An-Najah National University
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Confined hydrogen atom in a spherical cavity in N dimensions

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Dedication

الى روح أمي وأبي رحمهما الله

الى روح الشهداء الطاهرة

الى زوجي وأولادي

الى كل من علمني واضاء لي شعلة في طريق المعرفة

الى كل من يعلي من شأن الا نسانية

والى كل يد طاهره تبني في هذا الوطن

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إقـــرار

أنا الموقع أدناه مقدم الرسالة التي تحمل العنوان:

Confined hydrogen atom in a spherical cavity in N-dimensions

اقر بأن ما اشتملت عليه هذه الرسالة، انما هي نتاج جهدي الخاص، باستثناء ما تمت الاشارة اليه حيثما ورد، وأن هذه الرسالة ككل، او اي جزء منها لم يقدم من قبل لنيل اية درجة علمية او بحث علمي او بحثي لدى اية مؤسسة تعليمية او بحثية اخرى.

Declaration

The work provided in this thesis, unless otherwise referenced, is the researcher’s own work, and has not been submitted elsewhere for any other degree or qualification.

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Confined hydrogen atom in a spherical cavity in N- dimensions

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Abstract

In this research the Schrödinger equation for a confined hydrogen atom in a spherical cavity in N dimensional spatial space has been solved for N ≥ 3. The eigen functions as well as the eigen values have been determined.

We show that the Schrodinger equation here doesn't differ from that of the free hydrogen atom in N dimensions; therefore they have similar wave functions namely "$R_{\lambda l}(\rho) = A'\rho^{l}\, e^{(-\frac{\rho}{2})}\, {}_1F_1(l+\frac{N-1}{2} - \lambda;\, 2l + N - 1;\, \rho)$", while they differ in energy. A series solution of the Schrödinger equation is adopted here, and then, by applying the boundary conditions to the wave functions we found the energy eigen-values.

The dependence of the ground state energy eigen-values of a confined hydrogen atom for $l = 0$ for certain values of N, on the radius of the cavity S, has been examined. We found that they depend on the radius of the cavity S, we show that for a given N, if S increases the ground state

energies decreases until they approach a limiting value which approaches the energy eigen value of that N of the free hydrogen atom. While as S decreases, the ground state energy eigen values increases up until it approaches zero at a minimum value of S that is called the critical cage radius (S_c) at which the total energy of the confined hydrogen atom equals zero.

The critical values S_c are calculated for dimensions from (2-10), whose values are 0.722890, 1.835247, 3.296830, 5.088308, 7.200250, 9.617367, 12.35000, 15.36350, 18.68200 respectively, (all the values here are multiples of Bohr radius (a_0), where (a_0) = 0.529×10^{-10}meters.

It is shown here that S_c increases as N increases.

It is also shown that for a given S, the energy eigen-values for l=0 depend on the dimensionality of space N, that is, as N increases, the ground state energy eigen-values increase.

The dependence of bound states of a confined H-atom, for a given S, as a function of N is investigated, and it is found that it decreases as N increases, while if we choose a larger value of S, the number of the bound states increases for each value of N.

We found it interesting to compare the energy eigen-values of a confined hydrogen atom in a spherical cavity of a certain radius, with those energies of the corresponding energy eigen-states of a free hydrogen atom in the same dimension N. We found that the effect of confinement becomes more profound for larger N.

Finally, I considered the behavior of pressure on the cavity as the radius S is varied.

It has been shown that the pressure exerted on the atom increases as S decreases up to a certain maximum value which occurs at a radius value called $S_{P\ max}$, but then it decreases within a small range of S.

Chapter 1

Introduction

Chapter One

Introduction

One of the great developments in the human knowledge of the 20^{th} century is the Birth of a new theory in physics called quantum mechanics, which builds a new model of the atom that explains its structure and stability. Classical Mechanics couldn’t properly explain this, because there is nothing that will stop the electron from spiraling into the nucleus where no more stable atomic structure exists.

This model was mainly built on the simplicity of the hydrogen atom compared to other atoms. Solving the Schrödinger equation of the H-atom revealed its mystery, where many mathematical techniques were developed to solve the Schrödinger equation in three dimensions to get the energy eigen-values and the corresponding eigen-functions, and other relevant quantities.

We are three-dimensional observers, and this makes it easy for us to conceive the observed reality as 3-Dimensions. One can distinguish four types of directions, spatial dimensions, and time. But theories such as string theory predict that the space in general has in fact 10 dimensions, and universe, when measured along these additional dimensions is subatomic in size. In the 20^{th} century, the idea of the higher dimensional space was greatly investigated. Dimensions in both mathematics and physics refers to the parameters required to describe the position and relevant characteristics of any object within a conceptual space, where the dimensions of space are the total number of different parameters used for all possible objects considered in the model, in physics also dimensions are referred to degrees of freedom or the units of measurements. Many physical problems related to higher dimensional space have recently attracted the attention of many workers [1, 2, 3, 4], where it is widely believed that it plays an important role in the study of cosmology, group theory, many body problem, super symmetry, and the problem of unifying the four forces in nature together etc. Schrödinger equation, in the case of multi-dimensional problems, works very well as the starting point for general discussion in any multi-dimensional quantum problems.

Many studies were concerned in solving this equation in N-dimensions, to obtain the eigen-functions and the eigen-values, one of which showed a method that relates the solutions in 2- and 3-dimensional problems to higher dimensional cases for radial symmetric potentials [4], while some of the others used the series solution and other methods.

The radial Schrödinger equation of the H-atom in N-dimensions can be written as [1]:

$$\frac{\hbar^2}{2\mu}\,\nabla^2\psi(r) + \frac{Z\,e^2}{r}\,\psi(r) + E\,\psi(r) = 0 \qquad (1.1)$$

∇^2 is the Laplacian operator in N dimensions given by [1] :

$$\nabla^2 = r^{(1-N)}\frac{\partial}{\partial r}\left(r^{(N-1)}\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\Lambda^2 \qquad (1.2)$$

Λ^2 is a partial differential operator on the unit sphere S^{N-1}, which also is the square of the angular momentum operator.

