# IONISATION OF ATOMS BY EXTERNAL ELECTROMAGNETIC FIELDS

THESIS SUBMITTED TO

FACULTY OF WOMEN FOR
ARTS , SCIENCE AND EDUCATION

AIN SHAMS UNIVERSITY



FOR

THE AWARD OF THE (M.SC) DEGREE
(APPLIED MATHEMATICS)

BY

AZZA HASSAN AHMED
DEPARTEMENT OF MATH.

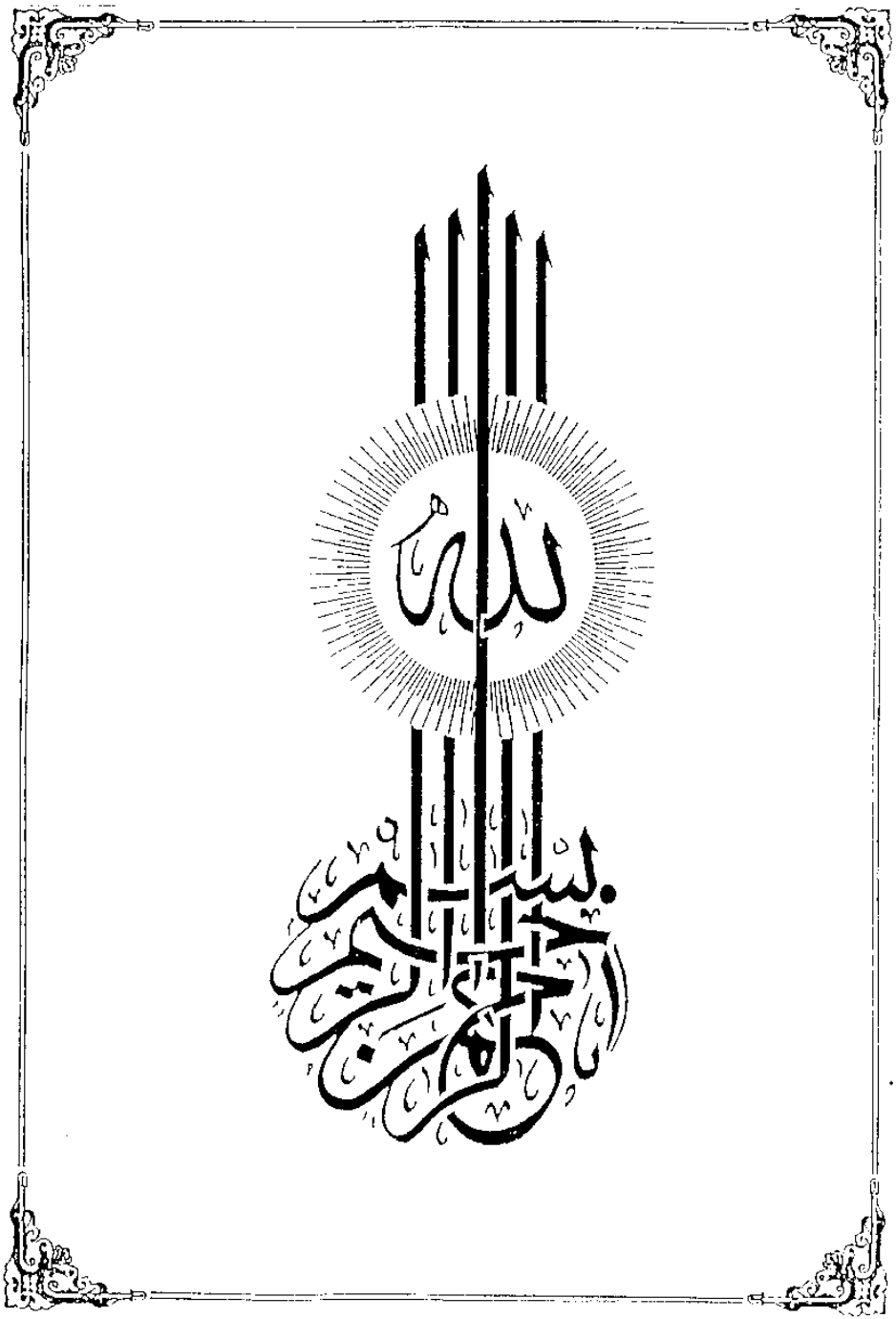
1989

بسم الله الرحمن الرحيم

"... رَبِّ أَوْزِعْنِي أَنْ أَشْكُرَ نِعْمَتَكَ الَّتِي أَنْعَمْتَ عَلَيَّ وَعَلَىٰ وَالِدَيَّ
وَأَنْ أَعْمَلَ صَالِحًا تَرْضَاهُ وَأَدْخِلْنِي بِرَحْمَتِكَ فِي عِبَادِكَ الصَّالِحِينَ"

صدق الله العظيم

"سورة النمل آيه ١٩"



A C K N O W L E D G M E N T

I am deeply grateful to Prof. Dr. Afaf A. Sabry for his valuable encouragement throughout the supervision of this work. I am greatly indebted to him for suggesting the problem involved in this work, stimulating advice and courteous help .

