Democratic and Popular Republic of Algeria

Ministry of Higher Education and Scientific Research
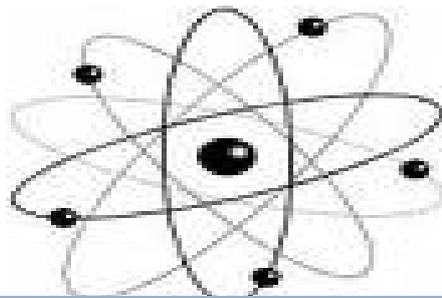
University Med Khider of Biskra

Department of Matter Sciences   Domain of Matter Sciences

Section of Physics

Speciality Physics of Photo-Voltaic

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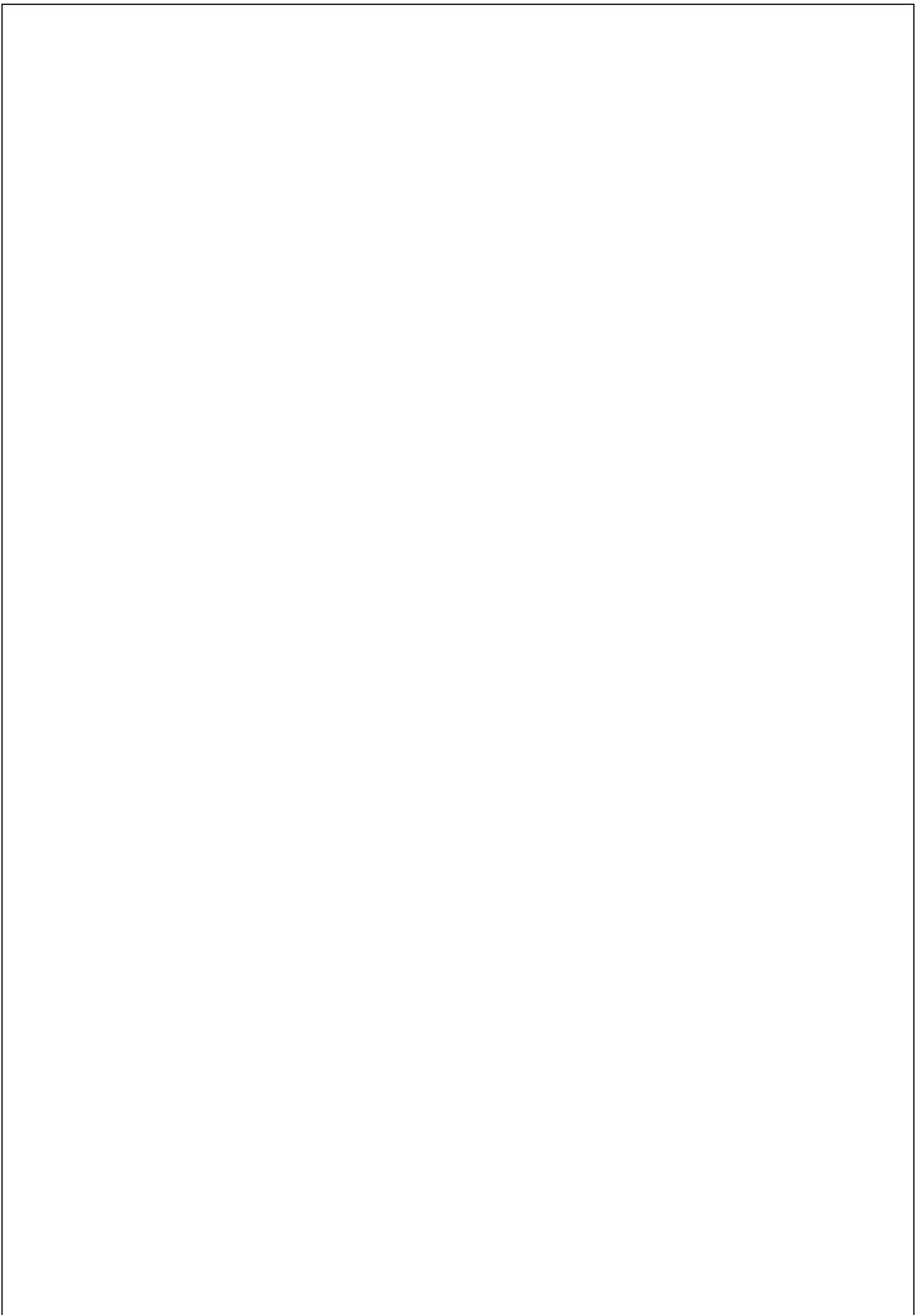
Dedication:

I dedicate this work to

My dear parents

My brothers, my sisters especially to my brother Hachem
for his help and his labor with me

To all my family

To my friends: R, S, F, S, SH, S, S, A

To all students of material science, specially to student of
Speciality Physics of Photo-Voltaic

Acknowledgement:

I thank Allah Almighty for having given me the courage and determination to achieve my memory, to make this work that we hope it will reach our aspirations, God willing.

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I wish to express my thanks to my colleague CHARROUF Randa helped me in making this work

Thank all those who, near or far I helped to carry out my work.

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Introduction

Introduction:

The interaction of a charged particle with a charged gathering (molecule, ion…) is a fundamental problem, which received a lot of attention since the early days of nuclear and molecular physics, that phenomenon was studies first by Fermi (1942).It has been shown that the electric dipole field is capable of supporting an infinite number of bound states for an electron if the dipole moment is greater than the critical value [1].

The important task of quantum mechanics is to find the exact bound state solutions of the Schrödinger equation for certain potentials of much physical interest. Generally speaking, there are a few main traditional methods for studying the exact solutions of quantum systems like the Coulomb potentials [2].

We present the exact energy bound state solutions of the Schrödinger equation in 3 dimensions for potential of the form $V(r) = \frac{a}{r} + \frac{b}{r^2} + \frac{c\cos^2\theta}{r^3}$, the solution of central potential was obtained analytically. But for approximation there are many of the quantum mechanical systems, the most popular approximation schemes are stationary perturbation theory [2].

We will begin with hydrogen-like atoms and ions that have only one electron, this problem is of importance because the hydrogen-like atom has certain features that will be common to all atomic systems; all other problems will involve both approximations and correction factors [3].

This study involves three sections:

> ➤ In section one: we present the Coulomb potential by the expansion of multipole (dipole and quadrupole) in spherical coordinate, for calculate this impact we use expansion of multipole where approach the gathering to charged punctual this model agrees the model of hydrogen atom.
> ➤ In section two: we present discussion with a review of the Schrödinger equation for a single electron in a central potential $V(r)$, we consider analytical solutions to the equation where it has three-term: the angular wave function, azimuthal wave function and radial component of the wave-function

Introduction

- ➢ In section three: we calculate the first and second order corrections of the last solution by time independent perturbation theory by using Mathematica software.

- ➢ In section four: we conclude and discus the results

Chapter I:

The Multipole Expansion

I-1-Expended Charge:

Far enough away from any charge distribution with net charge q, the potential is approximately that due to a point charge q located in the distribution.Consider an extended charge distribution $q(r')$, we wish to find the electrostatic potential due to this charge distribution at a given point r, we assume that point is at a large distance from the charge distribution, that is if r' varies over the charge distribution then $r \gg r'$ [5].

The Coulomb potential for this charge distribution is given by [4]:

$$V(r) = k\sum \frac{q}{r_i} \text{ where } k = \frac{1}{4\pi\epsilon_0}$$

I-2-Multipole Expansion:

I-2-1-Définition:

A multipole expansion is a mathematical series representing a function that depends on angles usually the two angles on a sphere. These series are useful because they can often be truncated, meaning that only the first few terms need to be retained for a good approximation to the original function. The function being expanded may be complex in general. Multipole expansions are very frequently used in the study of electromagnetic and gravitational fields, where the fields at distant points are given in terms of sources in a small region. The multipole expansion with angles is often combined with an expansion in radius. Such a combination gives an expansion describing a function throughout three-dimensional space [6]

The multipole expansion is expressed as a sum of terms with progressively finer angular features, for example, the initial term called the zeroth, or monopole moment is a constant independent of angle. The following term the first or dipole moment varies once from positive to negative around the sphere. Higher-order terms (like the quadrupole and octupole) vary more quickly with angles. A multipole moment usually involves powers (or inverse powers) of the distance to the origin, as well as some angular dependence [6]

In principle, a multipole expansion provides an exact description of the potential and generally converges under two conditions:

1- If the sources (ex. charges) are localized close to the origin and the point at which the potential is observed is far from the origin

2- The reverse, if the sources (ex. charges) are located far from the origin and the potential is observed close to the origin.

In the first (more common) case, the coefficients of the series expansion are called exterior multipole moments or simply multipole moments whereas, in the second case, they are called interior multipole moments. The zeroth-order term in the expansion is called the monopole moment, the first-order term is denoted as the dipole moment, and the third (the second-order), fourth (the third-order), etc. terms are denoted as quadrupole, octupole, etc. moments [6].