The radial part of the Schrödinger equation can be written as:

$$\frac{d^2R}{d\rho^2}+\frac{N-1}{\rho}\frac{dR}{d\rho}-\frac{l(l+N-2)}{\rho^2}R+\left(\frac{\lambda}{\rho}-\frac{1}{4}\right)R=0 \qquad (1.3)$$

The eigen-functions and the energy eigen-values for the free hydrogen atom are in terms of CGS system of units [1],

$$R_{nl}(\rho) = A' \, e^{\left(-\frac{\rho}{2}\right)} \rho^{l} \, {}_1F_1 \left(l+\frac{N-1}{2} - \lambda;\ 2l + N - 1;\ \rho \right) \qquad (1.4)$$

$$E_n = \left(-\mu e^4/2\hbar^2\right) \frac{1}{\left(n+\frac{N-3}{2}\right)^2} \qquad (1.5)$$

where μ is the reduced mass of the H-atom.

Some other aspects of the H-atom were investigated in N-dimensional space [1]. For example the degeneracy of the energy level of the N-dimensional hydrogen atom, the radial distribution function, expectation values ($< 1/r >$), ($<1/r^2>$), and the varial theorem were considered, it was shown that the effect of the effective potential manifests itself in some of those aspects. Also, the quantization of angular momentum in N-dimensions was described [1]. Romeo studied the Wentzel-Kramers-Brilliouin (WKB) approximation in connection with hyper spherical quantum billiards [5]. Yaniz et al. investigated the position and momentum information entropies of N-dimensional systems [6]. The generalization of Fermi pseudo potentials to higher dimensions was illustrated by

Wo’dkiewic [7]. Random walks and moments of inertia in N dimensions have been considered by Bender et al. and Bender and Mead [8]. Fukutaka and Kashiwa considered the formulation of path integrals and their quantization on N-dimensional sphere [9].

The problem of a hydrogen atom confined in a sphere in 3-dimensions has quite a long history in quantum physics. The concept of a confined quantum system originated with a model suggested by Michels et al [10], who proposed the idea of simulating the effect of pressure on an atom by enclosing it in an impenetrable spherical box. During the last 70 years this model has proved to be quite useful in a number of fields of physics: the effect of pressure on energy levels, polarizability and ionization potentials of atoms and molecules [10], the cell model of the liquid state, semiconductor quantum dots, and several other areas. Its value in astrophysics has also been proved, e.g. in the mass-radius relation in the theory of white dwarfs, and in the determination of the rate of escape of stars from galactic and globular clusters. For a partial listing of references in this field, the reader may consult FrÖman *et al* who gave a list of 64 such publications up to 1984 [11].The confined hydrogen atom model has also been used for studies on the equilibrium properties of a partially ionized plasma and the thermodynamic properties of non ideal gases. It is also relevant for other situations where dense matter is involved, such as laser-imploded plasmas and the interior of giant planets [11].

Somerfield and Welker recognized the importance of the model of Michels *et al* for astrophysics and carried out a detailed investigation of the properties of a hydrogen atom enclosed in a spherical box. Such an atom is frequently referred to as a compressed atom or a confined atom. Subsequently, there have been several other investigations on the compressed hydrogen atom with various techniques [11, 12].

Sommerfeld and Welker [12], studied it in detail and calculated the critical radius in 3 dimensions for which the binding energy becomes zero, they obtained a series expansions for the $l = 0$ case, which are exact, being full generalization from the situation where the boundary conditions apply rigorously in the non-relativistic case, namely when a node coincides with the confining boundary and the analytic solution is known. They showed that, as the radius of the cavity decreases, the binding energy diminishes and there is a critical value of the sphere radius at which the binding energy becomes zero. That was called, the critical cage radius r_c. Sommerfeld and Welker found that for the 1s state $r_c = 1.835\times a_0$. For $r < r_c$ the energy of the system is positive.

Over the years there has been a steady flow of papers on this and other closely related problems. The model of the confined hydrogen atom has often been used as a test problem for various perturbation methods. Using their boundary perturbation method, Hull and Julius [13], obtained a formula which expresses the change of energy for the eigen-states in the confined system in terms of the corresponding wave functions in free space [14].

The boundary correction for a hydrogen atom in a spherical well using an approximation method which is linear in energy was studied by Djajaputra and Cooper [14]. This method is used very often in solid-state physics has been widely used in electronic structure calculations, under the name of the linear muffin-tin orbital (LMTO) method. In this method the wave functions of a Hamiltonian with energies which are in close vicinity of the energy of a known wave function are calculated [14, 15, 16].

Also, the calculation method to solve the Schrödinger's equation of a confined or half-confined hydrogen atom in three dimensions, i.e., a hydrogen atom with wave function which vanishes at a given closed or opened surface, was investigated by Yang and Wang [17].

More recently it has also been considered the hydrogen atom within spherical boxes with penetrable walls. The application of the Rayleigh-Schrödinger perturbation theory to the hydrogen atom in a spherical box has been discussed. In particular, the ground-state energy up to the fifth order in e^2has been obtained by Aguilera-Navarro, Koo and Zimerman [18].

But the effect of the boundary conditions on the energy eigen-values of the confined hydrogen atom in a spherical cavity in N-dimensions has not been investigated yet. Therefore, in this study, the Schrödinger equation for the confined hydrogen atom in a spherical cavity in N-dimensions has been solved, the eigen-values are determined; the influence of the radius of the cavity on the eigen-values is examined for different dimensions, making use of numerical calculations using the mathematica 5.0 software. The critical radius for each dimension is determined, and then the S_c-N relation is plotted. The number of bound states for given radii of the cavity has been examined in this study, where we chose $S= 22a_0$ and $S= 44a_0$.

Also, a comparison between the energy eigen-values in the case of the free and the confined H-atom as a function of N for a given radius of the cavity is pointed out.

