THEORETICAL STUDY OF POSITRON-ATOM COLLISIONS

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

By

SALAH EL-DEEN MOHAMMAD YASEEN EL-BAKRY

To

Department of Physics, Faculty of Science
Ain Shams University

ACKNOWLEDGEMENT

I wish to express my sincere appreciation to Professor Dr. Ali H. Moussa, Professor of Theoretical Physics and Head of 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 course of study and development of this manuscript.

Sincere thanks are extended to Dr. M.A. El-Shabshiry for the many helpful discussions during this work.

I would also like to extend may appreciation to Dr. M.A. Abdel-Raouf, Lehrstühl Fur Theoretische Chemie, Friedrich-Alexander Universität Erlangen-Nürnberg, West Germany, for the valuable discussions and enlightened ideas especially during the initial and final stages of this work.

My thanks are due to the staff of the scientific computing centre of Ain-Shams University for their help.

بسم الله الرحمن الرحيم

CONTENTS

Note I

Abstract II

CHAPTER I
INTRODUCTION

1.1 Introduction 1

1.1.1. Positronium. 3

1.2 Scattering Cross Section. 3

1.3 Types of Collisions. 5

1.4 Channels 8

1.5 Alkali-Atoms 9

1.6 Review of Work Done in Theoretical Study of Positrons with Atoms 9

1.6.1 Positron-Hydrogen Scattering 9

1.6.2 Positron-Helium Scattering 14

1.6.3 Positron-Alkali Atom Collision 15

CHAPTER II
Development of the Coupled-Static Approximation for Positron-Lithium Atom Collisions

2.1 Introduction 19

2.2 Calculation of the Net Core Potential $V_c(r_0)$ 20

2.3 Calculation of the Ground-state Energy of the Target Model 22

2.4 Description of the Two Channel Problem 28

2.5 Mathematical Justification of the Coupled Integro-differential Equations 31

2.5.1 Calculation of the Static Potential of the First Channel $U_{st}^{(1)}(x)$ 34

2.5.2 Calculation of the Static Potential of the Second Channel $U_{st}^{(2)}(\sigma)$ 38

2.6 Reformulation of the Previous Calculations with the Exchange Effect ... 49

2.7 Determination of the Elements of the Reactance Matrix R 52

2.8 Calculation of the Partial and Total Cross Sections 54

CHAPTER III

Results and Discussion 57

Appendices
Appendix A: Analysis of the Potentials and Kernels
Appendix B: The Numerical Iterative Method
Appendix C: Short Notes on the Program for the Calculation of the Partial and Total Cross Sections of Positron-Lithium Collisions

References

Arabic Summary

NOTE

Beside the work carried out in this thesis, the candidate has attended a post-graduate course for one year (1985 - 1986) in the following topics:

I. GENERAL COURSES:

- Advanced quantum mechanics.
- Advanced electrodynamics.
- Statistical physics.
- Mathematical physics.
- Computational physics.

II. SPECIAL COURSES:

- Theoretical nuclear physics.
- General theory of relativity.
- Field theory.
- Computational systems.
- Theory of atomic collisions.

He has successfully passed an examination in these topics.

ABSTRACT

In the present work, theoretical treatment of positron-atom collisions is studied with special application to the lithium atom, where we deal with a two channel problem in which the positronium formation should be remarkably noticed within a wide region of the scattering energy even when the incident positron energy equals zero. Thus the total elastic and positronium formation cross-sections in low energy regions are considered. Both the coupled-static and frozen core approximations are used. The analysis of the coupled-static approximation is developed through the calculation of the core potential, the static potentials, the total energies, and the total Hamiltonians of the first and second channels with and without the exchange part of the core potential.