I-2-2-Applications of Multipole Expansions:

Multipole expansions are widely used in problems involving gravitational fields of systems of masses, electric and magnetic fields of charge and current distributions, and the propagation of electromagnetic waves. A classic example is the calculation of the exterior multipole moments of atomic nuclei from their interaction energies with the interior multipoles of the electronic orbitals [7].

Multipole expansions are also useful in numerical simulations, and form the basis of the fast multipole method of other method, a general technique for efficient computation of energies and forces in systems of interacting particles. The basic idea is to decompose the particles into groups, particles within a group interact normally (by the full potential), whereas the energies and forces between groups of particles are calculated from their multipole moments [7].

The multipole expansion of: $\|\vec{r_i}\|^{-1}$ or $\|\vec{r} - \vec{r_i}\|^{-1}$ shows the relation and demonstrates that at long distances $r \gg r'$, we can expand the potential as a multipole; we write

$$\|\vec{r_i}\| = \sqrt{\left\|\vec{r} - \vec{r'}\right\|^2} = \sqrt{r^2\left(\vec{u_r} - \frac{r'}{r}\vec{u'}\right)^2} \qquad I.1$$

$$\frac{1}{\|\vec{r_i}\|} = \frac{1}{r}\left(1 - 2\frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\right)^{-\frac{1}{2}} \qquad I.2$$
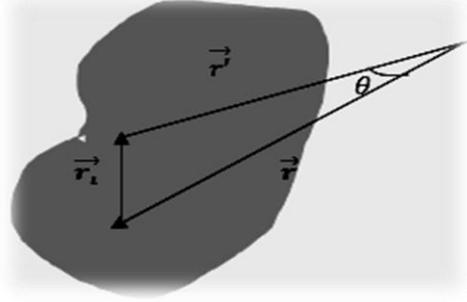
Figure I.1: Multipole Moments of a Point Charge

We use Taylor expansion [4]: $(1 + x)^n = 1 + \frac{nx}{1!} + \frac{n(n-1)x^2}{2!} + \cdots$ $\qquad$ *I.3*

$$(1 + x)^{\frac{-1}{2}} = 1 + \frac{\frac{-1}{2}x}{1!} + \frac{\frac{-1}{2}\left(\frac{-1}{2}-1\right)x^2}{2!} + \cdots = (1 + x)^{\frac{-1}{2}} = 1 + \frac{-1}{2}x + \frac{3}{8}x^2 + \cdots \qquad I.4$$

To express the r term in the potential:

$$\left(1 - 2\frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\right)^{\frac{-1}{2}} = 1 - \frac{1}{2}\left(-2\frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\right) + \frac{3}{8}\left(-2\frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\right)^2 + \cdots \qquad I.5$$

$$\left(1 - 2\frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\right)^{\frac{-1}{2}} = 1 + \frac{r'}{r}\cos\theta - \frac{1}{2}\frac{r'^2}{r^2} + \frac{3}{8}\left(4\frac{r'^3}{r^3}\cos^2\theta + \frac{r'^4}{r^4} - 4\frac{r'}{r}\cos\theta\frac{r'^2}{r^2}\right) \qquad I.6$$

We use the fact that $r \gg r' \Rightarrow \frac{r'^4}{r^4}, \frac{r'^3}{r^3} \approx 0$ to write the precedent expression in the following way and as before, we restrict ourselves to the second order for convenience and to the show the behaviour of the corrections induced by the dipole and the quadrupole and this is equivalent to not considering the octupole term.

$$\left(1 - 2\frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\right)^{\frac{-1}{2}} = 1 + \frac{r'}{r}\cos\theta - \frac{1}{2}\frac{r'^2}{r^2} + \frac{3}{2}\frac{r'^2}{r^2}\cos^2\theta \qquad I.7$$

$$\left(1 - 2\frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\right)^{\frac{-1}{2}} = 1 + \frac{r'}{r}\cos\theta + \frac{r'^2}{r^2}\left(\frac{3\cos^2\theta - 1}{2}\right) \qquad I.8$$

$$\frac{1}{\|\vec{r}\|} = \frac{1}{r}\left[\underbrace{1}_{monopole} + \underbrace{\frac{r'}{r}\cos\theta}_{dipole} + \underbrace{\frac{r'^2}{r^2}\left(\frac{3\cos^2\theta - 1}{2}\right)}_{quadrupole}\right] \qquad I.9$$

Using these relations, the potential is now writing as [4]:

$$V(r) = k \sum \frac{q}{r_i} = k \int_{v'} \frac{q(r')}{r_i} dv' = k \frac{1}{r} \int_v q(r') \left(1 + \frac{r'}{r} \cos\theta + \frac{r'^2}{r^2} \left(\frac{3\cos^2\theta - 1}{2} \right) \right) dv' \qquad I.10$$

$$V_{mono} = k \frac{1}{r} \int_{v'} q(r') dv' \qquad I.11$$

$$V_{dip} = k \frac{1}{r^2} \int_{v'} q(r') r' \cos\theta \, dv' \qquad I.12$$

$$V_{qua} = k \frac{1}{r^3} \int_{v'} q(r') r'^2 \left(\frac{3\cos^2\theta - 1}{2} \right) dv' \qquad I.13$$

I-3-The Monopole Part:

A point charge is a hypothetical charge located at a single point in space. While an electron can for many purposes be considered a point charge, its size can be characterized by length scale known as the electron radius [8].
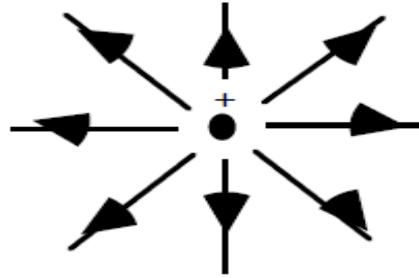
Figure I-2: A Point Electric Charge Field

A normal magnet has two poles, usually called the north and south poles. You might have one of these on your fridge. If you place it on your fridge door the right way it sticks as if by magic. If you turn it around it jumps out of your hand and lands on the floor [9].

A magnetic monopole doesn't have two poles. as its name suggests it's a monopole. It only has one pole. While the Human Design revelation says the magnetic monopole only attracts, there is no attraction or repelling force in the scientific version of the magnetic monopole because by its very nature it doesn't have a polarity [9].

The electric potential of an electric charge monopole is given by [4]:

$$V_{mono} = k \frac{1}{r} \int_{v'} q(r') dv'$$

I-4-Definition of Dipole:

A physical dipole consists of two equal and opposite point charges. Its field at large distances (distances large in comparison to the separation of the poles) depends almost entirely on the dipole moment. A point (electric) dipole is the limit obtained by letting the separation tending to 0 while keeping the dipole moment fixed. The field of a point dipole has a particularly simple form, and the order-1 term in the multipole expansion is precisely the point dipole field [10].

Figure I-3: An Electric Dipole Field

The electric potential of an electric charge dipole is given by [7]:

$$V_{dip} = k \frac{1}{r^2} \int_{v'} q(r') r' \cos \theta \ dv'$$

I-5-Definition of Quadrupole:

A quadrupole or quadrupole is one of a sequence of configurations of electric charge or current or gravitational mass that can exist in ideal form, but it is usually just part of a multipole expansion of a more complex structure reflecting various orders of complexity [11]

The simplest example of an electric quadrupole consists of alternating positive and negative charges, arranged on the corners of a square.

The monopole moment (just the total charge) of this arrangement is zero. Similarly, the dipole moment is zero, but the quadrupole moment of the arrangement in the diagram cannot be reduced to zero [12]

Figure 1. Electrodes and equipotential lines in an electrostatic quadrupole.
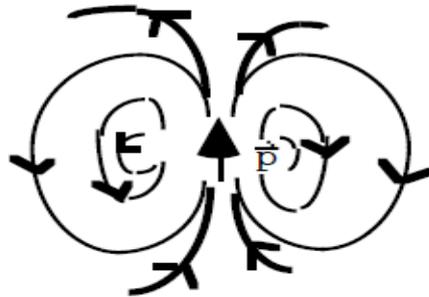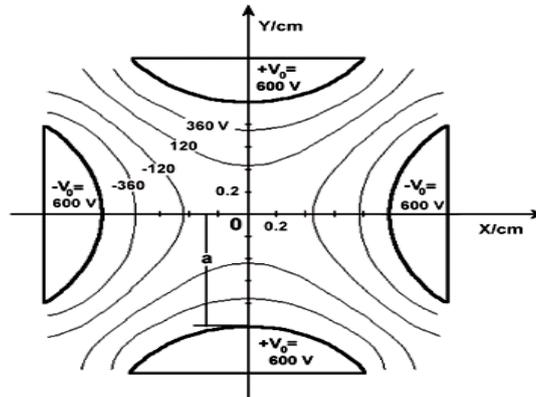
FigureI-3: the Equipotential Surfaces of an Electric Quadrupole Field

The electric potential of an electric charge quadrupole is given by [4]:

$$V_{qua} = k\frac{1}{r^3} \int_{v'} q(r')r'^2 \left(\frac{3\cos^2\theta - 1}{2}\right) dv'$$

Chapter II:

The Schrödinger Equation in Three Dimensions

II-1-Introduction:

In quantum mechanics, the Schrödinger equation is a partial differential equation that describes how the quantum state of quantum physical system changes with time. It was formulated in late 1925, and published in the beginning of 1926, by Austrian physicist Erwin Schrödinger [13].