Finally, the dependence of the pressure (exerted on the wall of the cavity) on the radius of the cavity for a given dimension of space, N, is examined

Most of the above aspects of the study were investigated for the ground state where l (the angular momentum quantum number) equals zero, and the energy of the confined H-atom is minimum.

This study is organized in four Chapters; Chapter One is an introduction to the subject that contains some of the previous work related to the study. Chapter Two contains 3 theoretical sections, where the Schrödinger equation of the confined hydrogen atom in the case of N=3 is solved in section one, in section two it has been solved in N dimensions, while in section 3, I derived a relation between the pressure, and N, and the radius of the cavity S. Through these sections some of the practical applications are mentioned.

Chapter three consists of four sections, I arranged the calculations in tables and graphs in section 1, through which the results about the energy eigen values are examined and discussed. In section two, a definition for the critical radius of the cavity is introduced, and its behavior as a function of space dimensionality is examined too. In section three, the number of bound states was determined for two specific values: S=$22a_0$, and $44a_0$, and thus the influence of space dimensionality and the radius of the cavity S on number of bound states is also examined. While in section four the pressure calculations are arranged in tables and represented by graphs.

Finally, in chapter four, conclusion of this study is given based on the discussion and results.

Chapter 2

Theoretical

Chapter Two

Theoretical Background

Solving the Schrödinger equation for a system in physics is one of the important things to do in quantum mechanics mainly in problems of multidimensional space. This process leads to determining the eigen-values, eigen-functions and eigen-energies of each state.

This chapter will include 4 sections; the first one contains a solution of the confined H-atom in 3-dimensions, which is similar to the solution of the Schrödinger equation of the free hydrogen atom in 3-dimensions.

In the second section, a solution of the Schrödinger equation in N dimensions is carried out.

In the third section a relation between the pressure exerted on the atom, the spatial dimensionality N, and the radius of the cavity S is worked out. As it was mentioned before, either for the free or the confined hydrogen atom, the wave functions will have the same form. But the free hydrogen atom will exhibit different energies other than those for the confined one.

2.1. Solution of the Schrödinger equation of a confined hydrogen atom in a spherical cavity in 3-dimensions.

Consider a H-atom in an impenetrable cavity, this condition simulates, practically, the physics of high pressure materials, and large classes of nanostructure systems such as quantum dots, and artificial atoms which are related to this problem. We mean by confined atoms that; those “atoms that experience external potentials which keep themselves in a region with length scales comparable to the atomic size” [19].

In this study I will first solve the Schrödinger equation for N=3, in order to simplify the understanding of the solution in N-dimensions.

Now, consider a hydrogen atom in an impenetrable spherical cavity. The potential of this system can be expressed as,

$$V(r) = \begin{cases} \dfrac{-ze^2}{4\pi\varepsilon_0 r} \quad , & 0 \le r \le S \\ \infty \quad , & \text{elsewhere} \end{cases} \tag{2.1}$$

Where S is the radius of the cavity, and Z=1 for the hydrogen atom. To examine the effect of the cavity on the energy eigen-values, one has to solve the Schrödinger equation to obtain a relation between the energy eigen values and the radius of the cavity.

After making separation of variables for the Schrödinger equation in spherical coordinates, the radial equation reads,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)R - \frac{l(l+1)}{r^2}R = 0 \tag{2.2}$$

For simplicity, I write $u(r) = r\,R(r)$ *to give,*

$$\frac{d^2u}{dr^2} + \frac{2\mu}{\hbar^2}\left[\frac{e^2}{4\pi\varepsilon_0 r} - \frac{l(l+1)\hbar^2}{2\mu r^2} + E\right]u(r) = 0 \tag{2.3}$$

μ is the reduced mass of the H-atom, *l* is the angular momentum quantum number.

Now it is convenient to define the dimensionless variables:

$$\rho = \sqrt{\frac{8\mu(-E)}{\hbar^2}}\,r \qquad \text{and} \qquad \lambda = \sqrt{\frac{\mu e^4}{2(4\pi\varepsilon_0)^2\hbar^2(-E)}} \tag{2.4}$$

One can easily notice that equation (2.3) is similar to that for the free hydrogen atom in three dimensions; therefore both will have the same form of the solution.

With these substitutions, equation (2.3) becomes,

$$\frac{d^2u}{d\rho^2} - \frac{l(l+1)u}{\rho^2} + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right) u\,(\rho) = 0 \tag{2.5}$$

The asymptotic behavior is obtained by solving equation (2.5) when $\rho \to \infty$, i.e. solving

$$\frac{d^2u}{d\rho^2} - \frac{1}{4}u = 0 \tag{2.6}$$

Then, $u\,(\rho) = Ae^{-\frac{\rho}{2}} + Be^{\frac{\rho}{2}}$, but $e^{\frac{\rho}{2}}$ is infinite for large ρ, then B is set to zero.

Thus $$\mathrm{u}\,(\rho) = A\,e^{\frac{-\rho}{2}} \tag{2.7}$$

In the vicinity of the origin ($\rho \to 0$), in this case, the $\frac{l(l+1)}{\rho^2}$ dominates over the other terms in equation (2.5), and thus it becomes

$$\frac{\mathrm{d}^2\mathrm{u}}{\mathrm{d}\rho^2} = \frac{l(l+1)u}{\rho^2} \tag{2.8}$$

The general solution of eq. (2.8) is

$$u(\rho) = D\rho^{-l} + C\rho^{(l+1)} \tag{2.9}$$

The term ρ^{-l} diverges, and hence D must be set to zero.

