ELECTRON AND POSITRON SCATTERING BY ATOMIC RUBIDIUM

CHIN JIA HOU

DISSERTATION SUBMITTED IN FULFILLMENT OF THE REQUIREMENT FOR THE DEGREE OF THE MASTER OF SCIENCE

INSTITUTE OF MATHEMATICAL SCIENCES
FACULTY OF SCIENCE
UNIVERSITY OF MALAYA
KUALA LUMPUR

2011

ABSTRACT

Electron and positron scattering from the Rubidium atom is studied using the coupled-channel optical method (CCOM). This method incorporates the continuum effect within the close coupling method (CC) by including an optical potential into the calculations. For electron-Rubidium scattering, a 5-state [Rb(5s, 5p, 4d, 6s, 6p)] and 8-state [Rb(5s, 5p, 4d, 6s, 6p, 5d, 7s, 7p)] CC and CCO calculations are carried out. For positron-Rubidium scattering, a 8-state [Rb(5s, 5p, 4d, 6s, 6p) + Ps(1s, 2s, 2p)], 11-state [Rb(5s, 5p, 4d, 6s, 6p) + Ps(1s, 2s, 2p, 3s, 3p, 3d) and Rb(5s, 5p, 4d, 6s, 6p, 5d, 7s, 7p) + Ps(1s, 2s, 2p, 3s, 3p, 3d)] calculations are carried out. The elastic, excitation, differential and total cross sections are reported and compared to other theoretical data and experimental measurements.

ABSTRAK

Penyerakan elektron dan positron pada Rubidium atom dikaji dengan menggunakan kaedah "coupled-channel optical" (CCOM). Kaedah ini mengaplikasikan pendekatan keupayaan optikal ke dalam kaedah "close-coupling" (CC). Bagi sistem penyerakan elektrondijalankan dengan menggunakan Rubidium, pengiraan 5-saluran dan 8-saluran [Rb(5s, 5p, 4d, 6s, 6p) dan Rb(5s, 5p, 4d, 6s, 6p, 5d, 7s, 7p)]. Bagi sistem penyerakan positron-Rubidium, pengiraan 8-saluran [Rb(5s, 5p, 4d, 6s,6p) + Ps(1s, 2s, 2p)], 11- saluran [Rb(5s, 5p, 4d, 6s, 6p)+Ps(1s, 2s, 2p, 3s, 3p, 3d) dan Rb(5s, 5p, 4d, 6s, 6p, 5d, 7s, 7p)+Ps(1s, 2s, 2p)] dan 14-saluran [Rb(5s, 5p, 4d, 6s, 6p, 5d, 7s, 7p)+Ps(1s, 2s, 2p, 3s, 3p, 3d)] telah dijalankan. Keratan rentas elastik dan bukan-elastik telah dipaparkan. Pembeza dan jumlah keratin rentas juga akan dipaparkan. Semua hasil pengiraan akan dibandingkan dengan hasil pengiran teori lain dan ukuran ujikaji.

LIST OF PUBLICATIONS

1. Chin, J. H., Ratnavelu, K., & Zhou, Y. (2011). Optical Potential Study of Electron Scattering by Rubidium. *Journal of Korean Physical Society*, *59*(4), 2877-2879.

ACKNOWLEDGEMENT

First of all, I would like to express my deepest gratitude to my supervisor Professor Kurunathan Ratnavelu for his guidance in completing this thesis. Throughout the entire course of this thesis, he provided a lot of useful and perceptive comments. I had gained much knowledge from his comments.

I would like to acknowledge the Postgraduate Research Grant (PPP) (Project No.: PS210-2009A) of University of Malaya that provided me with the research fund. I also want to thank all the staff of the Institute of Mathematical Sciences (ISM) for their helps during my research period in the department. I appreciate the atomic wavefunctions of rubidium atom provided by Dr. Y. Zhou and I would like to record my sincere thanks for her help. All the calculations were done using the Ultra 10 SUN and SUN-BLADE at ISM.

I want to extend my heartfelt gratitude to my parents, brother and sister for their unrivalled support all the time. This thesis cannot be completed without their blessing and understanding. Last but not least, I would like to thank my friends especially Mohd Zahurin Mohamed Kamali, Chin Lit Chien, Chang Phooi Yee and Chong Chee Hong for giving me valuable advices in my research.

