THEORETICAL STUDY OF POSITRON - EXCITED ALKALI ATOM COLLISIONS

Thesis

Submitted for Partial Fulfillment of the Requirements for M.Sc. Degree in Physics

By

Khadija Ali Mohamed Ali

(B.Sc., 7th October University - Libya)

To

Physics Department, Faculty of Science, Ain Shams University, Cairo-Egypt

2012

THEORETICAL STUDY OF POSITRON - EXCITED ALKALI ATOM COLLISIONS

By

Khadija Ali Mohamed Ali

B.Se. (Physics)

Faculty of science, 7th October University, Libya

Thesis Advisors

Approved

Prof. Dr. Salah Yaseen El-Bakry

Prof. of Theoretical Physics, Faculty of Science, Ain Shams University

Dr. El-Sayed A. El-Dahshan

Assist. Prof. of Computational Physics, Faculty of Science, Ain Shams University

Dr. Mahsan Mahsoup

Lecturer of Theoretical Physics, Faculty of Science, Ain Shams University

2012

دراسة نظرية لتصادم البوزيترونات مع ذرات قلوية مثارة

رسالة تكميلية

مقدمة للحصول على درجة الماجستير في العلوم في الفيزياء

مقرمة من

خديجة علي محمد علي

بكالوريوس العلوم — جامعة ٧ أكتوبر — ليبيا

فسم الفبزباء - كلبث العلوم جامعت عبن شمس ۲۰۱۲

CONTENTS

		Page
	ledgement	
Abstract		
1.1	• 1: Introduction The importance of scattering	1
1.1.1	Types of collisions	2
1.1.2	Definition of channel	2
1.2	The difference between electron and positron scattering	3
1.3	Positronium atom	6
1.4	Alkali metal atoms	7
1.5	Positron-alkali atom scattering	8
1.6	Survey of the previous work in positron alkali atom collisions	9
Chapter	2: Theoretical treatment of the two - channel problem of positron-excited lithium scattering.	
2.1	The bound-state wave functions	14
2.2	The total energy	15
2.3	The total Hamiltonian	15
2.4	Analyses of the two-channel scattering problem	18
2.4.1	Analysis of the first coupled integro - differential equation (eq. (2.18))	18
2.4.2	Analysis of the second coupled integro - differential equation (eq. (2.19))	21
2.5	Solution of the two-channel coupled integro - differential equations	23
2.6	Reactance and transition matrices	26
2.7	The partial and total cross-sections	27

CONTENTS (Cont...)

		Page
Chapter	3: Results and discussion	28
Summa	ry	63
Append	ix I: Analyses of the potentials	
1.1	The direct part of the core potential	66
1.2	The exchange part of the core potential	69
1.3	The static potential of the first channel $U_{st}^{1}(x)$	71
1.4	The static potential of the second channel $U_{st}^2(\sigma)$	80
1.5	The polarization potential of the second channel $V_{pol}^{Ps}(\sigma)$	81
1.6	Gauss quadrature formula	82
Appendix II: The coupling kernals of the two channel problem.		
II.1	The coupling kernel of the first channel (eq. (2.29)	84
II.2	The coupling kernel of the second channel (eq. (2.37)	88
II.3	Numerical treatment of the kernels	90
	References	95
	Arabic Summary	

LIST OF TABLES

Tab. No.	Title	Page No.
Table 3.1	Variation of the elements of the reaction matrix R with the number of iterations, at 0.5 eV and Integration Range (IR) = 48 a for the S-, P- and D- matrix waves	$\mathbf{k}_{1}^{2} =$
Table 3.2	Variation of the partial elastic cross section (in πa_0^2) of positron-excited lithium (Li *(2 scattering with the increase of the integrarange IR (in a.u.)	2p)) ation
Table 3.3	Variation of the partial positronium formators sections σ_{12} (in πa_0^2) of positron-excellithium (Li*(2p)) scattering with the increof the integration range IR (in $a.u.$)	cited rease
Table 3.4	Variation of the partial rearrangement of sections σ_{21} (in πa_0^2) of positronium – lith ion (Li ⁺) scattering with the increase of integration range IR (in a.u.)	nium f the
Table 3.5	Variation of the partial elastic cross section πa_0^2) of positronium – lithium ion σ_{22} (I scattering with the increase of the integrarange IR (in $a.u.$)	Li ⁺)
Table 3.6	Partial and total elastic cross sections σ_{11} πa_0^2) of positron-excited lithium (Li*(2 scattering without polarization pote calculated by the coupled-static approximating Integration range IR = 48 $a.u.$ and the number of iterations = 20	2p)) ntial tion. nber
Table 3.7	Partial and total positronium formation of sections σ_{12} (in πa_0^2) of positron-excited lith (Li*(2p)) scattering without polarization potential calculated by the coupled-sapproximation. Integration range IR = a.u. and the number of iterations = 20	eross nium ation static 48

LIST OF TABLES (Cont...)

