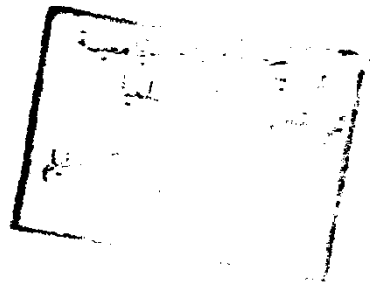
THEORETICAL STUDY OF MULTI-CHANNEL POSITRON-LITHIUM ATOM COLLISIONS



Thesis

Submitted for the degree of
Doctor of Philosophy
in physics

TO

Physics Department
Faculty of science
Ain Shams University

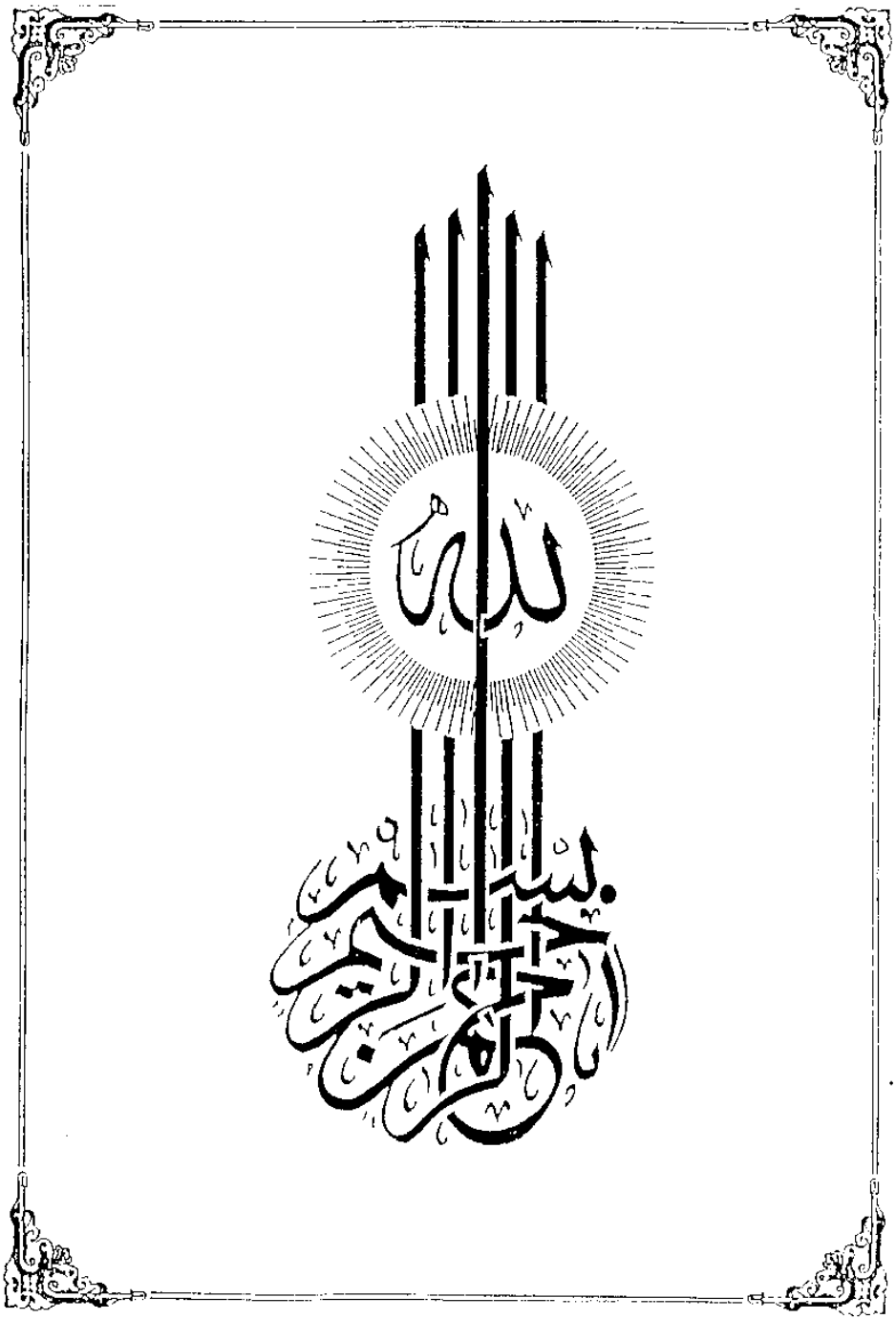
By

Salah El-Deen Mohammad Yaseen EL-Bakry

M. A. Abdel-Rahman

1993

CONTENTS



PAGE

PAGE

LIST OF FIGURES

LIST OF TABLES

ACKNOWLEDGEMENTS

I would like to express my gratitudes to **Prof. Dr. Karimat El - Sayed**, head of the Physics Department, for her help and encouragement.