TABLE OF CONTENTS

ABSTRACT				i
ABSTRAK				iii
LIST OF PUE	LIST OF PUBLICATIONS			iv
ACKNOWLE	DGEN	MENT		V
TABLE OF C	CONTE	ENTS		V
LIST OF FIG	URES			Х
LIST OF TAR	BLES			xiii
CHAPTER 1	INTR	ODUC'	ΓΙΟΝ	
	1.1	Genera	al Introduction	1
	1.2	Literat	ure Review	5
		1.2.1	Close-Coupling Approximation (CC)	5
		1.2.2	Coupled-Channel Optical Method (CCOM)	7
		1.2.3	R-matrix	Ģ
		1.2.4	Modified Galuber Approximation	11
		1.2.5	Distorted-Wave method (DWM)	12
		1.2.6	Other Methods	13
		1.2.7	Experimental Methods	14
CHAPTER 2	THE (CLOSE	-COUPLING THEORY	
	2.1	Termin	nology	17
	2.2	Type o	of Interaction	18
		2.2.1	Electron-atom scattering	19
		2.2.2	Positron-atom scattering	21
	2.3	Theore	etical Details	24
		2.3.1	Electron-Rubidium Scattering	24
		232	Positron-Rubidium Scattering	25

		2.3.3	The Interaction Matrix Elements	29
			a) Interaction between different positron channels	29
			b) Interaction between Ps and the residual ion	30
			c) Rearrangement matrix element	31
		2.3.4	Matrix elements in momentum space	33
		2.3.5	Partial Wave Analysis	35
		2.3.6	Experimental Quantities	39
			a) Differential Cross Section (DCS) and Total Cross Section (TCS)	39
			b) Total Reaction Cross Section	40
CHAPTER 3	THE	COUPI	LED-CHANNELS OPTICAL METHOD	
	3.1	Optica	al Potential Formalism	41
	3.2	Comp	utational Details of the Optical Potentials	47
CHAPTER 4 COMPUTATIONAL AND NUMERICAL DETAILS				
	4.1	Nume	rical solutions of Lippmann-Schwinger Equations	51
	4.2	Nume	rical Details in Electron-Rb Scattering Calculations	54
		4.2.1	Quadrature Points	54
		4.2.2	Convergence of the Cross Section	58
	4.3	Nume	rical Details in Positron-Rb Scattering Calculations	61
		4.3.1	Quadrature points	61
	4.4	Nume Soluti	rical Convergence of the Lippmann-Schwinger on	66
CHAPTER 5	RESU	JLTS A	ND DISCUSSION	
	5.1	List of	Calculations	77
		5.1.1	Electron-Rb Scattering	77
		5.1.2	Positron-Rb Scattering	78
	5.2	Electr	on-Rubidium Scattering	79

	5.2.1	Elastic and Inelastic Cross Sections	79
	5.2.2	Total Cross Section (TCS)	81
	5.2.3	Differential Cross Section (DCS)	83
		a) Elastic Transition	83
		i) 10 eV	83
		ii) 20 eV	83
		iii) 30-100 eV	85
		b) 5p Excitation Transition	87
		i) 10 eV	87
		ii) 20 eV	87
		iii) 30-100 eV	89
5.2	Positro	on-Rubidium Scattering	91
	5.3.1	Elastic and Excitation Cross Sections	91
		a) Elastic Transition	91
		b) 5p Excitation Transition	93
		c) 4d Excitation Transition	95
		d) 6s Excitation Transition	95
		e) 6p Excitation Transition	98
	5.3.2	Positronium (Ps) Formation Cross Sections	100
		a) Ps(1s) Formation	100
		b) Ps(2s) Formation	102
		c) Ps(2p) Formation	102
		d) Ps(n=3) Formation	105
		e) Total Positronium Cross Sections (TPCS)	105
	5.3.3	Total Cross Section (TCS)	108
	5.3.4	Differential Cross Section (DCS)	111

a)	Ps(1s) Formation	111
b)	5s Elastic Transition	113
c)	5p Excitation Transition	114
CHAPTER 6 CONCLUSION		116
APPENDICES		
Appendix I		119
Appendix II		120
Appendix III		122
Appendix IV		128
Appendix V		138
Appendix VI		140
Appendix VII		144
REFERENCES		145

LIST OF FIGURES

Fig. 1.1 :	Schematic of the apparatus used by Visconti's group.	15
Fig. 1.2 :	Schematic of the apparatus used by Stein's and Parikh's groups.	16
Fig. 1.3:	Schematic of the apparatus used by Surdutovich's group.	16
Fig. 2.1:	The concept of channel.	18
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.	19
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.	19
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.	20
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.	20
Fig. 2.6 :	Ionization in electron-atom scattering. The valence electron is removed from the atom. The atom is ionized and becomes an ion.	21
Fig. 2.7 :	Elastic positron-atom scattering.	21
Fig. 2.8:	Inelastic scattering in positron-atom scattering.	22
Fig. 2.9 :	Ionization in positron-atom scattering.	23
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.	23
Fig. 2.11 :	Positron-Rb scattering.	25