Tab. No.	Title	Page No.
Table 3.8	Partial and total rearrangement or sections σ_{21} (in πa_0^2) of positronium- lithium	ross ion
	(Li ⁺) scattering without polarization potential calculated by the coupled-static approximate. Integration range IR = $48 a.u.$ and the number iterations = 20	ion. r of
Table 3.9	Partial and total elastic cross sections σ_{22}	(in
	πa_0^2) of positronium-lithium ion (Lescattering without polarization potential calculated by the coupled-static approximation range IR = 48 a.u. and the number of iterations = 20.	tial on. ber
Table 3.10	Partial and total elastic cross sections σ_{11}^{P} πa_0^2) of positron-excited lithium (Li*(2 scattering with polarization potential calcula by the coupled-static approximati Integration range IR = 48 a.u. and the num of iterations = 20.	p)) ited on. ber
Table 3.11	Partial and total positronium formation of sections σ_{12}^{p} (in πa_0^2) of positron-excited lith	
	(Li*(2p)) scattering with polarization poter calculated by the coupled-static approximat Integration range IR = $48 a.u.$ and the number iterations = $20.$	ion. r of
Table 3.12	Partial and total rearrangement or sections σ_{21}^{p} (in πa_0^2) of positronium -lithing ion (Li ⁺) scattering with polarization potential calculated by the coupled-static approximate. Integration range IR = 48 $a.u.$ and the number	ntial ion.
	iterations = 20	42

LIST OF TABLES (Cont...)

Tab. No.	Title	Page No.
Table 3.13	Partial and total elastic cross sections σ_{22}^{p} πa_0^2) of positronium -lithium ion (Li ⁺) scatter with polarization potential calculated by coupled-static approximation. Integration range = $48 a.u.$ and the number of iterations = 20	ring the IR
Table 3.14	Partial and total elastic cross sections σ_{11}^{pl} πa_0^2) of positron-excited lithium (Li*(2) scattering with polarization potential calculated by the coupled-static approximate (intermediate energy region). Integration rate IR= 48 <i>a.u.</i> and the number of iterations = 20	p)) ited ion nge
Table 3.15	Partial and total positronium formation or sections σ_{12}^{pl} (in πa_0^2) of positron-excilithium (Li*(2p)) scattering with polarizate potential calculated by the coupled-standard approximation (intermediate energy region Integration range IR = 48 a.u. and the number of iterations = 20.	ited ion atic on). ber
Table 3.16	Partial and total rearrangement cross sections σ_2 (in πa_0^2) of positroninum- lithium ion (L scattering with polarization potential calculated the coupled-static approximation (intermed energy region). Integration range IR = 48 $a.u.$ the number of iterations = 20.	i ⁺) l by iate and
Table 3.17	Partial and total elastic cross sections σ_{22}^{pl} πa_0^2) of positronium- lithium ion (L scattering with polarization potential calcula by the coupled-static approximation (intermed energy region). Integration range IR = $a.u.$ and the number of iterations = 20	i ⁺) ated iate 48

LIST OF TABLES (Cont...)

Tab. No.	Title	Page No.
Table 3.18	Partial and total elastic cross sections σ_{11}^{I} (in π of positron-excited lithium (Li*(2p)) scatte	
	without polarization potential calculated by coupled-static approximation (intermediate en region). Integration range IR = $48 \ a.u.$ and number of iterations = $20.$	the ergy the
Table 3.19	Partial and total positronium formation consections σ_{12}^{I} (in πa_0^2) of positron-exc	
	lithium ($\text{Li}^*(2p)$) scattering with polarization potential calculated by coupled-static approximation (intermed energy region). Integration range IR = $a.u.$ and the number of iterations = 20	the iate 48
Table 3.20	Partial and total rearrangement cross sections $a = (in \pi a_0^2)$ of positronium- lithium ion (L scattering without polarization potential calcul by the coupled-static approximation (intermed energy region). Integration range IR = 48 $a.u.$ the number of iterations = 20.	i ⁺) ated liate and
Table 3.21	Partial and total elastic cross sections σ_{22}^{-1} πa_0^2) of positronium-lithium ion (L scattering without polarization poter calculated by the coupled-static approxima (intermediate energy region). Integration rather 48 $a.u.$ and the number of iterations = 2	i ⁺) ntial tion nge
Table 3.22	Comparison between various total positron formation cross sections (in πa_0^2) of positr lithium scattering determined by diffe authors.	ron- rent
Table II-1	Arguments of $G_l^{(j)}$ at different values of j	94

LIST OF FIGURES (Cont...)