I wish to express my deep thanks to **Prof. Dr. Ali H. Moussa,** for his continuous support, valuable comments, genius help and encouragement .

I would like to express my most heartful thanks and deep gratitude to **Prof. Dr. M. A. Abdel-Raouf**, for suggesting the research topics presented in this thesis. My deep thanks go also to **Prof. Abdel-Raouf** for his continuous help, valuable discussions and for continuous guidance and advices.

Thanks are also due to **Dr. A. Khazbak** for his fruitful help. My very warm gratitudes go to the members of the theoretical group at the Physics Department for many fruitful discussions as well as for their kind supports.

Great thanks are due to **Egyptian Meteorological Authority** and in particular to **Mr. M . A . Bekhiet**, Chairman Board of Directors, and to **Dr. A. A. Ibrahim** , The Director of The Computer Centre, for providing the computer facilities and for valuable cooperations. Thanks are also due to **Mr. Magdy Abbas**, head of the group of the computer centre, and to his colleagues for their help.

Finally, I would like to thank the staff of the computer centre, Ain Shams university, for their help.

ABSTRACT

Inelastic collision processes, in which elastic, rearrangement and excitation channels are open, are investigated for the first time within the framework of the coupled-static and frozen-core approximations. A generalised formalism, applicable to multi-channel collision of atoms with positive ions, is presented. The formalism is employed for calculating partial and total elastic, positronium formation and 2p-excitation cross sections of positrons scattered from lithium atoms at energies ranging from 2 eV (i.e. slightly above the 2p-excitation threshold) to 30 eV (which lies in the intermediate energy region). The results demonstrate the efficiency of our formalism as well as the computer codes created for treating such problems. They emphasize that positronium formation cross sections are leading in comparison with the the 2p-excitation cross sections in the energy region $2 \leq k_1^2 \leq 7$ eV. A fact which supports the importance of including the rearrangement channel in all treatments of e^+ - Alkali atom inelastic scattering processes in this energy region.

CHAPTER 1

INTRODUCTION

Recently , there has been an increasing interest among experimental and theoretical positron physicists in the study of positron - alkali atom collisions . The strongest justification of this interest is due to the possibility of positronium (Ps) formation even at zero incident energy. This means that we are facing from the beginning multi-channel scattering processes in which at least two channels, (the elastic and rearrangement ones) are open . This fact suggests that any serious theoretical treatment of these processes should consider , especially in the low energy region (i.e. below 10 eV) , the Ps formation channel . On The other hand np excitation channels occur at very low energies (very few eV 's above the Ps formation channel) and emphasize the importance of their consideration .

Lithium atom is the uppermost element of the alkali group and its inelastic collision with positrons can be treated theoretically with reasonable accuracy .

The first serious theoretical treatment of positron-lithium collisions was carried out by Guha and Ghosh [1] who applied the two - state close coupling approximation considering only the elastic scattering and the ground - state positronium formation . Taking the effect of the adiabatic polarization potential into account in both the direct and rearrangement channels , results for the differential , total and momentum - transfer cross sections were computed at

incident positron energies 0.5 - 10 eV . These authors found that the differential cross section for both the elastic scattering and positronium formation shows a deep minimum at low energies of positron impact and at certain values of scattering angles . Their elastic differential cross section curve becomes minimum at around the scattering angle 120° at incident energy of 2 eV .

Wadehra [2] and Khare and Vijayshri [3] were mainly interested in the behaviour of the total collisional cross sections of positron-lithium scattering at intermediate and high energies up to 1000 eV .They used Born and modified Glauber approximation (MGA) ,respectively ,and obtained the total cross-sections which are in fair agreement with the one of electron - lithium scattering calculated by Guha and Ghosh [4] .