TO MY PARENTS

Whose love and encouragement were among the incentives in accomplishing this hard work.

C O N T E N T S

## CHAPTER III

## POSSIBILITY OF IONISATION



## MATHEMATICAL APPENDICES

# INTRODUCTION

## The one electron atom under a constant external electric field (Stark effect):

When an atom is placed in an external electric field, its energy levels are altered; this phenomenon is known as the Stark effect.

The Stark effect in hydrogen atom has often been studied by perturbation theory. The first- order effect was derived by Schrödinger, the second- order by Epstein, the third- order by Doi and the fourth- order by Basu.

However the ionisation of the atom cannot be explained by using the perturbation theory due to the very nature of the bound state Raleigh- Schrödinger (R-S) perturbation method. Different methods have been applied to explain the ionisation (tunnel effect for example).

In this thesis we shall apply the WKB approximation method to explain the ionisation. In general this method, compared to the known R-S perturbation method, is not accurate enough for small fields, but it may prove important for very strong external fields for which the usual R-S perturbation method fails.

The Schrödinger wave equation for a one electron atom under an external field $\mathcal{F}$ is given by

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{Ze^2}{4\pi\epsilon R}\psi - (-e)\mathcal{F}z\psi = E\psi \qquad (1)$$

where $m$ , $-e$ are the reduced mass and charge of the electron, $Ze$ the charge of the nucleus, $R$ the distance between the

nucleus and the electron, and z the projection of this distance in the direction of the external field.

It is usual to use atomic units in order to have dimensionless quantities in the Schrödinger equation. We take for unit of length the Bohr first orbit radius of the hydrogen atom (Z = 1)

$$a = \frac{4\pi\epsilon_0\hbar^2}{me^2} \qquad (2)$$

For the unit of energy we also take the quantity $\frac{e^2}{4\pi\epsilon_0 a}$ Using these units equation (1) becomes

$$-\frac{1}{2}\Delta\psi + (-\frac{Z}{r} + Fz)\psi = E\psi \qquad (3)$$

where

$$F = \frac{\mathcal{F}}{\mathcal{F}_0} \quad , \quad \mathcal{F}_0 = \frac{e}{4\pi\epsilon_0 a^2} \qquad (4)$$

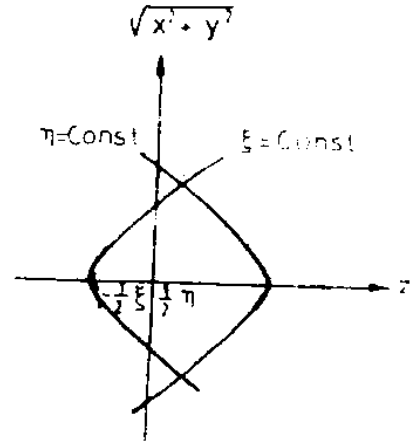
In this case (an atom in an external electric field) the separation of the variables is possible in what is called parabolic coordinates. The solution of the problem of motion in a Coulomb field in terms of parabolic coordinates is useful in investigating a number of problems where a certain direction in space is distinctive.

The parabolic coordinates $\xi, \eta, \chi$ are defined by the formula

$$\begin{aligned} x &= \sqrt{\xi\eta}\cos\chi \\ y &= \sqrt{\xi\eta}\sin\chi \\ z &= \frac{1}{2}(\eta - \xi) \\ r &= \frac{1}{2}(\xi + \eta) \end{aligned} \qquad (5)$$

$\xi$ and $\eta$ take values from 0 to $\infty$, and $\chi$ from 0 to $2\pi$.

The surfaces $\xi$ = const. and $\eta$ = const. are paraboloids of revolution about the z-axis, with focus at the origin. This system of coordinates is orthogonal.




(6) Parabolic coordinates

The Laplace operator is given by

$$\Delta = \frac{4}{\xi+\eta}\left[\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right)+\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)\right]+\frac{1}{\xi\eta}\frac{\partial^2}{\partial\chi^2}$$

Equation (3) can be expressed in parabolic coordinates

$$\frac{\partial}{\partial\xi}\left(\xi\frac{\partial\psi}{\partial\xi}\right)+\frac{\partial}{\partial\eta}\left(\eta\frac{\partial\psi}{\partial\eta}\right)+\frac{\xi+\eta}{4\xi\eta}\frac{\partial^2\psi}{\partial\chi^2}+\left[Z-\frac{F}{4}(\eta^2-\xi^2)+\frac{E}{2}(\xi+\eta)\right]\psi=0 \qquad (7)$$