Fig. No.	Title	Page No.
Fig 2.1	Configuration space of positron- excited lithiu scattering.	
Fig. 3.1	Comparison between our calculated total elast (σ_{11}) and total Ps formation cross sections (σ_{12}) of e^+ - Li*(2p) scattering without polarization potential.) on
Fig 3.2	Comparison between our calculated to rearrangement (reversal of the positronium formation) cross sections (σ_{21}) and total elast cross sections (σ_{22}) of Ps - Li ⁺ scattering without	im tic out
	polarization potential.	54
Fig 3.3	Same as Fig 3.1 but with polarization potential.	55
Fig 3.4	Same as Fig 3.2 but with polarization potential.	55
Fig 3.5	Same as Fig 3.1 but at intermediate energy regio	n56
Fig 3.6	Same as Fig 3.2 but at intermediate energy regio	n56
Fig 3.7	Same as Fig 3.3 but at intermediate energy regio	n57
Fig 3.8	Same as Fig 3.4 but at intermediate energy regio	n57
Fig 3.9	Shows the effect of polarization potential on t total elastic cross sections of e ⁺ - Li*(2 scattering.	p)
Fig 3.10	Shows the effect of polarization potential on t total Ps formation cross sections of e ⁺ - Li* (2 scattering.	p)
Fig 3.11	Shows the effect of polarization potential on t total rearrangement (reversal of the Ps formatio cross sections of Ps - Li ⁺ scattering	n)

LIST OF FIGURES (Cont...)

Fig. No.	Title	Page No.
Fig 3.12	Shows the effect of polarization potential on the total elastic cross sections of Ps - Li ⁺ scattering	
Fig 3.13	Comparison between various total positronium formation cross sections (in πa_0^2) of e^+ - I	
	scattering determined by different authors	62

Acknowledgement

I wish to express my sincere appreciation to professor Dr. Salah Yaseen El-Bakry, Professor of Theoretical Physics and Head of Theoretical Physics Group, Physics Department, Faculty of Science, Ain Shams University, and the major advisor, for suggesting the topics of this work and for his continuous guidance, encouragement, confidence and patience which gave me added incentive throughout the development of this manuscript.

Sincere thanks are extended to *Dr. El-Sayed A. El-Dahshan*, Assist. Prof. of Computational Physics, Physics Department, Faculty of Science, Ain Shams University, for the helpful guidance in progress of this work and help during the preparation of the computer codes of my work.

I would also like to extend my appreciation to *Dr. Mahasen Mahsoup*, Jecture of Theoretical Physics, Physics Department, Faculty of Science, Ain Shams University, for her fruitful help during the preparation of our programs.

I would like to express my gratitudes to **Prof. Dr. Adel**Abdel Sattar El-Saadany, Head of the Physics Department, for his help and encouragement

My very warm gratitudes go to **Dr. M. S. Al-Koth** and the members of the Theoretical Group at the Physics Department, Faculty of Science, Ain Shams University, for many fruitful discussion as well as for their kind supports.

On a person notice, I am indebted to my family for their support and encouragement over all these years.

ABSTRACT

The inelastic scattering of positrons by excited lithium alkali atoms $\mathrm{Li}^*(2\,\mathrm{p})$ have been investigated within the frame work of the coupled – static and frozen – core approximations with the assumption that the elastic and rearrangement channels are open. In the present work, a rather complicated computer code is developed based on the coupled – static, frozen – core and Green's function partial wave expansion technique. The partial and total elastic and positronium (Ps) formation cross sections of e^+ – $\mathrm{Li}^*(2\,\mathrm{p})$ are calculated through a wide range of incident energy of positrons ranging from 0.3 eV to 1000 eV. Also, we have calculated the partial and total elastic and rearrangement (reversal of the Ps formation) cross sections of Ps – Li^+ collisions through the low, intermediate and high energy regions.

The effect of polarization potential of the Ps atom is taken into our consideration. The total cross sections which corresponding to twelve partial cross sections (calculated at twelve values of the total angular momentu l=0 to l=11) are calculated for each channel. Our calculated total positronium formation cross sections are compared with experimental results and those calculated by other authors. The present calculations encourage the experimental physicists to carry out positron – lithium experiments by taking the excited lithium target into accounts in order to obtain more positronium especially in the low and intermediate energy regions.

Keywords: Positrons; Positronium formation; Alkali atoms; Collisions; Inelastic scattering; Cross-sections; Lithium; Polarization potential.

Chapter 1

INTRODUCTION

1.1 The importance of scattering

Atomic scattering (collision) is a very wide topic. The field of atomic scattering has a venerable history, since it was central to the development of quantum mechanics, and nuclear physics. Atomic scattering are the basic means for probing the atomic structure of matter. Almost every thing we know about nuclei and elementary particles has been discovered in scattering experiments, from Rutherford's surprise at finding that atoms have their mass and positive charge concentrated in almost point - like nuclei, to the more recent discoveries, on a far smaller length scale, that protons and neutrons are themselves made up of apparently point - like quarks. More generally, the methods that we have to probe the properties of condensed matter systems rely fundamental on the notion of scattering. Study of scattering processes is the main source of information about strong, electromagnetic and weak interactions [Burke].

The interaction of antimatter with matter is an interesting and active field of study. Positron interactions with matter play important roles in many physical processes of interest. Examples include the origin of astrophysical sources of annihilation radiation, the use of positron in medicine (e.g., positron emission tomography); the characterization of materials; and the formation of antihydrogen, which is the simplest of stable, neutral antimatter [Marler].