Walters' wave functions are used to describe the orbitals of the target atom. The two coupled integro-differential equations are also obtained with and without the exchange effect and their solutions are given formally by the Lipmann-Schwinger equation. An iterative method is applied for calculating the iterative partial cross-sections through the calculation of the iterative transition matrix which in turn is related to the reactance matrix. The partial cross-sections corresponding to 8 values of the total angular momentum l ($0 \leq l \leq 7$) are determined for 21 values of the incident energy lying between 0.1 and 1000 ev. Results illustrate the stability of the iterative numerical technique employed. They demonstrate the role played by each partial wave in the total cross-sections and emphasize the argument that the effect of positronium formation on the total collisional cross-sections diminishes when the incident energy is larger than 30 ev. We have succeeded in obtaining the positronium formation at very low energies where no threshold energy occurs. It was found that the exchange part of the core potential increases the positronium formation cross-sections and decreases the elastic scattering cross-sections of the first channel. The present results are compared with various results obtained by

different authors. These results have revealed good agreement with the results obtained by Guha and Ghosh (1981) and also agree well with those obtained by Mazumdar and Ghosh (1987).

CHAPTER I

INTRODUCTION

1.1. INTRODUCTION

The relativistic quantum mechanics of fermions (Particles of spin $\frac{1}{2}\hbar$) introduced by Dirac[1] predicts that for each kind of particle with a certain mass and charge there should exist a different kind of particle, termed an `antiparticle', with the same mass and with a charge of equal magnitude but opposite sign.

The subsequent discovery of the anti-particle to the electron, known as the positron, by Anderson[2] in 1932 and Blackett and Occhialine[3] in 1933, is rightly regarded as one of the triumphs of modern physics. Since that time, positrons have been studied from many points of view. First, verification of the fundamental properties of the particles were in accord with those predicted by theory, but later interest has centred on applications in which the positron is employed as a probe into problems of atomic or solid state physics.

The importance of the study of positron interactions in collision theory was perhaps first emphasized by Massey and Mohr[4] in 1954. Since that time, important advances have occurred, both theoretically and experimentally. The points of contact between the experiments and theory are not as many as could be wished and are somewhat indirect. The reason for this is that there are until 1982 no controlled mono-energetic beams of low energy positrons and the experiments have been performed with positrons arising from nuclear beta decay. The positrons produced from beta decay have an energy distribution which is peaked about some rather high energy. In our context, high and low energies are with respect to typical binding energies of electrons in atoms. The interaction of a positron, at non-relativistic velocities $\upsilon << c$, with an electron or with a nucleus is represented accurately by a Coulomb potential. Apart from the opposite sign of the interaction, electron positron scattering differs from electron-electron scattering in two respects:

i. As the particles are different, the wave function need not be antisymmetrical and there are no exchange terms in the scattering amplitude,

ii. the electron-positron pair can annihilate (subject to certain selection rules), as a rule into two photons. In principle, this absorptive process modifies the potential acting on the electron and positron by the addition of a positive imaginary part, but as the annihilation cross-section is much smaller than the cross-sections associated with characteristic atomic scattering, this modification of the Coulomb potential can be ignored. The attractive coulomb interaction between an electron and a positron supports a series of bound states. The bound system of a positron and an electron was named positronium by Ruark(5).

1.1.1. Positronium

Positronium (P_s) is a bound system composed of an electron e^- and a positron e^+. It can be said to be an isotope of hydrogen, with the proton being replaced by a positron. However, it must be noted that the situation is not quite the same: in the hydrogen atom, the proton (which is much heavier than the electron) remains almost motionless, while in P_s, the positron, has the same mass and consequently the same velocity as the electron when the centre of mass of P_s is fixed. The reduced mass associated with positronium is half the electron mass. For a given state of positronium, the average electron-positron distance is twice the electron-proton distance for the corresponding state of the hydrogen atom. The differences between the energies of the stationary states, however, are twice as small, and the optical line spectrum emitted by P_s is obtained by doubling all the wavelengths of that of hydrogen. The spin of P_s may be either para- or ortho-positronium and the fraction of formations are 25 to 75 percent, respectively. The life times are 1.5×10^{-10} sec and 1.47×10^{-7} sec, respectively. The mode of annihilation (number of γ-rays) are 2 and 3, respectively.

