu 2000, Kamali & Ratnavelu 2001 and Ratnavelu & Ng 2006). The present work will extend this method to study positron scattering by Rb.

1.2.2 Coupled-channel Optical Method (CCOM)

The Coupled-channel optical method (CCOM) for electron-atom scattering was first introduced by McCarthy and Stelbovics (1983a). The CCOM treats all the effects explicitly: the reaction channels are treated by a coupled-channels method in momentum space while the continuum channels are treated by adding an ab-initio complex-polarization potential into the calculation. The remaining significant discrete channels are treated by second-order polarization potentials. The optical potential is derived from the Schrodinger equation which is separated into 2 spaces, P space and Q space. P space consists of the atomic states and Q space consists of the remaining discrete and continuum states.

By using the CCOM, McCarthy and Stelbovics (1983a) successfully showed that the continuum effect is very important as the inclusion of the effect improved the calculations. McCarthy *et al.* (1983b, 1983c, 1985) extended the CCOM into the study of electron scattering on hydrogen, sodium and potassium. Bransden *et al.* (1985) applied the CCOM to positron-atom scattering. They attempted to treat the Q-space in 2 different ways: by using the CCOM complex-polarization potentials or by the pseudostates approach. In general, the CCOM calculations agree well with most of the experimental data. Bransden concluded that although the CCOM is a good approximation, it will be hard to improve the method.

Bray and co-workers (Bray *et al.* (1989, 1990, 1991a, 1991b, 1993a, 1993b)) extended the original CCOM by solving the coupled equation using the distorted wave representation. Both of the papers in 1991 (Bray *et al.* (1991a, 1991b)) showed that the CCOM improved the magnitude of the cross sections, thus the CCOM cross sections agree better with the experimental data compared to the CC calcuations. Bray and McCarthy (1993a) also showed that the inclusion of the continuum effect will affect the exchange during the collision.

The quantum scattering theory group of the University of Malaya also implemented the CCO method in the study of positron scattering on alkali atom. Ratnavelu and Rajagopal (1999) reported the first implementation of the CCOM within the CC formalism of Mitroy (1993a) to study positron-H scattering. Thus the CCO model of McCarthy and Stelbovics (1983a) was implemented within the formalism that explicitly includes the Ps channels in the CC expansion. Nevertheless, this CCO method is also an approximation as it does not include the continuum effects for the Ps coupling. Futher calculations have been reported for positron-alkali systems (Natchimuthu and Ratnavelu 2001 and Ratnavelu and Ng 2006).

Ratnavelu *et al.* (2002) calculated the DCS and TCS of positron scattering by hydrogen and lithium that yields reasonably good results, despite some discrepancies in the lithium TCS. The reduced Stokes parameters for electron impact excitation of 2p and 3p states of hydrogen were calculated by Kamali *et al.* (2008a). Their results are in good accord with the experimental measurements. By using the CCO, Kamali and Ratnavelu (2008b) reported DCS for positronium formation in positron-hydrogen scattering by using large states in the CC expansion.

The theoretical group from Jilin University also implemented CCOM in the study of positron-alkali atom scattering. Zhou and Pan (1997) reported their study of positron scattering by hydrogen, sodium and potassium atoms for energies ranging from ionization threshold to 300 eV. Nan *et al.* (2004) also calculated the positronium (Ps(n=1) and Ps(n=2)) formation cross section for positron-potassium scattering at low energies. Zhang *et al.* (2007) have studied positron-Rb scattering and their TCS display a few peaks in the vicinity of 47 eV.

1.2.3 R-matrix

The R-matrix theory has been implemented in various collision problems such as nuclear reactions, many-body scattering and electron-atom scattering (Lane and Thomas 1958, Burke and Robb 1975, Barrett *et al.* 1983, Burke *et al.* 1971, Berrington *et al.* 1978, Berrington and Kingston 1987, Sawey *et al.* 1990). A complete overview of the R-matrix theory as well as the applications of this method in the electron-atom scattering problems can be found in the book written by Burke and Berrington (1993).

In general, the concept of the R-matrix theory is to separate the configuration space of the physical system into several parts. After that, the system is solved part by part. The implementation of the R-matrix theory in the electron-atom scattering system is as follows: Firstly, the continuum states are expanded in a complete basis set orbital defined in a finite region where the exchange is important. Then, the Hamiltonian is diagonalized to obtain the R-matrix. By using the R-matrix, the *S*-matrix and cross sections can be obtained eventually.

Kernoghan *et al.* (1996b) applied the R-matrix method in the calculation of positron scattering by Rb and caesium (Cs). They used 6 Ps states : Ps(1s, 2s, 2p, 3s, 3p, 3d) and 5 atomic states : Rb(5s, 5p, 4d, 6s, 6p) and Cs(6s, 6p, 5d, 7s, 7p) in the calculations. By using the n^3 scaling rule, the Ps($n \ge 4$) formations are estimated from the calculated Ps(n=3) formations.

