

THESIS IN COMPUTATIONAL QUANTUM MECHANICS

SUBMITTED TO

MATHEMATICS DEPARTMENT AIN SHAMS UNIVERSITY

519.5 7.A

UNIVERSITY COLLEGE FOR WOMEN
FOR

THE DEGREE OF PH.D.IN APPLIED MATHEMATICS

BY

Zein El-Abdeen Ahmed Gaafar El-kotbi

M.SC. AIN SHAMS UNIVERSITY

CAIRO 1992

In memory of

my father



ACKNOWLEDGEMENT

All gratitude is due to god almighty who guided and aided me to bring forth to light this theses.

The author is heartily grateful to Prof. Dr. F.A. Ayoub Professor of Applied Math. For proposing and planning this investigation, and whose continuous encouragement, valuable suggestions, capable supervision and reading throughout the manuscript have rendered the realisation of this work to be possible.

I wish to express my gratitude to all Professors and Teachers who taught me.

CONTENTS

Summary	V
Introduction	1
Chapter I A general veim of scattering theory	.11
1 - 1: Introduction To Scattering	12
1 - 2 : The Destorted Wave Approximation	23
$I=3$: The Reaction Of μ^* -meson with tritium	26
Chapter II The Electronic Wave Functions .	32
2 - 1: The Two Wave Functions * And	33
2 - 2 : The Born - Oppenheimer Separation	34
2 - 3 : The Tritium Molecule—Ion	37
2 - 4 : The Vibration And Rotation	
Of Diatomic Molecule	40
2 - 5 : The Wave Functions F And G	48
Chapter III Integration Of the Electronic Wave	
Functions	-60
$3-i$: The Normalizing Factors N_1,N_2	
Of The Wave Functions 🛡 . 🗘	61
3 - 2 : Integration Over r'	63
$3-3$: Evaluation Of The Integral l_1	66
$3-4$: Evaluation Of The Integral I_2	82
Chapter IV Calculation Of The Cross Sections	88
$4-1$: The Wave Function X and Ω	89
4 - 2 : The Integration Over ρ , ρ'_{\bullet}	94
4 - 3 : Calculation	97
4 - 4 : Calculation Of The Differential	
Cross Sections	101
Appendix (1) Normalizing Factor	203
Appendix (2) Runge - Kutta Method	105
Appendix (3) Program	
5-4	777

SUMMARY

The present work has been based on the study of collisions of elementary particles.

An introduction gives a brief summery of the properties of tritium and u-mesons.

This thesis consists of four chapters.

The first chapter contains the mathematical derivation of the differential cross-section for the reaction,

$$(H_1^3)_2^* + \mu^* \rightarrow (\mu H_1^3)^* + (H_1^3)^*$$

using the distorted wave method.

The second chapter contains the calculations of the two wave functions corresponding to the relative motion of μ^* -meson in field of $(H_1^3)_2^*$ molecule and of $(\mu H_1^3)^*$ in the field of $(\mu H_1^3)^*$ molecule.

The difference between the corresponding levels of vibrational and rotational energies of $(\mu H_1^3)^*$ and $(\mu H_1^3)^*$ molecules has been calculated.

The third chapter contains the calculations of the two wave functions representing the motion of the electron in the field of $(H_1^3)^*$ and $(\mu H_1^3)^*$ molecules and the integrations of the electronic wave functions over the element of are calculated.

The fourth chapter contains the calculations for excited states of the two wave functions corresponding to vibrational and rotational motion of the nuclei of $(H_1^3)_2^*$ and $(\mu H_1^3)^*$ molecules. Also the integration over the elements ρ_e , ρ^* are calculated.

The differential cross-secton reaction are calculated for different values energy levels.

It is found that calculated cross sections comparable with the theoretical maximum ones.

Supervisor Prof Dr. F. A Ayonb EAjub

Central Library - Ain Shams University

INTRODUCTION

INTRODUCTION

In this thesis we are doing to study a chemical reaction, so we have to know first some properties of the components of this reaction. For the present section, these components are tritium and processors.

Tritium

The Tritium is the heaviest isotope of the element hydrogen and the only one which is radioactive. Tritium occurs in very small amounts in nature but is denerally prepared artificially by processes known as nuclear transmutations. It is widely used as a tracer in chemical and biological research and is a component of the so-called thermo-nuclear of hydrogen bomb. It is commonly represented by symbol \mathcal{H}^3 , indicating that it has an atomic number of 1 and an atomic mass of 3, or by the special symbol 7. For information about the other hydrogen isotopes properties.

Both molecular tritium, T_2 , and its counter part hydrogen, H_2 are gases under ordinary conditions. Because of the great difference in mass, many of the properties of tritium difference substantially from those of ordinary hydrogen.

chemically, tritium behaves quite similarly to hydrogen. However, because of its larger mass, many of its reactions take place more slowly than do those of hydrogen.

The nucleus of the tritium atom, often called a triton and symbolized t, consists of a proton and two neutrons. It has a mass of 3.01700 atomic mass units (amu), a nuclear spin of $\frac{1}{2}$, and a magnetic moment of 2.9788 nuclear magnetos.