II-2-Solution of Schrödinger Equation in Three Dimensions:

Although some physical systems can be described in one or two dimensions, the most general problems require the solution of the Schrödinger equation in three dimensions [13].

The stationary Schrodinger equation in three dimensions is a partial deferential equation involving three coordinates per particle. The mathematical complexity behind such an equation can be intractable by analytical means. However, there are certain high-symmetry cases when it is possible to separate variables in some convenient coordinate system and reduce the Schrodinger equation to one-dimensional problems [14]

The Schrödinger equation for the hydrogen like atom will not be separable unless the Hamiltonian is expressed in one of a number of non-Cartesian coordinates. (Write r as function of x, y, z and ask if separable.) .The simplest of these are spherical coordinates [15]

To generalize this to three dimensions, we can give the momentum its three components in each of the three spatial dimensions, so we get [13]

$$\frac{P^2}{2m}\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t} \longrightarrow P = -i\hbar\frac{\partial}{\partial x} \qquad\qquad II.1$$

To generalize this to three dimensions, we can give the momentum its three components in each of the three spatial dimensions, so we get [13]:

$$\left.\begin{array}{l} P_x = -i\hbar\frac{\partial}{\partial x} \\ P_y = -i\hbar\frac{\partial}{\partial y} \\ P_z = -i\hbar\frac{\partial}{\partial z} \end{array}\right\} \Rightarrow P^2 = -\hbar^2\left(\frac{\partial}{\partial x^2}^2 + \frac{\partial}{\partial y^2}^2 + \frac{\partial}{\partial z^2}^2\right) = -\hbar^2\nabla^2 \qquad II.2$$

If we assume that the potential $V = V(x, y, z)$ is independent of time, the Schrödinger equation in three dimensions can therefore be written as [13]:

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad\qquad II.3$$

Where, as before, the energy E takes on a set of discrete values for the bound states and a set of continuous values for the scattering, or unbound states. The spatial wave function ψ satisfies the time-independent Schrödinger equation [13]:

$$\frac{-\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \qquad\qquad II.4$$
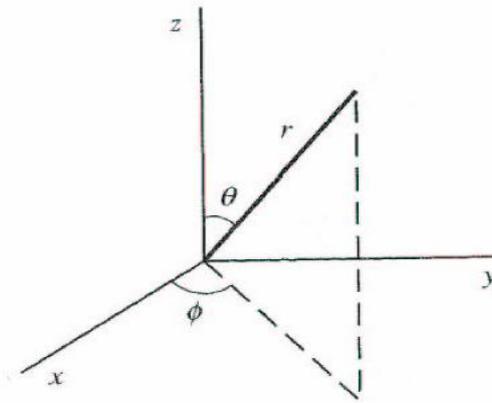
Figure II-1: Point Charge in Spherical Coordinate

Transformation to a spherical coordinate system [15]:

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$

Things get interesting when we consider the analysis relating to the three spatial dimensions. A common situation is that where the potential is spherically symmetric; it depends only on the radial distance for the origin (the electrostatic potential is one such case). In this case, it makes more sense to use spherical coordinates, so we need to rewrite (II.4) in spherical coordinates. There is a general method for transforming differential operators such as ∇^2 into other coordinate systems which we'll consider in another post. For now we'll just quote the result in spherical coordinates (r, θ, ϕ), where r is the distance from the origin (so

$r \geq 0$), θ is the angle from the positive z axis (so $0 \leq \theta \leq \pi$), and is the ϕ azimuthal angle measured from the x axis (so $0 \leq \phi \leq \pi$) [13]:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}(\sin\theta\frac{\partial}{\partial \theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right) \qquad II.5$$

Given this, the time-independent portion of the Schrödinger equation satisfies [13].

$$\left[\frac{-\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\frac{h^2}{2m_er^2}\frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right)\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}\right) V(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \quad II.6$$

This implies that our wave-function will be a function of r, θ and ϕ so Schrodinger equation becomes:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial\psi}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial \phi^2}\right) + \left[\frac{2m_e}{\hbar^2} E - V(r)\right]\psi = 0 \qquad II.7$$

II-3-Separation of Variables:

The equation can be separated in different independent equations when it is expressed in spherical coordinates. So the Schrödinger equation for a hydrogen atom is [16]:

$$\psi_{nlm} = R_{nl}(r)\, Y_l^m(\theta,\phi) \qquad\qquad II.8$$

$$\frac{1}{r^2}\frac{\partial^2}{\partial r^2}(r^2 R_{nl}(r)\, Y_l^m(\theta,\phi)) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\left(R_{nl}(r)Y_l^m(\theta,\phi)\right)\right)\right] + \quad II.9$$

$$\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}[R_{nl}(r)\, Y_l^m(\theta,\phi)] + \frac{2m_e}{\hbar^2}\,[E - V(r)\, R_{nl}(r)\, Y_l^m(\theta,\phi)] = 0$$

We multiply by $r^2\sin^2\theta$ to have:

$$\sin^2\theta r^2\frac{\partial^2 R_{nl}(r)}{\partial r^2}\, Y_l^m(\theta,\phi) + \sin^2\theta\frac{1}{\sin\theta}\left[\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial Y_l^m(\theta,\phi)}{\partial \theta} R_{nl}(r)\right) + \quad II.10$$

$$1\sin\theta\partial 2\,Ylm\theta,\phi\partial\phi 2Rnlr + \sin 2\theta\, 2mer2\hbar 2E - Vr\ Rnlr\ Ylm\theta,\phi = 0$$

$$\sin^2\theta\frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + sin^2\theta\frac{1}{\sin\theta\, Y_l^m(\theta,\phi)}\left[\frac{\partial}{\partial \theta}\sin\theta\frac{\partial Y_l^m(\theta,\phi)}{\partial \theta} + \frac{1}{\sin\theta}\frac{\partial^2\, Y_l^m(\theta,\phi)}{\partial \phi^2}\right] + \quad II.11$$

$$\sin^2\theta\frac{2m_er^2}{\hbar^2}(E - V(r)) = 0$$

$$\sin^2\theta \frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \frac{2m_e r^2}{\hbar^2}\left(E - V(r)\right) = -\frac{\sin^2\theta}{\sin\theta\, Y_l^m(\theta,\phi)}\left[\frac{\partial}{\partial\theta}\left(\left(\sin\theta\frac{\partial Y_l^m(\theta,\phi)}{\partial\theta}\right) + \right.\right. \qquad II.12$$

$$1\sin\theta\partial2\,Ylm\theta,\phi\partial\emptyset2$$

We put [15]: $Y_l^m(\theta,\phi) = F(\theta)P(\emptyset)$ $\qquad\qquad II.13$

To get:

$$\frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \frac{2m_e r^2}{\hbar^2}\left(E - V(r)\right) = -\frac{1}{\sin\theta F(\theta)P(\emptyset)}\left[\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right)P(\emptyset) + \right. \qquad II.14$$

$$1\sin\theta\partial2P\emptyset\partial\emptyset2F\theta$$

$$\sin^2\theta\frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \sin^2\theta\frac{2m_e r^2}{\hbar^2}\left(E - V(r)\right) + \frac{\sin\theta}{F(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right) = \frac{\partial^2 P(\emptyset)}{P(\emptyset)\partial\emptyset^2} \qquad II.15$$

II-4-Solution of Components:

II-4-1-Solution of Angular Components:

A   Solution of $\emptyset$:

The $\emptyset$ equation is [16]: $-\frac{1}{P(\emptyset)}\frac{\partial^2 P(\emptyset)}{\partial\emptyset^2} = m^2$ $\qquad\qquad II.16$

or: $\frac{\partial^2 P(\emptyset)}{\partial\emptyset^2} = -m^2 P(\emptyset)$ $\qquad\qquad II.17$

The equation is easily solved to give[16] :

$$P(\emptyset) = Ae^{-im\emptyset} \qquad\qquad II.18$$

Where A is some constant to be determined by normalization:

$$\int_0^{2\pi} P(\emptyset)P(\emptyset)^* d\emptyset = 1 \Rightarrow \int_0^{2\pi} Ae^{-im\emptyset}Ae^{im\emptyset}d\emptyset = 1 \Rightarrow A^2\int_0^{2\pi} d\emptyset = 1 \Rightarrow A = \frac{1}{\sqrt{2\pi}} \qquad II.19$$

$$P_m(\emptyset) = \frac{1}{\sqrt{2\pi}}e^{-im\emptyset}; m \in \mathbb{Z} \qquad\qquad II.20$$

B   -Solution of θ:

$$\sin^2\theta\left[\frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \frac{2m_e r^2}{\hbar^2}\left(E - V(r)\right) + \frac{1}{\sin\theta F(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right)\right] = m^2 \qquad II.21$$

$$\Rightarrow \frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \frac{2m_e r^2}{\hbar^2}\left(E - V(r)\right) + \frac{1}{\sin\theta F(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right) = \frac{m^2}{\sin^2\theta} \qquad II.22$$

$$-\frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \frac{2m_e r^2}{\hbar^2}\left(E - V(r)\right) = \frac{m^2}{\sin^2\theta} - \frac{1}{\sin\theta\, F(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right) = -l(l+1) \qquad II.23$$

$$\Rightarrow \frac{m^2}{\sin^2\theta} - \frac{1}{\sin\theta\, F(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right) = -l(l+1) \qquad II.24$$

$$\Rightarrow m^2 + l(l+1)\sin^2\theta - \frac{\sin\theta}{F(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right) = 0 \qquad II.25$$