Thus $u(\rho) = \mathrm{C}\ \rho^{(l+1)}$

Therefore the solution of eqn. (2.5) is assumed to take the form,

$$u\ (\rho) \propto \rho^{l+1} e^{-\frac{\rho}{2}}\ v(\rho) \tag{2.10}$$

After differentiation and Substitution in equation (2.5), the radial equation in terms of $v\ (\rho)$ becomes:

$$\frac{d^2 v}{d\rho^2} + \left[\frac{2(l+1)}{\rho} - 1\right]\frac{dv}{d\rho} + \left[\frac{\lambda - (l+1)}{\rho}\right] v = 0 \tag{2.11}$$

A series expansion of $v\ (\rho)$,

$$v\ (\rho) = \sum_0^\infty a_j\, \rho^j \tag{2.12}$$

gives us the recursion relation

$$a_{j+1} = \left[\frac{(j+l+1) - \lambda}{(j+1)(j+2l+2)}\right] a_j \tag{2.13}$$

We want to determine the coefficients $(a_0, a_1, a_2 \ldots)$

For the function $v\ (\rho)$ to be terminated for very large values of j, the series must be terminated, i.e.

$$\lim_{j \to \infty} \frac{a_j + 1}{a_j} = \frac{j}{j^2} = \frac{1}{j}$$

This is the same ratio of coefficients as those of the expansion of e^{ρ}.

This leads to that $v(\rho) \propto e^{\rho}$. Thus $u(\rho) \propto \rho^{l+1} e^{\frac{\rho}{2}}$ [This shows that u (ρ) must terminate, but the series blows up as $\rho \longrightarrow \infty$].

Therefore, let j_{max} indicates the term of termination, then $a_{j\,max} + 1 = 0$, or the last term of the series is, $a_{j\,max}$. From equation (2.13) we have

$$j_{max}+l+1-\lambda = 0 \quad \text{, or} \qquad \lambda = j_{max}+l+1 \qquad (2.14)$$

where λ here corresponds to n (the principal quantum number in the case of the free H-atom).

But λ determines E, where ($\lambda = \sqrt{\frac{\mu e^4}{2(4\pi\varepsilon_0)^2\hbar^2(-E)}}$).

With, $\rho = qr$ and, $q = \sqrt{\frac{8\mu(-E)}{\hbar^2}}$ then

$$E = \frac{-\hbar^2 q^2}{8\mu} = \frac{-\mu\, e^4}{2(4\pi\varepsilon_0)^2\hbar^2\lambda^2}\text{, or}$$

$$E = \frac{E_0}{\lambda^2} \qquad (2.15)$$

where $E_0 = \frac{-\mu e^4}{2(4\pi\varepsilon_0)^2\hbar^2} = -13.6\, eV$ is the ground state energy of the free hydrogen atom.

Keeping in mind that $a_0 = \frac{(4\pi\varepsilon_0)\hbar^2}{\mu e^2} = 0.529\, x\, 10^{-10}\, m$, is the Bohr radius, we also have,

$$\frac{-\hbar^2}{2\mu} = E_0\, a_0^2 \qquad (2.16)$$

The previous equation can be used to compute the energies in this problem, but yet we need to find the eigen-functions. Going back to equation (2.11), and comparing it with the associated Lagurre differential equation

$$\{\frac{d^2}{d\rho^2} + [\frac{P+1}{\rho} - 1]\frac{d}{d\rho} + [\frac{(q-P)}{\rho}]\}\, L_q^P(\rho) = 0 \qquad (2.17)$$

shows,

$$P = 2l+1 \qquad and \qquad q = \lambda + l \qquad (2.18)$$

Thus equations (2.19) give the radial solution, which is

$$R_{\lambda\, l}(\rho) = A\, \rho^{l+1}\, e^{-\frac{\rho}{2}}\, L^p_{q-p}(\rho)$$

$$R_{\lambda l}(\rho) = A\, \rho^{l+1}\, e^{-\frac{\rho}{2}}\, L^{2l+1}_{\lambda-l-1}(\rho) \qquad (2.19)$$

Where A is the normalization constant whose value is determined from the requirement,

$$A^2 \int_0^\infty [e^{-\frac{\rho}{2}} \rho^{l+1} L^{2l+1}_{\lambda-l-1}(\rho)]^2 r^2 dr = 1 \qquad (2.20)$$

and after making use of,

$$\int_0^\infty e^x\, x^{k+1} L_n^k(x)\, L_n^k(x)\, dx = \frac{(n+k)!}{n!}(2n+k+1)$$

We will get:

$$A = \sqrt{(\frac{2}{\lambda a_0})^3 \frac{(\lambda-l-1)!}{2\lambda[(\lambda+l)!]}} \qquad (2.21)$$

The radial solution can also be expressed in terms of the confluent hyper geometric polynomials as (see appendix B)

$$R_{\lambda\, l}(\rho) = \qquad (2.22)$$

$$\sqrt{\left(\frac{2}{\lambda a}\right)^{3}\frac{(\lambda-l-1)!}{2\lambda[(\lambda+l)!]}}\; e^{\left(-\frac{\rho}{2}\right)}\,\rho^{l+1}\,\frac{(\lambda+l)!}{(\lambda-l-1)!(2l+1)}\,{}_1F_1\,(1+l-\lambda;\,2l+2;\rho)$$

The boundary conditions at r = S, where S is the radius of the cavity can be written as,

$$R_{\lambda l}\,(\rho)\,|_{r=S}= R_{\lambda l}\,(qS) = \text{Zero}, \qquad (2.23)$$

Because the potential at the walls of the cavity is ∞, and the wave function diminishes there.

Unfortunately, those zeros (namely the roots of the confluent hyper geometric polynomials) are not nice numbers (not integers), as in the case of the free hydrogen atom in 3-dimensions which gives the principal quantum numbers. The roots of the wave function are determined using mathematica software, version 5.0.

The zeros of $R_{\lambda\, l}(\rho)$ are those of the confluent hyper geometric polynomials, and they are calculated using mathematica software, version 5.0.

Note that a subscript $\lambda\, l$ is given to $R(\rho)$ because it depends on both of them, and the information that it holds depend on the value of λ and l, while λ itself depends on the radius of the cavity S as follows.

It can easily show that

$$\lambda = \frac{2S}{\rho a_0} \qquad (2.\ 24)$$

Since $q = \frac{2}{a_0\,\lambda}$ and, $\rho = \frac{2}{a_0\,\lambda}\ r$

ρ indicates the roots, and thus at r = S, we have,

$$\rho = \frac{2S}{a_0\,\lambda} \qquad (2.25)$$

This gives eqn. (2.24).