Fig. 4.1:	Partial-wave cross section for 5s channel in the unit of πa_0^2 obtained from the CC8 calculation for 100 eV. <i>JMAX</i> =100 and UBA is the uniterized Born approximation.	59
Fig. 4.2 :	PW cross section for 5s channel in the unit of πa_0^2 for the CC8 calculation at 100 eV.	61
Fig. 4.3:	The quadrature points are distributed among the 5 regions as shown. The regions are determined by the values of smk1, smk2, smk3, dmk1 and dmk2.	62
Fig. 4.4 :	The illustration of the on-shell coordinates for CC(5,3) calculations at 15 eV.	66
Fig. 4.5:	The illustration of the on-shell coordinates for CC(5,3) calculations at 6 eV. The grey area is the overlapping region of atomic and Ps on-shell coordinates.	66
Fig. 5.1 :	The total, elastic and inelastic cross sections of the electron-Rb scattering.	79
Fig. 5.2:	TCS of electron-Rb scattering for energy ranged from 10 eV to 100 eV.	82
Fig. 5.3 :	DCS of electron-Rb elastic scattering at 10 eV.	84
Fig. 5.4 :	DCS of electron-Rb elastic scattering at 20 eV.	84
Fig. 5.5 :	DCS of electron-Rb elastic scattering from 30 eV to 60 eV.	86
Fig. 5.6 :	DCS of electron-Rb elastic scattering from 70 eV to 100 eV.	86
Fig. 5.7 :	DCS of electron-Rb 5s-5p excitation at 10 eV.	88
Fig. 5.8 :	DCS of electron-Rb 5s-5p excitation at 20 eV.	88
Fig. 5.9 :	DCS of electron-Rb 5s-5p excitation at 30 eV to 60 eV.	90
Fig. 5.10:	DCS of electron-Rb 5s-5p excitation at 70 eV to 60 eV.	90
Fig. 5.11 :	Elastic cross sections of positron-Rb scattering.	92
Fig. 5.12 :	5s - 5p excitation cross sections of positron-Rb scattering.	94
Fig. 5.13:	5s – 4d excitation cross sections of positron-Rb scattering.	96
Fig. 5.14 :	5s – 6s excitation cross sections of positron-Rb scattering.	97
Fig. 5.15:	5s – 6p excitation transition of positron-Rubidium scattering.	99

Fig. 5.16 :	Ps(1s) formation of positron-Rb scattering.	101
Fig. 5.17 :	Ps(2s) formation of positron-Rb scattering.	103
Fig. 5.18 :	Ps(2p) formation of positron-Rb scattering.	104
Fig. 5.19 :	Ps(n=3) formation of positron-Rb scattering.	106
Fig. 5.20 :	Total Ps cross section of positron-Rb scattering.	107
Fig. 5.21 :	Total cross section of positron-Rb scattering.	109
Fig. 5.22 :	DCS of Ps(1s) formation for positron-Rb scattering at 5 eV.	112
Fig. 5.23:	DCS of Ps(1s) formation for positron-Rb scattering at 10 eV.	112
Fig. 5.24 :	DCS of elastic scattering for positron-Rb scattering at 5 eV.	113
Fig. 5.25 :	DCS of elastic scattering for positron-Rbscattering at 10 eV and 20 eV.	114
Fig. 5.26 :	DCS of 5p excitation for positron-Rb scattering at 10 eV.	115
Fig. 5.27 :	DCS of 5p excitation for positron-Rb scattering at 20 eV.	115