By multiplying with $F(\theta)$, we get:

$$F(\theta)[m^2 + l(l+1)\sin^2\theta] - \sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F(\theta)}{\partial\theta}\right) = 0 \qquad II.26$$

We put $x = \cos\theta$ &$\sin^2\theta = 1 - \cos^2\theta = 1 - x^2$ to write [15]:

$$(1-x^2)\frac{d^2 F}{dx^2} - 2x\frac{dF}{dx} + F(\theta)\left[\frac{m^2}{1-x^2} + l(l+1)\right] = 0 \qquad II.27$$

This equation has as a solution the Legendre polynomial [17]:

$$F_m^l(x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1) \qquad II.28$$

So we have the following expression for the angular part of the wave-function:

$$Y_l^m(\theta,\phi) = F(\theta)P(\emptyset) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)\frac{1}{\sqrt{2\pi}}e^{-im\emptyset} \qquad II.29$$

II-4-2-Solution of The Radial Part

$$-\frac{r^2}{R_{nl}(r)}\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \frac{2m_e r^2}{\hbar^2}\left(E - V(r)\right) = -l(l+1) \qquad II.30$$

$$\Rightarrow -\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \left[\frac{2m_e}{\hbar^2}\left(E - V(r)\right) + \frac{l(l+1)}{r^2}\right]R_{nl}(r) = 0 \qquad II.31$$

With the expressions [3]: $E = \frac{-z^2 q^4 m_e}{2(4\pi\varepsilon_0)^2\hbar^2 n^2}$ & $V(r) = -z\frac{q^2}{4\pi\varepsilon_0 r}$, we can write:

$$-\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \left[\frac{2m_e}{\hbar^2}\left(-\frac{z^2 q^4 m_e}{2(4\pi\varepsilon_0)^2\hbar^2 n^2} + z\frac{q^2}{4\pi\varepsilon_0 r}\right) + \frac{l(l+1)}{r^2}\right]R_{nl}(r) = 0 \qquad II.32$$

$$-\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \left[\frac{2m_e}{\hbar^2}\frac{-z^2 q^4 m_e}{2(4\pi\varepsilon_0)^2\hbar^2 n^2} + \frac{2m_e}{\hbar^2}z\frac{q^2}{4\pi\varepsilon_0 r} + \frac{l(l+1)}{r^2}\right]R_{nl}(r) = 0 \qquad II.33$$

$$-\frac{\partial^2 R_{nl}(r)}{\partial r^2} + \frac{l(l+1)}{r^2} R_{nl}(r) + \frac{1}{r}\frac{zq^2}{4\pi\varepsilon_0} R_{nl}(r) - \frac{2m_e}{\hbar^2}\frac{z^2q^4m_e}{2(4\pi\varepsilon_0)^2\hbar^2n^2} R_{nl}(r) = 0 \qquad II.34$$

We use the asymptotic behavior to find the solution:

$$\Rightarrow -\frac{\partial^2 R_{nl}(r)}{\partial r^2} = \frac{2m_e}{\hbar^2} E\, R_{nl}(r) \Rightarrow R_{nl}(r) = r^{l+1}\, e^{-\frac{2m_e}{\hbar^2}Er} \sum A_n\, r^n \qquad II.35$$

And finally we have [15]:

$$R_{nl}(r) = y^l e^{-y/2}\, L_{n-l-1}^{2l+1}(y) \qquad II.36$$

$$y = 2\sqrt{\frac{-2m_e E_n}{\hbar^2}}r = 2\sqrt{\frac{Z^2}{n^2 a_0{}^2}}r = \frac{Z}{na_0}r;\, a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e q^2}$$

$L_{n-l-1}^{2l+1}(y)$ is the Laguerre polynomial of degree $n-l-1$. We can also use the Laguerre function [17]:

$$\Rightarrow R_{nl}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}}\, y^l e^{-y/2}\, L_{n-l-1}^{2l+1}(y) \qquad II.37$$

II-3-4-Solution ofψ_{nlm}:

We compile all the precedent expression to write the final expression of the solutions:

$$\psi_{nlm} = R_{nl}(r)\, Y_l^m(\theta,\phi) \qquad II.38$$

$$= \sqrt{\left(\frac{2}{n\,a}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}}\, e^{\frac{-r}{n\,a}}(y)^l\, L_{n-l-1}^{2l+1}(y)\, Y_l^m(\theta,\phi) \qquad II.39$$

Chapter III:

Time Independent Perturbation Theory

-III-1-Introduction:

Very often, a mathematical problem cannot be solved exactly or, if the exact solution is available, it exhibits such an intricate dependency in the parameters that it is hard to use as such. It may be the case, however, that a parameter can be identified, say such that the solution is available and reasonably simple for $\varepsilon = 0$ then, one may wonder how this solution is altered for non-zero but small ″. Perturbation theory gives a systematic answer to this question [18]

III-2-Introduction to Regular Perturbation Theory:

Perturbation theory for algebraic equations **.**Consider the quadratic equation

$$x^2 - 1 = \varepsilon x \qquad\qquad 1.III$$

The two roots of this equation are:

$$x_1 = \frac{\varepsilon}{2} + \sqrt{1 + \frac{\varepsilon^2}{4}} \, x_2 = \frac{\varepsilon}{2} - \sqrt{1 + \frac{\varepsilon^2}{4}} \qquad\qquad 2.III$$

For small, these roots are well approximated by the first few terms of their Taylor series expansion

$$x_1 = 1 + \frac{\varepsilon}{2} + \frac{\varepsilon^2}{8} + O(\varepsilon^2) \, x_2 = -1 + \frac{\varepsilon}{2} - \frac{\varepsilon^2}{8} + O(\varepsilon^2) \qquad\qquad 3.III$$

One can obtain (3) without prior knowledge of the exact solutions of (1) using regular perturbation theory:

$$x = X_0 + \varepsilon X_1 + \varepsilon^2 X_2 + O(\varepsilon^2) \qquad\qquad 4.III$$

Another review topic that we discuss here is time-independent perturbation theory because of its importance in experimental solid state physics in general and transport properties in particular.

There are many mathematical problems that occur in nature that cannot be solved exactly. It also happens frequently that a related problem can be solved exactly. Perturbation

theory gives us a method for relating the problem that can be solved exactly to the one that cannot. This occurrence is more general than quantum mechanics many problems in electromagnetic theory are handled by the techniques of perturbation theory. In this course however, we will think mostly about quantum mechanical systems, as occur typically in solid state physics [18].

III-3-Definition of Time Independent Perturbation Theory:

In quantum mechanics, perturbation theory is a set of approximation schemes directly related to mathematical perturbation for describing a complicated quantum system in terms of a simpler one in time-independent. Perturbation theory is an important tool for describing real quantum systems, as it turns out to be very difficult to find exact solutions to the Schrodinger equation for Hamiltonians of even moderate complexity. The Hamiltonians to which we know exact solutions, such as the hydrogen atom [19].

III-4-Applications of Perturbation Theory:

Using perturbation theory, we can use the known solutions of these simple Hamiltonians to generate solutions for a range of more complicated systems. For example, by adding a perturbative electric potential to the quantum mechanical model of the hydrogen atom, we can calculate the tiny shifts in the spectral lines of hydrogen caused by the presence of an electric field (the Stark effect). This is only approximate because the sum of a Coulomb potential with a linear potential is unstable although the tunnelling time (decay rate) is very long. This shows up as a broadening of the energy spectrum lines, something which perturbation theory fails to reproduce entirely.

The expressions produced by perturbation theory are not exact, but they can lead to accurate results as long as the expansion parameter. Typically, the results are expressed in terms of finite power series in that seem to converge to the exact values when summed to higher order. After a certain order, however, the results become increasingly worse since the series are usually divergent (being asymptotic series). There exist ways to convert them into convergent series, which can be evaluated for large-expansion parameters, most efficiently by variational method.

The time-independent Schrödinger equation predicts that wave functions can form standing waves, called stationary states (also called "orbitals", as in atomic orbitals or

molecular orbitals). These states are important in their own right, and moreover if the stationary states are classified and understood, then it becomes easier to solve the time-dependent Schrödinger equation for any state. The time-independent Schrödinger equation is the equation describing stationary states. (It is only used when the Hamiltonian itself is not dependent on time. In general, the wave function still has a time dependency.)[19].

III-5-The Perturbation Series:

We begin with an unperturbed Hamiltonian H_0, which is also assumed to have no time dependence. It has known energy levels and eigenstates, arising from the time-independent Schrodinger equation [20]:

$$H_0|\psi^{(0)}\rangle = E_n^{(0)}|\psi^0\rangle \qquad \textit{5.III}$$

$$H_0|n^{(0)}\rangle = E_n^{(0)}|n^0\rangle \qquad \text{6.III}$$

Where $E_n^{(0)}$ and n^0 are energies and eigenstates of the levels for the unperturbed Hamiltonian.