Figure (1) below shows a graph of one of those wave functions of the confined H-atom for *l* =0, space dimensionality N=3, S=6a_0.

In such graphs, there might be more than one zero (or root), the last intercept is the one coincides with the surface of the walls of the cavity, and hence it indicates the ground state energy for each S, as will be shown later.

Let x_n be the n^{th}root of the confluent hyper geometric polynomials

$${}_1F_1\,(1 - \frac{2S}{\rho a_0};\, 2;\ \rho).$$

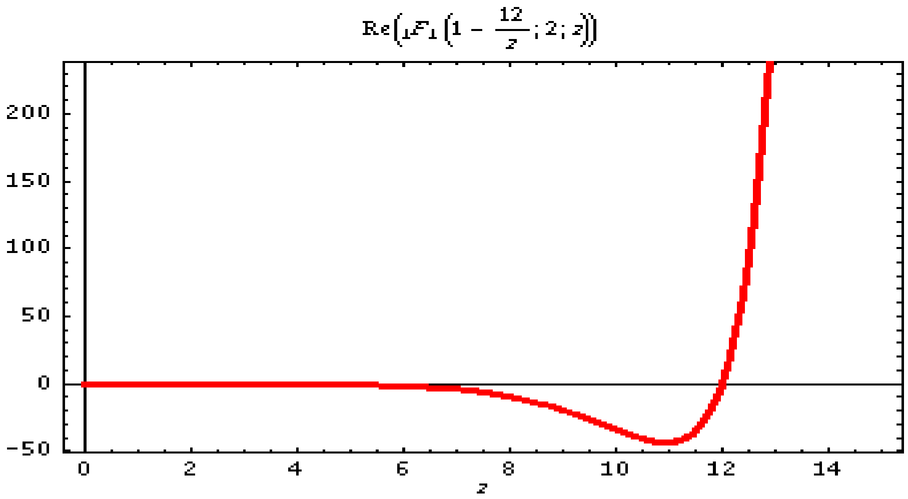

Fig. (1): Mathematica plot which shows one of the zeros (horizontal-axis intercepts) of the function${}_1F_1$ (1-12/z; 2; z).

From equation (2.25) we can easily relate the zeros and the radius of the cavity with λ to get the energy eigen values of this problem.

$$x_n = \frac{2}{a_0\,\lambda}\,S \tag{2.26}$$

Then $\lambda = \dfrac{2S}{a_0 x_n}$ (2.27)

From equation (2.27) we can compute the values of λ which corresponds to different values of S. Then eqn. (2.15) yeilds, $E_n = \dfrac{E_0}{\lambda^2}$ in eV units.

Also by using $\rho = \sqrt{\dfrac{8\mu(-E)}{\hbar^2}}\,r$, we can easily show that

$$E_n = -\frac{\hbar^2}{8\mu}\frac{x_n{}^2}{S^2} = -\frac{\hbar^2}{2\mu}\frac{x_n{}^2}{4S^2} \tag{2.28}$$

and with $E_0 = \dfrac{\hbar^2}{2\mu a_0{}^2}$ we can write E_n in the form

$$E_n = \frac{x_n{}^2\,a_0{}^2}{4S^2}\,E_0 \tag{2.29}$$

The energy eigen-values will be calculated numerically for the N-dimensional case in the next section.

2.2. Solution of the Schrödinger equation for the confined hydrogen atom in N-dimensional space.

"The problem of the confined atoms, would be equivalent to the problem of many-body Schrödinger equation with given boundary conditions" [19]. For the hydrogen atom enclosed within an impenetrable spherical cavity in N-dimensions, the potential is:

$$V(r) = \begin{cases} \frac{-ze^2}{4\pi\varepsilon_0 r} , & 0 \le r \le S \\ \\ \infty , & \text{elsewhere} \end{cases} \qquad (2.31)$$

The radial part of the Schrödinger equation in N-dimensions for the confined hydrogen atom in N-dimensions is [1]:

$$r^{1-N} \frac{d}{dr}\left(r^{(N-1)} \frac{dR}{dr}\right) - \frac{\beta}{r^2} R + \frac{2\mu}{\hbar^2} (\frac{Ze^2}{4\pi\varepsilon_0 r} + E) R = 0 \qquad (2.32)$$

Where $\beta = l(l+N-2)$, and $l = 0, 1, 2$ ….is the angular momentum quantum number for the H-atom.

Now we introduce $\rho = \frac{\sqrt{8\mu(-E)}}{\hbar} r$ or $\rho = qr$, (2.33)

and $\lambda = (\frac{z^2 e^4 \mu}{2\hbar^2 (4\pi\varepsilon_0)^2 (-E)})^{\frac{1}{2}}$ (2.34)

and using $\frac{dR}{dr} = \frac{dR}{d\rho} \frac{d\rho}{dr} = q \frac{dR}{d\rho}$ and $\frac{d^2R}{dr^2} = q^2 \frac{d^2R}{d\rho^2}$,

The radial part of the Schrödinger equation in N-dimensions becomes:

$$\frac{d^2R}{d\rho^2}+(\frac{N-1}{\rho}\frac{dR}{d\rho})-\frac{l(l+N-2)}{\rho^2}R+\left(\frac{\lambda}{\rho}-\frac{1}{4}\right)R=0 \qquad (2.35)$$

Same as before, notice that equation (2.35) is similar to that one for a free H- atom, but in N-dimensions. Accordingly, it has wave functions similar to those of the free H- atom in N-dimensions.