Following Kernoghan et al. (1996b), the wavefunction of the collision system is:

$$\Psi = \sum_{a} F_a(r_p)\psi_a(r) + \sum_{b} G_b(R)\phi_b(t)$$

where $\psi_a(r)$ and $\phi_b(t)$ are the bound eigenstates of the atom and positronium, respectively. In order to determine $F_a(r_p)$ and $G_b(R)$, the coupled equations are defined:

$$(\nabla_{p}^{2} - 2V_{p}(r_{p}) + k_{p}^{2})F_{a}(r_{p}) = 2\sum_{a'}V_{aa'}(r_{p})F_{a'}(r_{p}) + 2\sum_{b'}\int K_{ab'}(r_{p}, R)G_{b'}dR$$
$$(V_{R}^{2} + p_{b}^{2})G_{b}(R) = 4\sum_{b'}U_{bb'}(R)G_{b'}(R) + 4\sum_{a'}\int K_{a'b}^{*}(r_{p}, R)F_{a'}(r_{p})dr_{p}$$

The coupled equations are transformed into the partial wave forms and then they are solved using the R-matrix. Kernoghan *et al.* (1996b) reported the Ps formation, elastic, inelastic and total cross sections of positron-Rb scattering. They showed that the Ps(n=2) and Ps(n=3) cross sections are larger in magnitude than the Ps(n=1) cross

section. Their model diplays a peak in the TCS at around 6eV. They explained that the peak is due to the peaks in the TCS for excited state Ps formation.

1.2.4 Modified Glauber Approximation

Gien had studied the electron/positron-Rb scattering using the modified Glauber (MG) approximation in the model potential approach. The modified Glauber approximation is a method introduced to study the electron-hydrogen scattering by Gien (1976). The idea of the method is to replace the approximated second-order term of eikonal expansion with an exact second-order Born term. Later, Gien (1987) improved his modified Glauber approximation and simplified the calculation of the scattering amplitude. The new approach allows the inclusion of core-interaction effects which will reduce the difficulty of the calculation so that only a one-electron wave function is used in the calculation.

The main equation in the MG approximation is the scattering amplitude:

$$F_{MG} = F^{Core} + F_{MG}^{CC}$$

where F^{Core} is the amplitude of elastic scattering by the core potential and F_{MG}^{CC} is the core-corrected amplitude for electron or positron scattering from Rb valence electron. F_{MG}^{CC} can be partitioned into 3 parts:

$$F_{MG}^{CC} = F_{G}^{CC} - F_{G2}^{CC} + F_{B2}^{CC}$$

 F_G^{CC} is the conventional Glauber amplitude, F_{G2}^{CC} is the second-order eikonal term of conventional Glauber amplitude and F_{B2}^{CC} is the second-order Born amplitude. The model potential approach is included in the F_G^{CC} term.

Gien extended his modified Glauber approximation in model potential approaches to several alkali atom such as sodium (Na), lithium (Li), potassium (K) and

Rb (Gien (1989a, 1989b, 1990, 1993)). His calculations agree reasonably well with the experimental measurements and theoretical data at high energies but it does not show good agreement at lower energies.

1.2.5 Distorted-Wave method (DWM)

Pangantiwar and Srivastava (1987, 1988) implemented the DWM in the calculation of the DCS and the coincidence parameters, λ and χ for electron and positrons scattered by alkali atoms. Following Pangantiwar and Srivastava (1987), the coincidence parameters can provide an in-depth investigation of electron and positron scattering by the Rb atom.

A general formalism of DWM is as follow:

The T-matrix of a single-electron system from an initial state i to a final state f by incident particle impact (direct interaction) is expressed as:

$$T^{dir} = \left\langle \chi_f^{-}(r_1)\psi_f(r_2) \middle| V(r_1, r_2) \middle| \chi_i^{+}(r_1)\psi_i(r_2) \right\rangle$$

and the exchange interaction as:

$$T^{ex} = \left\langle \chi_f^-(r_1)\psi_f(r_2) \middle| V(r_1, r_2) \middle| \chi_i^+(r_2)\psi_i(r_1) \right\rangle \delta_{Z', -1}$$

where ψ_i and ψ_f are the initial state and final state wavefunctions of the alkali atom. $V(r_1, r_2)$ is the projectile-target alkali atom interaction potential. χ_i^+ and χ_f^- are the distorted waves which are the solutions to:

$$\left(-\frac{1}{2}\nabla^2 - \frac{1}{2}k_i^2 + U_i\right)\chi_i^+ = 0$$
$$\left(-\frac{1}{2}\nabla^2 - \frac{1}{2}k_f^2 + U_f\right)\chi_f^- = 0$$

By obtaining χ_i^+ and χ_f^- , the direct and exchange interaction T-matrices can be obtained, which is later used to calculate the DCS. The DCS for sodium, potassium, Rb and Cs is:

$$\left(\frac{d\sigma}{d\Omega}\right)_{np \to (n+1)s} = \frac{1}{4\pi^2} \frac{k_f}{k_i} \sum_{m=-1}^{+1} \left(\frac{1}{4} \left|T_{np \to (n+1)s}^{dir} + T_{np \to (n+1)s}^{ex}\right|^2 + \frac{3}{4} \left|T_{np \to (n+1)s}^{dir} - T_{np \to (n+1)s}^{ex}\right|^2 \right)$$

where $T_{np \to (n+1)s}^{dir}$ is the direct T-matrix and $T_{np \to (n+1)s}^{ex}$ is the exchange T-matrix.