We can put $|\psi\rangle$ in series format:

$$|\psi\rangle = |n^0\rangle + |a\rangle + |b\rangle + \cdots \qquad \textit{7.III}$$

Where $|a\rangle$ and $|b\rangle$ are the first and second order correction to function n^0.

We assume the energy value E so nearby than unperturbed energy value $E_n^{(0)}$ where we can put it en series form [20]:

$$E = E_n^{(0)} + \epsilon_1 + \epsilon_2 \qquad \textit{8.III}$$

Where ϵ_1 , ϵ_2 are the first and second order corrections to energy $E_n^{(0)}$, for we assumed integer parameter λ that has two values: zero and one. If $\lambda = 0$, this eliminates the perturbation and if $\lambda = 1$, this indicates a presence of perturbation.

The perturbed Hamiltonian is:

$$H = H_0 + \lambda H' \qquad \text{9.III}$$

Equations (7), (8) become:

$$|\psi\rangle = |n^{(0)}\rangle + \lambda|a\rangle + \lambda^2|b\rangle + \cdots \qquad 10.III$$

$$E = E_n^{(0)} + \lambda\epsilon_1 + \lambda^2\epsilon_2 + \cdots \qquad 11.III$$

Substituting equations (9), (11) in equations (5)

$$(H_0 + \lambda H')\left(|n^{(0)}\rangle + \lambda|a\rangle + \lambda^2|b\rangle + \cdots\right) = (E_n^{(0)} + \lambda\epsilon_1 + \lambda^2\epsilon_2 + \cdots)\left(|n^{(0)}\rangle + \quad 12.III\right.$$
$$\lambda a + \lambda 2b + \ldots$$

Our goal is: the first order correction depended to H' and the second order correction depended to H'^2. That derives from equating the power of λ with parts of equation (12)

Equating λ^1 gives:

$$H_0|a\rangle + H'|n^0\rangle = E_n^{(0)}|a\rangle + \epsilon_1|n^0\rangle \qquad 13.III$$

Equating λ^2 gives:

$$H_0|b\rangle + H'|a\rangle = E_n^{(0)}|b\rangle + \epsilon_1|a\rangle + \epsilon_2|n^0\rangle \qquad 14.III$$

III-6- The First Order Corrections:

We begin with an unperturbed Hamiltonian H_0, which is also assumed to have no time dependence. It has known energy levels and eigenstates, arising from the time-independent Schrodinger equation [21].

For simplicity, we have assumed that the energies are discrete. The superscripts denote that these quantities are associated with the unperturbed system.

Using the multiply in the left of equation (13) by function $|n^0\rangle$ [21]:

$$\langle n^0|H_0|a\rangle + \langle n^0|H'|n^0\rangle = \langle n^0|E_n^{(0)}|a\rangle + \langle n^0|\epsilon_1|n^0\rangle \qquad 15.III$$

Using the partnerships property we find:

$$H = H^\dagger \tag{16.III}$$

$$\langle n^0|H_0|a\rangle = \langle n^0|H_0^\dagger|a\rangle \tag{17.III}$$

$$\langle n^0|H_0|a\rangle = \left(\langle a|H_0^\dagger|n^0\rangle\right)^* = E_n^{(0)*}\langle n^0|a\rangle \tag{18.III}$$

Whereas $E_n^{(0)}$ is real value

$$E_n^{(0)} = E_n^{(0)*} \tag{19.III}$$

So we can write this equation:

$$\langle n^0|H_0|a\rangle = E_n^{(0)}\langle n^0|a\rangle \tag{20.III}$$

$$E_n^{(0)}\langle n^0|a\rangle + \langle n^0|H'|n^0\rangle = E_n^{(0)}\langle n^0|a\rangle + \epsilon_1 \underbrace{\langle n^0|n^0\rangle}_{=1} \tag{21.III}$$

The first order corrections give:

$$\epsilon_1 = \langle n^0|H'|n^0\rangle \tag{22.III}$$

III-7-The Second-Order Corrections:

To find the second-order correction to the energy, Using the multiply in the left of equation (14) by function: $|n^0\rangle$ [21]

$$\langle n^0|H_0|b\rangle + \langle n^0|H'|a\rangle = \langle n^0|E_n^{(0)}|b\rangle + \langle n^0|\epsilon_1|a\rangle + \langle n^0|\epsilon_2|n^0\rangle \tag{23.III}$$

Calculation the five parts we fine [21]

$$E_n^{(0)}\langle n^0|b\rangle + \langle n^0|H'|a\rangle = E_n^{(0)}\langle n^0|b\rangle + \epsilon_1\langle n^0|a\rangle + \epsilon_2\langle n^0|n^0\rangle \tag{24.III}$$

the second-order correction is given:

$$\epsilon_2 = \langle n^0|H'|a\rangle - \underbrace{\epsilon_1\langle n^0|a\rangle}_{=0} \tag{25.III}$$

because $\langle n^0| \perp |a\rangle$

$$\epsilon_2 = \langle n^0|H'|a\rangle \qquad\qquad 26.\text{III}$$

It gives

$$|a\rangle = -\sum_{\substack{m=0 \\ n\neq n}}^{\infty} |m^0\rangle \frac{\langle m^0|H'|n^0\rangle}{E_m^{(0)} - E_n^{(0)}}$$

Where $|a\rangle$first-order correction to the energy

$|m^0\rangle$ is the Eigen-states of the Hamiltonian H_0,and $|m^0\rangle \neq |n^0\rangle$

Substitute value of $|a\rangle$in equation (26)

$$\epsilon_2 = \left\langle n^0 \left| H' \right| - \sum_{\substack{m=0 \\ n\neq n}}^{\infty} |m^0\rangle \frac{\langle m^0|H'|n^0\rangle}{E_m^{(0)} - E_n^{(0)}} \right\rangle \qquad\qquad 27.\text{III}$$

$$\epsilon_2 = \sum_{\substack{m=0 \\ n\neq n}}^{\infty} \frac{\langle n^0|H'|m^0\rangle\langle m^0|H'|n^0\rangle}{E_m^{(0)} - E_n^{(0)}} \qquad\qquad 28.\text{III}$$

$$\epsilon_2 = \sum_{\substack{m=0 \\ n\neq n}}^{\infty} \frac{|\langle n^0|H'|m^0\rangle|^2}{E_m^{(0)} - E_n^{(0)}} \qquad\qquad 29.\text{III}$$

Remarks:

1- Equation (28) contains the square of H' as we suppose already [21].

2- $E_m^{(0)}$ is never equal $E_n^{(0)}$ otherwise $\epsilon_2 \to \infty$,we put the condition $m \neq n$ to obviate this status [21].

3- The sum contains to unlimited parts, but experimentally we take a limited number [21].

Chapter IV:

Results and Discussion

The Confirmation of $\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \, \psi \left(\frac{cos\theta}{r^2}\right) \psi^* r^2 \, sin\theta = 0$ **in all Situations for the Dipole:**

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}} \, e^{\frac{-r}{na_0}} (y)^l \, L_{n-l-1}^{2l+1}(y) \, Y_l^m(\theta, \phi)$$

We have:

$$y = 2\sqrt{\frac{-2m_e E_n}{\hbar^2}} \, r = \frac{z}{na_0} \, r; \qquad E_n = -\frac{z^2 q^4 m_e}{2(4\pi\epsilon_0)^2 \hbar^2 n^2} \; ; \qquad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e q^2} \; ;$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \, \psi \left(\frac{cos\theta}{r^2}\right) \psi^* r^2 \, sin\theta =$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \left(\sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}} \, e^{\frac{-r}{na_0}} (y)^l \, L_{n-l-1}^{2l+1}(y) \, 1\right)^2 \, Y_l^m(\theta, \phi) \left(\frac{cos\theta}{r^2}\right) Y_l^m(\theta, \phi)^* r^2 \, sin\theta$$

$$Y_l^m(\theta, \phi)^* = (-1)^m \, Y_l^{-m}(\theta, \phi)$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \, \psi \left(\frac{cos\theta}{r^2}\right) \psi^* r^2 \, sin\theta = \qquad 1.IV$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \left(\sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}} \, e^{\frac{-r}{na_0}} (y)^l \, L_{n-l-1}^{2l+1}(y)\right)^2 \, Y_l^m(\theta, \phi) \left(\frac{cos\theta}{r^2}\right) (-1)^m \, Y_l^{-m}(\theta, \phi) r^2 \, sin\theta$$

$$cos\theta \, Y_l^m = b_{l,m} \, Y_{l+1}^m + b_{l-1,m} \, Y_{l-1}^m$$

$$b_{l,m} = \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}}$$

$$b_{l-1,m} = \sqrt{\frac{(l-1+m+1)(l-1-m+1)}{(2(l-1)+1)(2(l-1)+3)}} = \sqrt{\frac{(l+m)(l-m)}{(2l-1)(2l+1)}}$$