As was done in the previous section, the asymptotic behavior is obtained by solving equation (2.35) when $\rho \rightarrow \infty$, i.e. solving

$$\frac{d^2R}{d\rho^2}-\frac{1}{4}R=0 \qquad \longrightarrow \qquad R\,(\rho)\ \propto\ e^{-\frac{\rho}{2}} \qquad (2.36)$$

In the vicinity of the origin $\rho \longrightarrow 0$, $\frac{d^2R}{d\rho^2}-\frac{l(l+N-2)}{\rho^2}R=0$ (2.37)

We are seeking a solution of Equation (2.37) of the form,

$$R\,(\rho)=\rho^l e^{-\frac{\rho}{2}}\,\nu(\rho) \qquad (2.38)$$

Substitution of eqn. (2.38) in equation (2.35) gives:

$$\frac{d^2\nu}{d\rho^2}+\left[\frac{2l+N-1}{\rho}-1\right]\frac{d\nu}{d\rho}+\left[\frac{\lambda-l-\frac{N-1}{2}}{\rho}\right]\nu=0 \qquad (2.39)$$

A series expansion of $\nu\,(\rho)$ can be write as,

$$\nu(\rho)=\sum_{j=0}a_j\,\rho^j \qquad (2.40)$$

The substitution of eqn. (2.40) in equation (2.39), gives,

$$\sum_{j=0} j(j-1)a_j\,\rho^{j-2} + \left[\frac{2l+N-1}{\rho}\right]\sum_{j=0} j\,a_j\rho^{j-1} -$$

$$\sum_{j=0} ja_j\rho^{j-1} + \frac{\lambda - l - \frac{N-1}{2}}{\rho}\sum_{j=0} a_j\rho^{j} = 0 \qquad (2.41)$$

$$\sum_{j=0} j(j-1)a_j\,\rho^{j-2} + [2l+N-1]\sum_{j=0} ja_{j\rho^{j-2}} -$$

$$\sum_{j=0} ja_{j\rho^{j-1}} + \left(\lambda - l - \frac{N-1}{2}\right)\sum_{j=0} a_j\rho^{j-1} = 0 \qquad (2.42)$$

In the first and the second term, let j be j+1 to get,

$$\sum_{j=-1} j(j+1)a_{j+1}\,\rho^{j-1} + [2l+N-1]\sum_{j=-1}(j+1)\,a_{j+1}\rho^{j-1}$$

$$-\sum_{j=0} ja_j\rho^{j-1} + \left(\lambda - l - \frac{N-1}{2}\right)\sum_{j=0} a_j\rho^{j-1} = 0 \qquad (2.43)$$

Substitute for j = -1 into equation (2.43) to get

$$\sum_{j=0} j(j+1)a_{j+1}\,\rho^{j-1} + [2l+N-1]\sum_{0}(j+1)\,a_{j+1}\rho^{j-1} -$$

$$\sum_{j=0} ja_j\rho^{j-1} + \left(\lambda - l - \frac{N-1}{2}\right)\sum_{j=0} a_j\rho^{j-1} = 0 \qquad (2.44)$$

Equating the coefficients of equal powers of (ρ), we get

$$\{j(j+1)+[2l+N-1](j+1)\}a_{j+1} = \left[j-\left(\lambda - l - \frac{N-1}{2}\right)\right]a_j \qquad (2.45)$$

Finally we get the recursion relation in the form of

$$a_{j+1} = \frac{j-\left(\lambda - l - \frac{N-1}{2}\right)}{j(j+1)+(2l+N-1)(j+1)}$$

Or, $$a_{j+1} = \frac{j+l+\frac{N-1}{2}-\lambda}{(j+1)(j+2l+N-1)}a_j$$

Taking into consideration that the series must terminate at $n_r = j_{max}$, then

$$J_{max} + l + \frac{N-1}{2} - \lambda = 0 \qquad (2.46)$$

Define n_r the radial quantum number, we can write

$$n_r + l + \frac{N-1}{2} = \lambda, \qquad (2.47)$$

Let ń to be the principal quantum number in N-dimensions.

then, $\acute{n} = \lambda = n_r + l + \frac{N-1}{2}$ (2.48)

But λ determines E, where ($\lambda = \sqrt{\frac{\mu e^4}{2(4\pi\varepsilon_0)^2\hbar^2(-E)}}$).

With, $\rho = qr$ and, $q = \sqrt{\frac{8\mu(-E)}{\hbar^2}}$ then

$$E = \frac{-\hbar^2 q^2}{8\mu} = \frac{-\mu e^4}{2(4\pi\varepsilon_0)^2\hbar^2\lambda^2},$$

$$E = \frac{E_0}{\lambda^2} \qquad (2.49)$$

Remember that $a_0 = \frac{(4\pi\varepsilon_0)\hbar^2}{\mu e^2} = 0.529\ x\ 10^{-10}\ m$

$E_0 = \frac{-\mu e^4}{2(4\pi\varepsilon_0)^2\hbar^2} = -13.4\ eV$ which is the ground state energy of the free hydrogen atom.

And $\frac{-\hbar^2}{2\mu} = E_0\, a_0^2$ (2.50)

What we have done here is getting a relation to compute the energies in this problem eqn. (2.49). By looking at equation (2.48) one can easily notice the dependence of the energy on the space dimensionality N through λ. For more visualizing we need to indicate the eigen-functions from which we can find the points where we can calculate the energy eigen-values.

Comparing equation (2.39) with the associated Lagurre differential equation

$$\left(\frac{d^2}{d\rho^2} + \left[\frac{P+1}{\rho} - 1\right]\frac{d}{d\rho} + \left[\frac{(d-p)}{\rho}\right]\right)L^{p}_{d-p}(\rho) = 0 \qquad (2.51)$$

We get $p = 2l + N - 2 \quad , \quad d - p = \lambda - l - \frac{N-1}{2}$ (2.52)

Now equation (2.39) has a solution of the form,

$$\mathrm{R}_{\lambda \mathrm{L}}(\rho) = A\,\rho^{l}\,e^{\left(-\frac{\rho}{2}\right)}\,L^{2l+N-2}_{\lambda - l - \frac{N-1}{2}}(\rho) \qquad (2.53)$$

Or,

$$R_{\lambda l}(\rho) = A'\rho^{l}\,e^{\left(-\frac{\rho}{2}\right)}\,{}_1F_1\left(l + \frac{N-1}{2} - \lambda;\ 2l + N - 1;\ \rho\right) \qquad (2.54)$$

Where $A' = A\,\dfrac{\left(\lambda + l + \frac{N-3}{2}\right)!}{\left(\lambda - l - \frac{N-1}{2}\right)!\left(2l + N - 2\right)!}$ (see Appendix B)

We need to apply the boundary conditions at r = S, where S is the radius of the cavity. Since the potential at the walls of the cavity is ∞, and the wave function diminishes there, thus, we can write

$$R_{\lambda l}(\rho)\big|_{r=S} = R_{\lambda l}(qS) = \text{Zero}, \qquad (2.55)$$

Here we need to indicate the values of ρ where the wave function $R_{\lambda l}$ vanishes; therefore one has to plot graphs. In this research, mathematica software, version 5.0, has been used for this purpose.