It undergos radioactive decay by emission of a β -particle to leave a helium nucleus of mass 3. No γ - rays are emitted in this process. The nalf-life for the decay is 12.26 years. The most energetic of the β -particles emitted by tritium have the comparatively low energy of 18.6 Kilo electron volts (KeV). β -particles are completely stopped by 7 mm of air or by 0.01 mm of paper or similar material. The average energy of the β -particle is 5.69 KeV.

When tritium is bombarded with deuterons of sufficient energy, a nuclear reaction known as tusion occurs and energy considerably dreater than that of the bombarding particle is released. The reaction may be written as

$$H^3 + H^2 \rightarrow H_2 e^4 + n_2^4 - 18 MEV$$

one of those which supply the energy of the thermo-nuclear bomb. It is also of major importance

in the development of controlled informational reactors. Enormous quantities of tritium will be required if such reactors are perfected and prought into use as electric power generators.

Natural Occurrence

Before the start of thermo-nuclear weapons testing in 1954, rainwater contained approximately 1-10 atoms of tritium per 10% atoms of hydroder. Such tritium origin atom largely from the bombardment of hitrogen in the upper atmosphere with neutrons and protons from cosmic rays, as in reaction (2), because the half-life

$$N_{7}^{14} + N_{5}^{12} \rightarrow H_{1}^{3} + C_{5}^{12}$$

of tritium is short in comparison with the time required for mixing of the ocean waters. The concentration of tritium in the ocean is much lower than in rainwater-before 1954 the total amount of tritium on the Earth's surface was estimated at 1800 g. Of which about 11g was in the atmosphere and 13g in groundwaters. Testing of thermo-nuclear weapons has resulted in sharp rises in the tritium content of rainwater to values as righ as 500 atoms per 10% atoms of hydrogen.

Preparation

Tritium was first produced in the laboratory by bombarding compounds of deuterium with high-energy deuterons, as in the reaction

$$H^2 - H^2 \rightarrow H^3 + H^1$$

A number of other nuclear reactions also give rise to tritium. The most important of these is the absorption of slow neutrons by the lithium isotope of mass 6. According to reaction . By irradiating

$$Li_3^6 + n_2^4 \rightarrow H_1^3 - He_2^4$$

enviched lithium—6. in the form of an allov with magnesium or alaminum, with neutrons from a nuclear reactor, tritium may be prepared on a large scale. bees As a result of its production for use in nuclear weapons. tritium has become available in large quantities at very low cost. It is used in admixture with zinc sulfige in the production of luminous paints, which have largely replaced the radium formerly used on watch dials, such mixtures are also used to produce small, permanent light sources.

Tritium absorbed on metals is used in tardets for the production of fast neutrons by nomberdment with deuterons. Tritium has been much used in hydrological studies, since it is an ideal tracer for water movement.

Some studies depend on natural tritium or that introduced by weapons testing in other cases target amounts of tritium are deliberately added.

Investigations include the distribution of groundwater in oil fields: the tracing of springs, rivers, and lakes: water seepage and loss from reservoirs; and the movement of glaciers.

Tritium has also been used as a tracer for hydrogen in the study of chemical reactions. The most widespread used of tritium has probably been in biological research, where it has been used both as a hydrogen tracer and as a molecular label in studies of metabolism, biosynthesis, and cytology. In particular, tritiated thymidine and other nucleotides and nucleosides have been extensively used in studies of the formation of DNA and KNA.

Compounds, very few compounds of pure tritium have been prepared and studied. Such compounds would under go decomposition quite rapidity under the action of the tritium \S -radiation. Fritium $0 \times 10^{10} \times 10^{10}$

are employed in tracer studies, such as those indicated above. Tritium-labelled compounds may be prepared by ordinary synthetic chemical methods, such as the catalytic addition of tritium-hydrogen mixtures to unsaturated compounds. Tritium may be exchanged for hydrogen in the presence of a catalyst such as platinum or a strong acid.

In recoil labelling, a mixture of an ordanic compound and a lithium selt are irradiated with neutrons in a nuclear reactors; some of the energetic tritons produced are incorporated into the ordanic compound.

Another important labelling procedure consists of the exposure of an organic compound to tritium question a sealed vessel; the tritium 3-radiation tacilitates the exchange of hydrogen in the compound with tritium in the gas. Some compounds of biological interest have been prepared by growing organisms in tritiated water.

Analysis

Because of its weak β -radiation, tritium is not readily measured by the ordinary design-mulley counter. More efficacious is the introduction of tritium as a gas in side the counting tube. Alternatively, the lonization of a gas caused by the β -radiation may be measured in an lonization

chamber, or the tritium compound may be dissolved in a suitable solvent containing a phosphor and the light pulses excited by the β -particles then may be counted with a scintillation counter. Fritium das containing only small amounts of ordinary hydroden may be analyzed with a mass spectrometer or by measuring the density of the das. Because of the very short range of the tritium β -particle, auto-radio-graphy, the exposure of radioactive material to a photographic plate is often used to locate precisely the position tritium in biological material.

The μ -meson

Studies of cosmic rays began after the first world was and it has been one of the most fruited; in modern physics leading to the discovery of the positron, the pir and num metons and the stronge particles. The importance of cosmic rays in deophysical and cosmological research generally is also very great.

A search was made for particles of this order of mass in the radiation at sea level and Angelein. The followed shortly after by Street and Stevenson, did discover them include chamber photographs produced by the hard component, because their masses are intermediate between those of electrons and or