$$cos\theta \, Y_l^m = \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}} \, Y_{l+1}^m + \sqrt{\frac{(l+m)(l-m)}{(2l-1)(2l+1)}} \, Y_{l-1}^m$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \, \psi \left(\frac{cos\theta}{r^2}\right) \psi^* r^2 \, sin\theta = \qquad 2.IV$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \left(\sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}} \, e^{\frac{-r}{na_0}} (y)^l \, L_{n-l-1}^{2l+1}(y) \,\right]\right)^2 \left(\sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}} \, Y_{l+1}^m + \right.$$

$$\left. \sqrt{\frac{(l+m)(l-m)}{(2l-1)(2l+1)}} \, Y_{l-1}^m\right) (-1)^m \, Y_l^{-m}(\theta, \phi) \, sin\theta$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi\, \psi \left(\frac{\cos\theta}{r^2}\right) \psi^* r^2 \sin\theta = \quad 3.\text{IV}$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi \left(\sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}}\, e^{\frac{-r}{na_0}}(y)^l\, L_{n-l-1}^{2l+1}(y)\right)^2 \left(\sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}}\,\, Y_{l+1}^m\, (-1)^m\, Y_l^{-m}(\theta,\phi)\, + \right.$$

$$l+ml-m2l-12l+1 \ Yl-1m \ -1m \ Yl-m\theta,\phi \ \sin\theta$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi\, \psi \left(\frac{\cos\theta}{r^2}\right) \psi^* r^2 \sin\theta = \quad 4.\text{IV}$$

$$\left(\sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}}\right)^2 \int_0^{+\infty} \left(e^{\frac{-r}{na_0}}(y)^l\, L_{n-l-1}^{2l+1}(y)\ \right)^2 dr \left(\sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}}\ \right)\int_0^\pi \int_0^{2\pi}\ Y_{l+1}^m\, (-1)^m\, Y_l^{-m}(\theta,\phi)\sin\theta\, d\theta\, d\phi\, + $$

$$l+ml-m2l-12l+10\pi02\pi \ Yl-1m \ -1m \ Yl-m\theta,\phi\sin\theta d\theta \ d\phi$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi\, \psi \left(\frac{\cos\theta}{r^2}\right) \psi^* r^2 \sin\theta = \quad 5.\text{IV}$$

$$\left(\sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)}}\right)^2 (-1)^m \int_0^{+\infty} \left(e^{\frac{-r}{na_0}}(y)^l\, L_{n-l-1}^{2l+1}(y)\right)^2 dr \left(\sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}}\ \right)\int_0^\pi \int_0^{2\pi}\ Y_{l+1}^m\, Y_l^{-m}(\theta,\phi)\sin\theta\, d\theta\, d\phi\, + $$

$$l+ml-m2l-12l+10\pi02\pi \ Yl-1m \ Yl-m\theta,\phi\sin\theta d\theta \ d\phi$$

This is orthogonality:

$$\int_0^\pi \int_0^{2\pi} Y_l^m\, Y_{l'}^{m'*}\, d\Omega = \delta_{ll'}\, \delta_{mm'}\, ;\, d\Omega = \sin\theta\, d\theta\, d\phi \qquad\qquad 6.\text{IV}$$

$$if \begin{cases} l = l'\ and\ m = m' \to\ \delta_{ll'}\, \delta_{mm'} = 1 \\ l \neq l'\ and\ m \neq m' \to\ \delta_{ll'}\, \delta_{mm'} = 0 \end{cases}$$

$$\int_0^\pi \int_0^{2\pi}\ Y_{l+1}^m\, Y_l^{-m}(\theta,\phi)\sin\theta\, d\theta\, d\phi = 0 \qquad\qquad 7.\text{IV}$$

$$\int_0^\pi \int_0^{2\pi}\ Y_{l+1}^m\, Y_l^{-m}(\theta,\phi)\sin\theta\, d\theta\, d\phi = 0 \qquad\qquad 8.\text{IV}$$

$$\int_0^\infty dr \int_0^{2\pi} d\theta \int_0^\pi d\phi\, \psi \left(\frac{\cos\theta}{r^2}\right) \psi^* r^2 \sin\theta = 0\ \ in\ all \qquad 9.\text{IV}$$

IV-Results and Discussion:

We present in this section results of our study of the multipole potential (monopole, dipole and quadrupole potential). We have calculated the exactly the unperturbed potential (Coulomb potential) and the perturbed potential, the corrections were calculated using perturbation theory.

We have used the software Mathematica for the calculations.

IV-2-For The Monopole: this party identified as the Coloumb potential, it is given with the following relations

$$V_c = -\frac{Zq^2}{4\pi\epsilon_0 r}$$
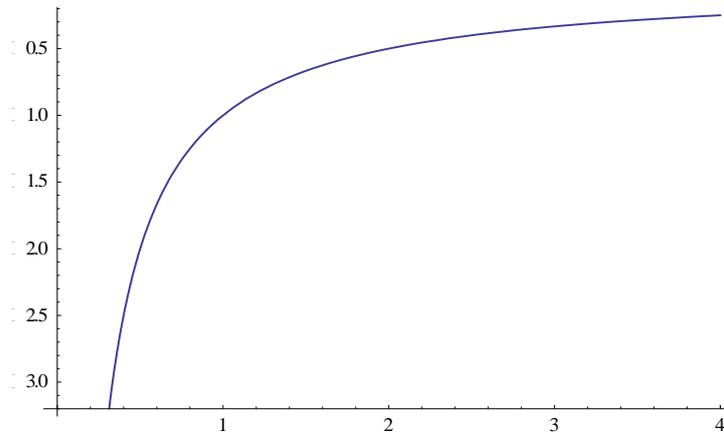
We plot the potential using Mathematica:

Figure IV-1: Monopole potential

And the energy is:

$$E_c = -\frac{Z^2 q^4 m_e}{2(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^2} = -2.180 \times 10^{-18} \frac{Z^2}{n^2} \frac{\text{Kilogram Meter}^2}{\text{Second}^2}$$

IV-3-For The Dipole: The dipole potential is

$$V_{dip} = -\frac{Zq^2}{4\pi\epsilon_0} \frac{\cos\theta}{r^2}$$

The first order correction for this term is always zero in all situations, so we go to second order correction.

We compute the corrections for different levels and we use these abbreviations:

$$E_n = -\frac{z^2 q^4 m_e}{2(4\pi\epsilon_0)^2 \hbar^2 n^2} \;; E_{n'} = -\frac{z^2 q^4 m_e}{2(4\pi\epsilon_0)^2 \hbar^2 n'^2} \;; a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e q^2} \;; Z = 1$$
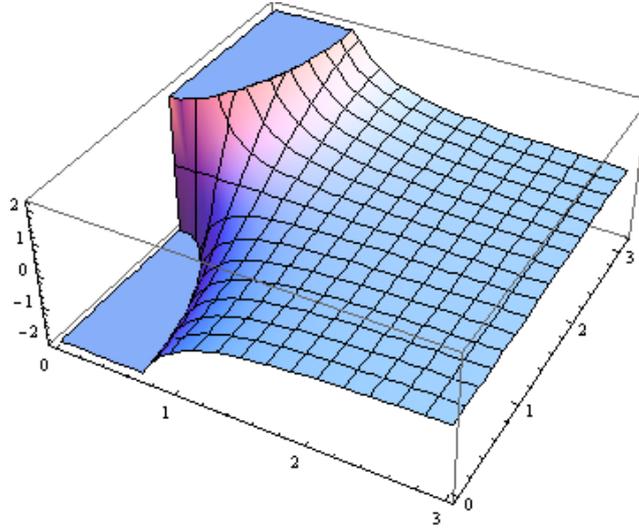
$D = qd$ where d the distance between the charges

Figure IV-2: Dipole Potential $V(r,\theta) = -\cos\theta/r^2$

For the first level (100): $n = 1; \; l = 0; \; m = 0$

$$\sum_{n'=2}^{5} \sum_{l'=0}^{n'-1} \frac{\left(\iiint_{000}^{\infty\pi2\pi} \sqrt{\left(\frac{2}{n'a_0}\right)^3 \frac{(n'-l'-1)!\,Z}{2n((n'+l')!)}} \, e^{\frac{-r}{n'a_0}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}(y) Y_{l'}^{m'}(\theta,\phi) \left(\frac{\cos\theta}{r^2}\right) \left(\frac{qD^2}{4\pi\epsilon_0}\right) r^2 \sin\theta \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!\,Z}{2n((n+l)!)}} \, e^{\frac{-r}{na_0}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}(y) Y_l^m(\theta,\phi) dr d\theta d\phi \right)^2}{(E_n - E_{n'})}$$

$$= -2.539 \times 10^{39} D^2 \frac{Kg}{C^2 S^2}$$

For the second level (200) we have the $n' = 2;\ l' = 0;\ m' = 0$; we get:

$$E_D = -1.848 \times 10^{37} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

We have also the level (210) with $n' = 2;\ l' = 1;\ m' = 0$:

$$E_D = -3.244 \times 10^{37} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

For the third level (300) $n' = 3;\ l' = 0;\ m' = 0$:

$$E_D = -1.898 \times 10^{36} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