Unfortunately, those zeros (roots of the confluent hyper geometric polynomials) are not nice numbers (not integers).

The zeros here are those of the confluent hyper geometric polynomials in $R_{\lambda\, l}(\rho)$, namely ${}_1F_1$ $(\frac{N-1}{2}$ - $\frac{2S}{\rho a_0}; N-1;\ \rho)$ which joins all the variables of this problem (N, S, ρ) together.

One can easily show that

$$\lambda = \frac{2S}{\rho a_0} \tag{2.56}$$

In such graphs, there might be more than one zero (or root), Let x_n be the n^{th} root, the last intercept is the one coincides with the surface of the walls of the cavity, and hence it indicates the ground state energy for each S,

Since $q = \frac{2}{a_0\, \lambda}$ and, $\rho = \frac{2}{a_0\, \lambda}\, r$

ρ indicates the roots, and r indicates S,

$$\rho = \frac{2}{a_0\, \lambda}\, S \tag{2.57}$$

From equation (2.57) we can easily relate the zeros and the radius of the cavity with λ to get the energy eigen-values of this problem.

$$x_n = \frac{2}{a_0\, \lambda}\, S \tag{2.58}$$

Then $\lambda = \frac{2S}{a_0 x_n}$ (2.59)

For any given S and N we can plot the ${}_1F_1\,(\frac{N-1}{2} - \frac{2S}{\rho a_0}; N-1;\ \rho)$ and get the zeros, then using equation (2.59) we can compute the values of λ which correspond to these values of S and N. Then compute E from $E_n = \frac{E_0}{\lambda^2}$ in eV units.

Also we have, $E_n = -\frac{\hbar^2}{8\mu}\frac{{x_n}^2}{S^2} = -\frac{\hbar^2}{2\mu}\frac{{x_n}^2}{4S^2}$ (2.60)

With $E_0 = \frac{-\hbar^2}{2\mu {a_0}^2}$

Finally we can write ,

$$E_n = \frac{{x_n}^2\,{a_0}^2}{4S^2}\,E_0 \qquad (2.61)$$

Which is another formula to compute the energy eigen-values.

Equation (2.61) predicts that the ground state energy belongs to the largest x_n which corresponds to the largest value of n, and smallest λ because E_0 is a negative value, see eqns. (2.59), and (2.61).

This implies that either we have to use eqn. (2.49), or (2.61) to calculate the energy for a given state, we have to suggest different values of the cavity radius which practically means trapping the hydrogen atom (or other types of atoms) within atomic scale confinement of other substance (doping process).

For later comparison between the energies of the confined hydrogen atom and the free one, we write the energy of the free hydrogen atom in N dimensions [1], namely

$$E_{nfree} = \frac{E_0}{(n+\frac{N-3}{2})^2} \qquad (2.62)$$

In the above equation, n refers to the principal quantum number for the free hydrogen atom.

For example considering the values of $N=4$, $l=0$, $S= 9a_0$ we locate the zeros of the wave function by mathematica plots, just plot

${}_1F_1$ (1.5 – 18/ ρ; 3; ρ) to determine the zeros in order to find the energy eigen values from eqn. (2.60), or (2.61).

A mathematica graph for illustrative purposes is shown in figure (2), but one should be careful in locating the zeros, because for a given period of ρ it might not show all of the zeros (i.e. In the graph below there is another zero at $Z \cong 1.78$ which is not shown).

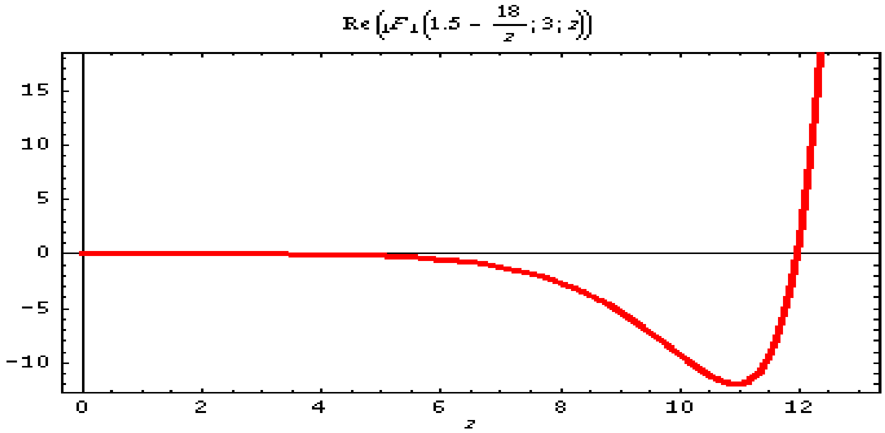

Fig.(2): Mathematica plot which shows one of the zeros (horizontal-axis intercepts) of the function ${}_1F_1$ (1.5 – 18/ ρ; 3; ρ).