The cross section is defined as:

$$\sigma = \int_0^\pi \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin\theta \, d\theta \, d\phi$$

1.2.6 Other Methods

Reid and Wadehra (1998) used the parameter-free model potentials approach to calculate the differential, elastic and total cross sections for positron-Rb scattering. In this method, the positron-Rb system is modelled using an interaction potential, V(r). V(r) consists of 3 potentials, which are the static potential, $V_{St}(r)$, the correlation-polarization potential, $V_{CP}(r)$, and the absorption potential, $V_{abs}(r)$. V(r) is defined as:

$$V(r) = V_{St}(r) + V_{CP}(r) + iV_{abs}(r)$$

The main problem in this method lies in the derivation of the average binary collision cross section which is one of the terms in $V_{abs}(r)$. The derivation is explained in detail by Reid and Wadehra (1998) in the paper. The calculated V(r) is substituted into the radial Schrodinger equation, followed by integrations. Some phase shifts are obtained and they are used to obtain the scattering amplitude. Finally, the DCS is

obtained from the scattering amplitude while the TCS are calculated using the optical theorem. The calculated TCS agree reasonably well with the experiments.

Guha and Mandal (1980) calculated the Ps(1s) formation of Rb using the distorted–wave approximation. In their paper, they define the total wavefunction as:

$$\Psi(r_1, r_2) = \Phi_{1s}(r_2)F(r_1) + \eta_{1s}(R)G(S)$$

where $\Phi_{1s}(r_2)$ and $\eta_{1s}(R)$ are the ground-state wave function of the target and Ps atoms. The scattering equations, $F(r_1)$ and G(S), describe the positron and Ps relative to the target nucleus. $F(r_1)$ and G(S) are defined as:

$$\left(\nabla_{r_1}^2 + k_i^2\right) F(r_1) = U(r_1) F(r_1)$$
$$\left(\nabla_s^2 + k_f^2\right) G(S) = 2\mu_f \int \eta_{1s}^*(R) (H - E) \Phi_{1s}(r_2) F(r_1) dR$$

Guha and Mandal (1980) defined the post and prior forms of the interaction potential. The prior and post forms require the Hamiltonian, H, to be operated from the right and left hand side in the G(S) equation, respectively. The partial-wave scattering amplitudes are obtained and used to get the DCS. The TCS is then obtained by integrating the DCS over the solid angle.

1.2.7 Experimental Methods

Some experiments on electron or positron scattering by Rb have been done. One of the earliest experiments on electron-Rb scattering was done by Visconti *et al.* (1971). By using the atom-beam recoil technique, they successfully measured the absolute TCS of large alkali atoms such as potassium, Rb and Cs at low energy. The systematic error in the measurement is $\pm 9\%$ which is affected by various values.

Vuskovic *et al.* (1984) measured the DCS of electron-Rb scattering by employing a crossed-electron-beam-atom beam scattering geometry. An electron gun which contains a hemispherical energy selector and cylindrical electrostatic lens elements is used to generate electrons. A channeltron detector is used to detect the



Fig. 1.1 : Schematic of the apparatus used by Visconti's group.

scattered electrons. It is placed at the exit of an electrostatic energy analyzer system, which also consists of a hemispherical energy selector. Their measurement uncertainties lay between 20% to 50% at various scattering angles. This group pioneered the measurement of the DCS of electron-Rb scattering.

Stein *et al.* (1990) conducted experiments to measure the TCS of positrons and electrons scattered by alkali atoms. They utilized the beam-transmission technique to measure the TCS of electrons and positrons scattered by sodium, potassium and Rb in the 1-102 eV energy range. Parikh *et al.* (1993), who are from the same group as Stein *et al.* (1990) improved the original scattering apparatus and produced the TCS of positrons and electrons scattered by potassium and Rb in 1-102 eV energy range. Their measurements do not include the angular-discrimination considerations.

Surdutovich *et al.* (1996) is the first experimental group to report Ps formation cross sections (upper and lower limits) for positrons scattered by the Rb atom. They reported the total Ps cross section measured using a different experimental techniques, which produced Lower Limit (LL), Upper Limit (UL) and Better Upper Limit (UL-R) ross sections. Their measurements agree reasonably well with the calculations of Kernoghan *et al.* (1996b) with both determinations showing a peak in the cross section at around 6 eV.



Fig. 1.2 : Schematic of the apparatus used by Stein's and Parikh's groups.



Fig. 1.3 : Schematic of the apparatus used by Surdutovich's group.