Mazumdar and Ghosh [5] applied the distorted wave approximation (DWA) for determining positronium formation cross-sections of e^{+}- Li scattering at few incident energies between 2 and 100 eV . The Ps formation cross sections decreases with the increase of incident positron energies and at about 100 eV , Ps formation is found to be negligible .

Gien [6] investigated the inelastic scattering of positrons by lithium atom using a modified Glauber (MG) and second Born (SB) approximations at energies ranging from 40

to 1000 eV . He employed Peach's pseudo-potentials [7] for describing the interaction between the valence electron and the rest of the alkali atom . The inert-core and frozen-core assumption and the use of the Clementi wavefunction [8] to represent the target electrons are considered . His comparison between positron and electron cross-sections calculated by the same approach showed that those of positrons are somewhat smaller .

Nahar and Wadehra [9] have investigated the inelastic scattering of positrons by lithium atoms using first Born (FB) and distorted wave Born (DWB) approximations . They calculated the positronium differential and total cross-sections at very few intermediate energies using a Hellmann-type pseudo-potential for representing the interaction between the valence electron and the core of the target .

Abdel-Raouf [10] has presented a detailed investigation of the inelastic scattering of positrons by lithium using coupled-static and frozen core approximations . In this work , the Clementi-Roetti wave functions are employed for describing the one-valence electron model of the target . The partial and total cross-sections are calculated for eight values of the total angular momentum ℓ , (corresponding to $0 \leq \ell \leq 7$) at 25 values of the incident energy k_i^2 ($0.1 \leq k_i^2 \leq 1000$ eV) . His results show that the S - and P - wave cross-sections dominate all other cross-sections below 1.0 eV , while the

roles of the D - and F - waves increase gradually up to the lower limit of the intermediate-energy region (k_i^2 = 30 eV) where all higher partial waves become important . The results show also that the total elastic cross-sections decrease monotonically , apart from a dip at k_i^2 = 0.5 eV and a local minimum at k_i^2 = 3 eV where regions of resonance could be expected . Abdel - Raouf has also obtained the partial and total positronium formation cross-sections which show the oscillating behaviour and the monotonic decrease in the region $0.1 \leq k_i^2 \leq 60$ eV. The Ps formation has a larger cross-section than elastic scattering at k_i^2 = 0.1 eV .

Recently , Abdel-Raouf et al [11] have investigated the inelastic collisions of positrons with lithium atoms within the frame work of the coupled-static and frozen-core approximations by employing Walters' wave funtions [12] for describing the target . They calculated the partial cross-sections for the first eight partial waves at 21 values of the incident energy laying between 0.1 and 1000 eV . The results show that the S- and P- waves have very large contributions to the total cross-sections below 1 eV ; the P- , D- and F- waves , respectively , produce the important parts of the total cross-sections between 3 and 50 eV and the higher partial waves become important at higher energies .The results show also that the D- ,P- ,F- and S- waves , respectively , play the most important role in the total Ps formation cross-sections

below 3 eV , while the higher partial waves are important in the region $3 \leq k_i^2 \leq 10$ eV . The results illustrate the fact that the value of the total Ps formation cross-section diminishes beyond 10 eV, a matter which supports the argument that the Ps formation does not play a fundamental role in the total collisional cross-sections of positron-lithium inelastic scattering in the intermediate and high energy regions . The total elastic cross-section falls off steadily with the increase of the incident energy , while the Ps formation cross-section increases (after 0.1 eV) steadily until it reaches its maximum around 0.9 eV , and then , falls off smoothly .

Ward et al [13] have performed five-state close- coupling calculations for e^- - Li (2S - 2P - 3S - 3P - 3d) scattering in the energy range 0.5- 50 eV . They used two different types of target wave functions namely : (i) numerical frozen-core Hartree-Fock wavefunctions , and (ii) wavefunctions derived from the model potential of Peach [7] . However , the authors neglected the positronium formation channel and focused their attention to the 2p , 3d , etc excitation channels .The model potential wavefunctions employed give excitation thresholds at 1.844 , 3.367 , 3.829 and 3.874 eV , respectively . They calculated the elastic , excitation and total integrated cross-sections .A sharp minimum is shown in the elastic differential cross-section in the vicinity of 40- 50° at