For the level (310) $n' = 3;\ l' = 1;\ m' = 0$

$$E_D = -1.309 \times 10^{37} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

For the level (320) $n' = 3;\ l' = 2;\ m' = 0$

$$E_D = -2.443 \times 10^{37} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

IV-4-For Quadrupole: The quadrupole potential is given, as shown before, by the expression:

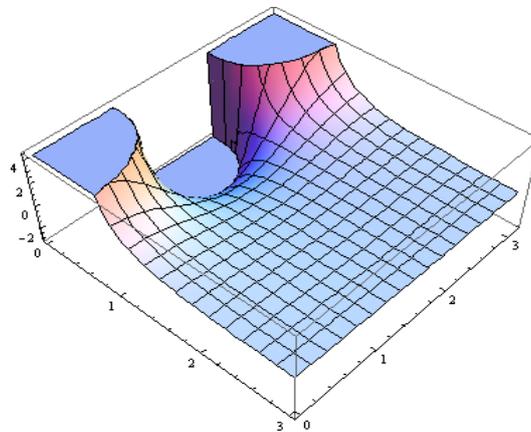$$V_{qua} = \frac{Zq^2}{4\pi\varepsilon_0} \frac{(3\cos^2\theta - 1)}{r^3}$$

Figure IV-3: Quadrupole potentiel $V(r,\theta) = (3\cos^2\theta - 1)/r^3$

The first order gives us value which are non-vanishing in general and that are in the same order as the second order of the dipole term, so we restrict ourselves to it.

For first level(100):$n = 1$; $l = 0$; $m = 0$, the correction vanishes:

$$\int\limits_{0}^{\infty}\int\limits_{0}^{\pi}\int\limits_{0}^{2\pi} \left(\sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!\,Z}{2n((n+l)!)}}\, e^{\frac{-r}{na_0}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}(y) \right)^2 Y_l^m(\theta,\phi) \left(\frac{3cos^2\theta-1}{r^3}\right) \left(\frac{qD^2}{4\pi\epsilon_0}\right)(-1)^m Y_l^{-m}(\theta,\phi) r^2 sin\theta\, dr\, d\theta\, d\phi$$

$= 0$

For second level(200): $n = 2$; $l = 0$; $m = 0$, The correction is also zero:

$$\int\limits_{0}^{\infty}\int\limits_{0}^{\pi}\int\limits_{0}^{2\pi} \left(\sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!\,Z}{2n((n+l)!)}}\, e^{\frac{-r}{na_0}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}(y) \right)^2 Y_l^m(\theta,\phi) \left(\frac{3cos^2\theta-1}{r^3}\right) \left(\frac{qD^2}{4\pi\epsilon_0}\right)(-1)^m Y_l^{-m}(\theta,\phi) r^2 sin\theta\, dr\, d\theta\, d\phi$$

$= 0$

For second level(210):$n = 2$; $l = 1$; $m = 0$;

$$E_D = 2.021 \times 10^{39} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

For third level(300): $n = 3$; $l = 0$; $m = 0$;

$$E_D = 0$$

For the level(310)$n = 3$; $l = 1$; $m = 0$;

$$E_D = 5.990 \times 10^{38} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

For the level(320)$n = 3$; $l = 2$; $m = 0$;

$$E_D = 8.557 \times 10^{37} D^2 \frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

We note that for the quadrupole term, the contribution is always zero when l = 0 for all levels.

IV-5-For The Total Energy:

The total energy given by the following relation $E_T = E_C + E_D + E_Q$ and it corresponds to the total potential:

$$V(r) = -\frac{Z\,q}{4\pi\epsilon_0}\left(q\frac{1}{r} + D\frac{\cos\theta}{r^2} + qD^2\left(\frac{3\cos^2\theta - 1}{2r^3}\right)\right)$$
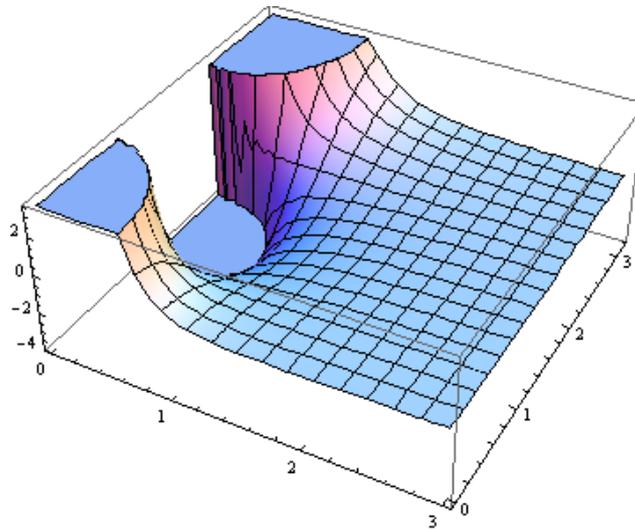
We plot it using Mathematica software:

Figure IV-4: Potential $V(r,\theta) = -1/r - \cos\theta/r^2 + (3\cos^2\theta - 1)/r^3$

$$E_T(100) = -2.179\times10^{-18}\frac{\text{Kg}}{\text{C}^2\text{S}^2} + 2.539\times10^{39}D^2\frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

$$E_T(200) = -2.179\times10^{-18}\frac{\text{Kg}}{\text{C}^2\text{S}^2} + 1.848\times10^{37}D^2\frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

$$E_T(210) = -2.179\times10^{-18}\frac{\text{Kg}}{\text{C}^2\text{S}^2} + 2.054\times10^{39}D^2\frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

$$E_T(300) = -2.179\times10^{-18}\frac{\text{Kg}}{\text{C}^2\text{S}^2} + 1.898\times10^{36}D^2\frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

$$E_T(310) = -2.179\times10^{-18}\frac{\text{Kg}}{\text{C}^2\text{S}^2} + 6.121\times10^{38}D^2\frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

$$E_T(320) = -2.179\times10^{-18}\frac{\text{Kg}}{\text{C}^2\text{S}^2} + 1.100\times10^{38}D^2\frac{\text{Kg}}{\text{C}^2\text{S}^2}$$

One can see an interesting phenomenon from the above relation and it is when the total energy goes to zero $E_T = E_C - E_D + E_Q = 0$, or when its bound state disappears.

We will compute the dipole potential value that makes this happens for all the precedent levels and then the characteristic dimension of the system from the relation $D = qd$ by taking the charge equal to the elementary one.

$$E_T(100) = 2.539 \times 10^{39} D^2 \frac{\text{Kg}}{\text{C}^2 \text{S}^2} - 2.179 \times 10^{-18} \frac{\text{Kg}}{\text{C}^2 \text{S}^2} = 0$$

$$\Rightarrow D = 2.929 \times 10^{-29} \text{CoulombMeter} \Rightarrow d = D/q = 3.455 \, a_0$$

$$E_T(200) = 1.848 \times 10^{37} D^2 \frac{\text{Kg}}{\text{C}^2 \text{S}^2} - 2.179 \times 10^{-18} \frac{\text{Kg}}{\text{C}^2 \text{S}^2} = 0$$

$$\Rightarrow D = 3.434 \times 10^{-28} \text{CoulombMeter} \Rightarrow d = D/q = 40.507 \, a_0$$

$$E_T(210) = 2.054 \times 10^{39} D^2 \frac{\text{Kg}}{\text{C}^2 \text{S}^2} - 2.179 \times 10^{-18} \frac{\text{Kg}}{\text{C}^2 \text{S}^2} = 0$$

$$\Rightarrow D = 3.257 \times 10^{-29} \text{CoulombMeter} \Rightarrow d = D/q = 3.842 \, a_0$$

$$E_T(300) = 1.898 \times 10^{36} D^2 \frac{\text{Kg}}{\text{C}^2 \text{S}^2} - 2.179 \times 10^{-18} \frac{\text{Kg}}{\text{C}^2 \text{S}^2} = 0$$

$$\Rightarrow D = 1.071 \times 10^{-27} \text{CoulombMeter} \Rightarrow d = D/q = 126.400 \, a_0$$

$$E_T(310) = 6.121 \times 10^{38} D^2 \frac{\text{Kg}}{\text{C}^2 \text{S}^2} - 2.179 \times 10^{-18} \frac{\text{Kg}}{\text{C}^2 \text{S}^2} = 0$$

$$\Rightarrow D = 5.967 \times 10^{-29} \text{CoulombMeter} \Rightarrow d = D/q = 7.038 \, a_0$$

$$E_T(320) = 1.100 \times 10^{38} D^2 \frac{\text{Kg}}{\text{C}^2 \text{S}^2} - 2.179 \times 10^{-18} \frac{\text{Kg}}{\text{C}^2 \text{S}^2} = 0$$

$$\Rightarrow D = 1.407 \times 10^{-28} \text{CoulombMeter} \Rightarrow d = D/q = 16.603 \, a_0$$

We summarize the results in this table and we use these consideration ($n' = 2 \rightarrow 5$ and $l' = 0 \rightarrow n' - 1$):

$$E_C = -\frac{Z^2 q^4 m_e}{2(4\pi\epsilon_0)^2 \hbar^2}\frac{1}{n^2} = -2.180 \times 10^{-18}\frac{Z^2}{n^2}\frac{\text{Kg}}{\text{C}^2\text{S}^2}; E_T = E_C - E_D + E_Q$$

n	l	m	E_D	E_Q	D	d
1	0	0	$-2.539\ 10^{39}D^2$	0	2.929×10^{-29}	$16.603\ a_0$
2	0	0	$-1.848\ 10^{37}D^2$	0	3.434×10^{-28}	$40.507\ a_0$
2	1	0	$-3.244\ 10^{37}D^2$	$2.012\ 10^{39}D^2$	3.257×10^{-29}	$3.842\ a_0$
3	0	0	$-1.898\ 10^{36}D^2$	0	1.071×10^{-27}	$126.400\ a_0$
3	1	0	$-1.309\ 10^{37}D^2$	$5.940\ 10^{38}D^2$	5.967×10^{-29}	$7.038\ a_0$
3	2	0	$-2.443\ 10^{37}D^2$	$8.557\ 10^{37}D^2$	1.407×10^{-28}	$16.603\ a_0$

We remark that the values of energies of dipole is negative and very close, except the energies for the level (100) and (300).For quadrupole the energies are positive and same magnitude of dipole energies, but are equal to zero when $l = 0$.