1.2. SCATTERING CROSS SECTION

Scattering is defined to be the deviation of a particle from its original direction of motion caused by its interaction with another particle (the scatterer). In connection with the fact that scattering is caused by the interaction (collision) of two particles, the scattering theory is also known as the collision theory. The great majority of collision phenomena, however, involve some reaction of the scattered particle on the scatterer. The proceeding of a scattering process in time consists in that two initially infinitely remote particles move towards each other, next, upon approaching, they interact, and, finally, fly away in different directions. Instead of considering how a scattering process goes on in time, it is often convenient to deal with an equivalent stationary picture. The transition from a temporal to a stationary description is performed with the aid of the assumption that there is a continuous flux of particles flying from infinity that, because of interaction with a scattering centre, transforms into a flux of scattered particles flying away from this centre in different directions. The density of the particles in the flux must be sufficiently low for the interaction between the incident particles to be negligibly small. In the stationary treatment, the scattering problem consists in calculation of the flux of scattered particles (at an infinitely great distance from the scattering centre) as a function of the incident particle flux when we know the scattering force field.

Scattering is characterized by the differential scattering cross section

$$d\sigma(\theta,\phi) = \frac{dN_{scat}(\theta,\phi)}{J_{inc}}$$

where

$dN_{scat}(\theta,\phi)$ = the number of particles scattered in unit time within the solid angle $d\Omega$ taken in the direction (θ,ϕ)

and

J_{inc} = the density of the incident particle flux.

Let

$J_{scat}(r,\theta,\phi)$ = the density of the scattered particle flux at large distances "r" from the scattering centre.

$$\therefore\ dN_{scat}(\theta,\phi) = J_{scat}(r,\theta,\phi)\, dA_r$$

$$= J_{scat}(r,\theta,\phi)\, r^2 d\Omega$$

Then,

$$d\sigma(\theta,\phi) = \frac{J_{scat}(r,\theta,\phi)r^2 d\Omega}{J_{inc}}$$

In quantum mechanics, J_{scat} and J_{inc} are understood to be the relevant densities of the probability fluxes. Integrating the previous expression over all the angles, we obtain the quantity

$$\sigma = \frac{1}{J_{inc.}} \oint J_{scat}(r,\theta,\phi)\, dA_r$$

$$= \frac{\Phi_{scat}}{J_{inc}} = \frac{\text{the total prob. of scattering of a particle (in unit time)}}{\text{the density of the prob. flux in incident beam}}$$

which is called the total effective scattering cross section.

dA_r = the area of an elementary surface at the distance r from the scattering centre and corresponding to the solid angle $d\Omega$,

and

Φ_{scat} = the scattered particle flux through the closed surface enveloping the scattering centre.

The surface over which the integral is evaluated is assumed to be at a great distance from the centre. Therefore, it is considered that at each point of this surface the scattered particles fly in a radial direction.

1.3. TYPES OF COLLISIONS

Let us consider a typical collision experiment in which a beam of particles, well collimated and nearly monoenergetic, is directed towards a target. The target usually consists of a macroscopic sample containing a large number of scatterers. The distances between these scatterers are in general quite large with respect to the de Broglie wavelength of the incident particle, in which case one can neglect coherence effects between the waves scattered by each of the scattering centers. In addition, if the target is sufficiently thin, multiple scattering by several scatterers can be neglected. Then, one may consider that each scatterer acts as if it were alone, and focus one's attention on the study of a typical collision between a particle of the incident beam and a scatterer of the target. After the collision, some or all outgoing particles are registered by detectors, located at a macroscopic distance from the target.

Several processes can occur:

1) ***Elastic Scattering***: the two colliding particles A and B are scattered without any change in their internal states and composition,

$$A + B \rightarrow A + B \tag{1.1}$$

2) ***Inelastic Scattering***: the two colliding systems A and (or) B undergo a change of their internal quantum state during the collision process. Denoting by A' and B' these new internal states, we may have

$$\begin{aligned} & A + B \rightarrow A' + B \\ \text{OR} \quad & A + B \rightarrow A + B' \\ \text{OR} \quad & A + B \rightarrow A' + B' \end{aligned} \tag{1.2}$$

3) ***Reactions:*** the composite system (A + B) splits into two (or more) particles different from A and B.