LIST OF TABLES

Table 3.1 :	Convergence of the continuum polarization potential for 5s-5s coupling for various momentum transfers and incident energies.	50
Table 4.1 :	3 sets of 24 quadrature points for electron-Rb scattering at 50 eV with different scale parameter a and fixed bunching parameter b . The columns (setA 2 - setA 1) and (setA 3 - setA 2) is the values of difference of each quadrature point between different set of quadrature points.	56
Table 4.2 :	3 sets of 24 quadrature points for electron-Rb scattering at 50 eV with different bunching parameters b and fixed scale parameter a . The columns (1.886 - set 1), (1.886 - set 2) and (1.886 - set 3) are the absolute difference between the scale parameter a with each quadrature points.	57
Table 4.3 :	On-shell coordinate for electron-Rb scattering at 50 eV. $a = 1.886$ and $b = 0.063$.	58
Table 4.4 :	TCS for each channel in the unit of πa_0^2 obtained from the CC8 calculation at 100 eV. <i>JMAX</i> used for the calculation is 60. PW is the short form for partial-wave.	59
Table 4.5 :	TCS for each channel in the unit of πa_0^2 obtained from the CC8 calculation for 100 eV. <i>JMAX</i> used for the calculation is 180.	59
Table 4.6 :	TCS for each channel in the unit of πa_0^2 . <i>JMAX</i> used for the CC8 calculation is 180. The <i>JMAX</i> used is the new <i>JMAX</i> after the merging.	60
Table 4.7 :	The effects of varying smk1 on the distribution of quadrature points in Region 2. The smk1 of set B differs from set A by -0.03 and set C differs from set A by $+0.02$.	63
Table 4.8 :	The effects of varying smk2 on the distribution of quadrature points in Region 4. The smk2 of set B differs from set A by -0.03 and set C differs from set A by $+0.02$.	63
Table 4.9 :	The effects of varying dmk1 on the distribution of quadrature points in Region 2. The dmk1 of set B differs from set A by -0.001 and set C differs from set A by +0.002.	64
Table 4.10 :	The effects of varying dmk2 on the distribution of quadrature points in Region 4. The dmk2 of set B differs from set A by -0.001 and set C differs form set A by +0.002.	64

Table 4.11 :	The on-shell coordinates for the CC(5,3) calculation at 6 eV and 15 eV.	65
Table 4.12a :	The numerical convergence for $CC(5,3)$ calculation at 5 eV ($JMAX = 10$).	68
Table 4.12b :	The absolute errors between 48 Q-points mesh with the other meshes for $CC(5,3)$ calculation at 5 eV ($JMAX = 10$).	68
Table 4.13a :	The numerical convergence for $CC(5,3)$ calculation at 10 eV $(JMAX = 10)$.	69
Table 4.13b :	The absolute errors between $R(24,12,10,12,10)$ mesh with the other meshes for $CC(5,3)$ calculation at 10 eV ($JMAX = 10$).	69
Table 4.14a :	The numerical convergence for $CC(5,3)$ calculation at 20 eV ($JMAX = 10$).	70
Table 4.14b :	The absolute errors between $R(24,12,10,12,10)$ mesh with the other meshes for $CC(5,3)$ calculation at 20 eV ($JMAX = 10$).	70
Table 4.15a :	The numerical convergence for $CC(8,6)$ calculation at 5 eV ($JMAX = 10$).	73
Table 4.15b :	The absolute errors between 48 Q-points mesh with the other meshes for $CC(8,6)$ calculation at 5 eV ($JMAX = 10$).	73
Table 4.16a :	The numerical convergence for $CC(8,6)$ calculation at 10 eV $(JMAX = 10)$.	74
Table 4.16b :	The absolute errors between $R(24,12,10,12,10)$ mesh with the other meshes for $CC(8,6)$ calculation at 10 eV ($JMAX = 10$).	74
Table 4.17a :	The numerical convergence for $CC(8,6)$ calculation at 20 eV ($JMAX = 10$).	75
Table 4.17b :	The absolute errors between $R(24,12,10,12,10)$ mesh with the other meshes for $CC(8,6)$ calculation at 20 eV ($JMAX = 10$).	75
Table 5.1 :	The cross sections for different channels at various energies for the CC8 calculations of electron-Rb scattering.	80
Table 5.2 :	The cross sections for different channels at various energies for the CCO8 calculations of electron-Rb scattering.	81
Table F.1 :	The cross sections of the CC(5,3) calculation.	140
Table F.2 :	The cross sections of the CCO(5,3) calculation.	140
Table F.3 :	The cross sections of the CC(5,6) calculation.	141

Table F.4 :	The cross section of the CCO(5,6) calculation.	141
Table F.5 :	The cross sections of the CC(8,3) calculation.	142
Table F.6 :	The cross sections of the CCO(8,3) calculation.	142
Table F.7 :	The cross sections of the CC(8,6) calculation.	143
Table F.8 :	The cross sections of the CCO(8,6) calculation.	143
Table G.1 :	The contributions of channels to the TCS for the CCO(8,6) calculation.	144
Table G.2 :	The contributions of channels to the TCS for the CC(8,6) calculation.	144