Let us seek the eigenfunction $\psi$ in the form

$$\psi = e^{im\chi}u_1(\xi)u_2(\eta) \qquad (8)$$

where $m$ is the magnetic quantum number. Substituting this expression in equation (8) multiplied by $\frac{\xi+\eta}{4}$ and separating the variables $\xi$ and $\eta$, we obtain for $u_1$ and $u_2$ the equations

$$\begin{aligned}&\frac{d}{d\xi}\left(\xi\frac{du_1}{d\xi}\right)+\left[Z_1+\frac{F}{4}\xi^2+\frac{E}{2}\xi-\frac{m^2}{4\xi}\right]u_1=0\\&\frac{d}{d\eta}\left(\eta\frac{du_2}{d\eta}\right)+\left[Z_2-\frac{F}{4}\eta^2+\frac{E}{2}\eta-\frac{m^2}{4\eta}\right]u_2=0\end{aligned} \qquad (9)$$

where the separation parameters $Z_1$, $Z_2$ are related by

$$Z_1+Z_2=Z \qquad (10)$$

In zero order (when $F = 0$), the solution of equation (9) is known to be

$$U_1^{(0)}(\xi) = \xi^{\frac{m}{2}} \; e^{-\frac{\epsilon}{2}\xi} \; {}_1F_1(-n_1, m+1, \epsilon\xi)$$
$$U_2^{(0)}(\eta) = \eta^{\frac{m}{2}} \; e^{-\frac{\epsilon}{2}\eta} \; {}_1F_1(-n_2, m+1, \epsilon\eta) \qquad (11)$$

where ${}_1F_1(a,b,c)$ is the confluent hypergeometric function,

$$Z_1^{(0)} = \epsilon\left(n_1 + \frac{m}{2} + \frac{1}{2}\right)$$
$$Z_2^{(0)} = \epsilon\left(n_2 + \frac{m}{2} + \frac{1}{2}\right) \qquad (12)$$
$$\epsilon = \sqrt{-2E}$$

and $n_1$, $n_2$ are the parabolic quantum numbers.

For small $F$ we can use the R-S perturbation procedure to find the energy levels and the wave function in successive orders of approximation in powers of $F$.

The energy levels for the one electron atom in the presence of external field are known to be (Refrence (17))

$$E = -\frac{Z^2}{2n^2} - \acute{n}\frac{3n}{2Z}F - \frac{n^4}{16Z^4}(17n^2 - 3\acute{n}^2 - 9m^2 + 19)F^2 - \frac{3n^7}{32Z^7}\acute{n}(23n^2 - \acute{n}^2 + 11m^2 + 39)F^3$$
$$- \frac{n^{10}}{1024Z^{10}}(5487n^4 + 1806n^2\acute{n}^2 + 147\acute{n}^4 + 35182n^2 + 5754\acute{n}^2 + 16211 - 18m^2(169n^2 + 63\acute{n}^2 + 439) - 549m^4)F^4 \qquad (13)$$

where

$$\acute{n} = n_1 - n_2$$
$$n = n_1 + n_2 + |m| + 1 \qquad (14)$$

In the present work we used the WKB method to obtain the expansion of the energy levels in powers of $F$, (for $E < 0$) and compare it with the R-S perturbation.

It was found that the zero and first orders approximation using both methods are the same, for the second and for the third orders are different in the constant term only. For very small values of F the WKB method has shown that there exists an essential singularity at the threshold $F = 0$ in a certain function (equation (3.10)).

Carrying out numerical computation for an external field on using the results of applying the WKB approximation, it was found that the ionisation stops when the external field attains certain critical values. The reason that ionization can happen for very small fields tending to zero is that the ionization depends on the energy that the electron gains from the field. So as the field tends to zero and the dimension of the space where the field prevails tends to infinity then a possible finite energy can be extracted from the field.

# CHAPTER 1

# ENERGY LEVELS SHIFTS USING WKB APPROXIMATION

CHAPTER I

# ENERGY LEVELS SHIFTS USING WKB APPROXIMATION

## Introduction:

In this chapter we will discuss the conditions of applicability of the WKB approximation. Then we will find the approximate solution of Schrödinger equation solved in parabolic coordinates.

Using the WKB approximation we will obtain an implicit formula to find the energy levels shifts as the results of the external field. Then we shall discuss simple cases of this formula, corresponding to the quantum numbers $n, n_1, n_2$.

Finally the expressions of partial derivatives of the implicit formula will be used in calculating numerically the energy shifts as functions of the external field.

## 1.1 Approximate solution of the Schrödinger equation:

In equation (9) we carry out the substitution

$$u_1 = \xi^{-\frac{1}{2}} f(\xi)$$
$$u_2 = \eta^{-\frac{1}{2}} g(\eta) \qquad (1.1)$$

Equations (9) are brought into the form

$$\frac{d^2 f}{d\xi^2} + \left(\frac{Z_1}{\xi} + \frac{F}{4}\xi + \frac{E}{2} + \frac{1-m^2}{4\xi^2}\right) f = 0$$
$$\frac{d^2 g}{d\eta^2} + \left(\frac{Z_2}{\eta} - \frac{F}{4}\eta + \frac{E}{2} + \frac{1-m^2}{4\eta^2}\right) g = 0 \qquad (1.2)$$