We have to compare between the shapes of the potential according to the parameter D and we use natural units for convenience where: $q_e = 1; \hbar = 1; m_e = 1$
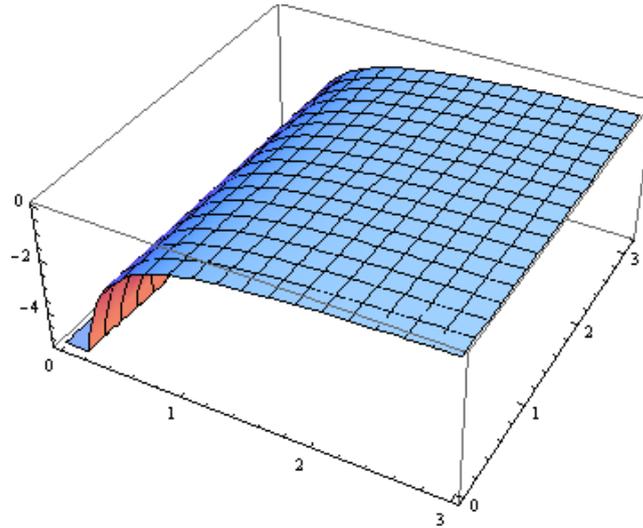

Figure IV-5: Potential $V(r, \theta) = -1/r - D\cos\theta/r^2 + D^2(3\cos^2\theta - 1)/r^3$ for $D = 0$

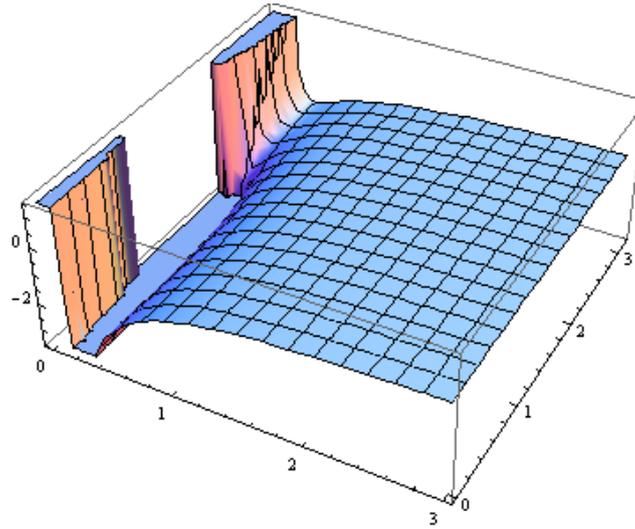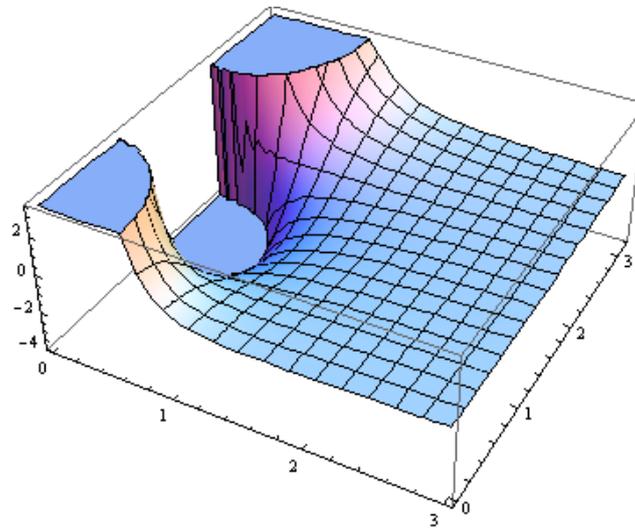Figure IV-6: Potential $V(r,\theta) = -1/r - D\cos\theta/r^2 + D^2(3\cos^2\theta - 1)/r^3$ for $D = 0.1$

Figure IV-7: Potential $V(r,\theta) = -1/r - D\cos\theta/r^2 + D^2(3\cos^2\theta - 1)/r^3$ for $D = 1$

We see that the well becomes less deep with increasing dipole moment. This makes the bound states disappearing one after the other; here the dipole and quadrupole terms play a role that is opposed to that of the Coulomb potential, which is binding the system because the well in infinite while it is finite when we add multipolar contributions.

Conclusion

Conclusion:

An important problem in quantum mechanics is to find the exact bound state solutions of the Schrödinger equation for certain potentials. In this work we calculate the spectrum of the potential of multipole for the highest resolution possible where we calculate approximations by the time-independent perturbation theory.

We write exact solutions for the coulomb potential considered as a monopole potential, and look to dipole and quadrupole as its corrections, we use multipole expansion so as to obtain the values of potential where we find:

$$V(r) = k \sum \frac{q}{ri} = k \int_{v'} \frac{q(r')}{r_i} dv' = k \frac{1}{r} \int_{v'} q(r') \left(1 + \frac{r'}{r} \cos\theta + \frac{r'^2}{r^2} \left(\frac{3cos^2\theta - 1}{2} \right) \right) dv''$$

Where V_{mono} is equal Coulomb potential and is proportional to r^{-1}; V_{dipole} is proportional to r^{-2} and $V_{quadrupole}$ is proportional to r^{-3}. We get the analytic solution ψ_{nlm} whichis solution of the Schrödinger equation for the Coulomb potential in three dimensions when it has three variables: angular component $\theta, \emptyset$ and radial r.

We use time-independent perturbation theory to get the solution with a high degree of accuracy. We study the energies for the first three levels. For the dipole, we demonstrate using orthogonality relation that energy it zero in all situation for first order correction. This is why we go to second order corrections where they are of magnitude $(10^{37}D^2 - 10^{39}D^2 Joules)$ $(dimD = CoulombMeter)$. For quadrupole term, the first order gives us value of same magnitudes for dipole in the second order, but when $l = 0$ the energies are zero.

There is a special case where the corrections equal the energies of the Coulomb potential and this gives us unstable or unbounded states because the total energy here is equal to zero. We put for these levels $E_T = 0$ to find the critical values of D and d (distance between the charges if we consider a dipole with two elementary charges) that makes this happens; we found that it is of the same magnitude of atomic dimensions.

By comparing between the shapes of the potential according to the parameter D, we remark that the bound states disappear one after the other when D increases. This is due to the fact

Conclusion

that the depth of the well decreases according to D which limits the number of bound states until theydisappear completely for $D \approx 1$.

We have used Mathematica software in all calculations and plots.

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Abstract:

In this work, we calculate the spectrum of multipole potential by perturbation theory (monopole, dipole and quadrupole potential); for monopole case the potential equal Coulomb potential. We apply time independent perturbation theory to find analytical solutions of the Schrödinger equation in three dimensions in order to write corrections of the first three levels. For the dipole we find the first order correction is zero so we go to second order correction which. For quadrupole energy we get values of the same magnitude of dipole energy except when $l = 0$ where the corrections of energy vanish.

Keywords: monopole, dipole and quadrupole potential, perturbation theory, Schrödinger equation in three dimensions

الملخص:

في هذا العمل قمنا بحساب طيف كمون متعددات الأقطاب (كمون أحادي.وثنائي ورباعي القطب). ونلك بتطبيق نظرية الاضطرابات المستقرة أي غير المتعلقة بالزمن على الحل التحليلي لمعادلة شرودنجر في ثلاث أبعاد من اجل المستويات الثلاث الأولى.من اجل ثنائيات الأقطاب نجد أن التصحيح من الدرجة الأولى معدوم فننتقل إلى التصحيح من الدرجة الثانية لنجده في حدود $10^{-37} D^2$. أما من اجل رباعيات الأقطاب فنجد أن قيم التصحيح من الدرجة الأولى هي من نفس رتبة ثنائيات الأقطاب عدا الحالات $l = 0$ أين تكون تصحيحات الطاقة معدومة.

كلمات مفتاحيه كمون أحادي.ثنائي ورباعي القطب.نظرية الاضطرابات المستقرة.معادلة شرودنجر في ثلاث أبعاد