In this study, the calculated energies correspond to *l*=0. In another words, the 1s state. Here it is worth mentioning that for each value of *l*, when substituted in the hyper geometric part of the wave function, there are different roots, one or many, but the ground state of the problem corresponds to the largest x_n for *l=0.*

The radial wave function $R_{\lambda l}(\rho) = A\,\rho^{l}\, e^{(-\frac{\rho}{2})}\, L^{2l+N-2}_{\lambda-l-\frac{N-1}{2}}(\rho)$ must be normalized. Now to calculate A, the normalization constant, we know that the total probability to find the particle within the cavity is 1,

Thus;

$$|A^2| \int_0^{\infty} e^{(-\rho)}\ \rho^{2l} |\, L^{2l+N-2}_{\lambda-l-\frac{N-1}{2}}(\rho)\,|^2\, r^{N-1} dr = 1 \tag{2.63}$$

From eqn. (2.57) we get,

$$dr = \frac{\lambda a_0}{2} d\rho \tag{2.64}$$

$$r^{N-1} = (\frac{\lambda a_0}{2})^{N-1} \rho^{N-1} \tag{2.65}$$

Making use of $\int_0^{\infty} e^{-x}\, x^k L_n^k(x) L_m^k(x) dx = \frac{(n+k)!}{n!}\delta_{mn}$ (2.66)

and $\int_0^{\infty} e^{-x}\, x^{k+1} L_n^k(x) L_n^k(x) dx = \frac{(n+k)!}{n!}(2n+k+1)$ (2.67)

gives,

$$|A|^2 \int_0^{\infty} e^{(-\rho)}\ \rho^{2l} \left| L^{2l+N-2}_{\lambda-l-\frac{N-1}{2}}(\rho) \right|^2 (\frac{\lambda a_0}{2})^N \rho^{N-1}\, d\rho = 1 \tag{2.68}$$

$$= |A|^2 \int_0^\infty e^{(-\rho)} \left| L^{2l+N-2}_{\lambda - l - \frac{N-1}{2}}(\rho) \right|^2 (\frac{\lambda a_0}{2})^N \rho^{2l+N-1}\, d\rho \qquad (2.69)$$

$$= |A|^2 (\frac{\lambda a_0}{2})^N \int_0^\infty e^{(-\rho)} \left| L^{2l+N-2}_{\lambda - l - \frac{N-1}{2}}(\rho) \right|^2 \rho^{2l+N-1}\, d\rho \qquad (2.70)$$

$$= |A|^2 \,(\frac{\lambda a_0}{2})^N \frac{\left(\lambda - l + 2l + N - 2 - \frac{N-1}{2}\right)!}{(\lambda - l - \frac{N-1}{2})!} [2\lambda - 2l - N + 1 + 2l + N - 2 + 1]$$

(2.71)

Therefore,

$$|A|^2 = (\frac{2}{\lambda a_0})^N \frac{(\lambda - l - \frac{N-1}{2})!}{\left(\lambda + l + \frac{N-3}{2}\right)!(2\lambda)} \qquad (2.72)$$

This yields the 3- dimensional case, namely

$$A = [(\frac{2}{\lambda a_0})^3 \frac{(\lambda - l - 1)!}{(\lambda + l)!(2\lambda)}]^{\frac{1}{2}} \qquad (2.73)$$

2.3. Expressing the relation between the pressure exerted on the H-atom and the radius of the cavity:

“The recent development in nanotechnology has generated intensive research activity in modeling spacially confined quantum systems, when an atom is or a molecule is trapped inside any kind of microscopic cavity, or is placed in a high pressure environment, it experiences special confinement that affects its physical and chemical properties.”[20]

An atomic system under very high pressure simulates a confined system. The interaction of the atom with the surroundings was suggested to be replaced by a uniform pressure on a sphere within which the atom is considered to be enclosed. [20]

Knowing the dependence of the ground state energy on the radius of the cavity, equation (2.61), allows us to calculate the pressure needed to ‘compress’ a hydrogen atom in the ground state in a certain size of the cavity.

It is known that $P = \frac{-dE}{dV}$ (2.74)

Substitute for the value of E_n from equation (2.61) to get

$$P = \frac{-d}{dV}\left(\frac{X_n{}^2 a_0{}^2}{4S^2}\right)E_0 \qquad (2.75)$$

But $dV = A\,dS$, then

$$P = \frac{-d}{A\,dS}E_n = \frac{-1}{A}\frac{dE_n}{dS} \qquad (2.76)$$

Now, in N dimensions the area of the hyper sphere is,

$$A_N(S) = \frac{2(\pi)^{N/2}}{\left(\frac{N}{2}-1\right)!} S^{N-1} \qquad (2.77)$$

and $$P_N = \frac{-1}{\frac{2(\pi)^{N/2}}{\left(\frac{N}{2}-1\right)!} S^{N-1}} \frac{dE_n}{dS} \qquad (2.78)$$

$$= \frac{-\left(\frac{N}{2}-1\right)!}{2(\pi)^{N/2}\, S^{N-1}} \frac{2{x_n}^2{a_0}^2}{4S} \frac{-1}{S^2} E_0 \qquad (2.79)$$

$$= \frac{\left(\frac{N}{2}-1\right)!}{2(\pi)^{N/2}\, S^{N-1}} \frac{2{x_n}^2{a_0}^2}{4S} \frac{1}{S^2} E_0 \qquad (2.80)$$

Finally

$$P_N = \frac{\left(\frac{N}{2}-1\right)!}{\pi^{N/2}} \frac{{x_n}^2{a_0}^2}{4S^{N+2}} E_0 \qquad (2.81)$$

When N=3,

$$P_{N=3} = \frac{\left(\frac{1}{2}\right)!}{\pi^{3/2}} \frac{{x_n}^2{a_0}^2}{4S^5} E_0 = \frac{\sqrt{\pi}}{2\pi^{3/2}} \frac{{x_n}^2{a_0}^2}{4S^5} E_0 = \frac{1}{8\pi} \frac{{x_n}^2{a_0}^2}{S^5} E_0 \qquad (2.82)$$

Equation (2.81) shows the dependence of the pressure exerted on the confined H-atom on the space dimension N, where more pressure is exerted on it with increasing N.

Chapter 3

Results and Discussion

Chapter Three

3.1. Results of the energy eigen-values.

In the previous Chapter, the formulae for the wave functions and for the energy eigen-values were determined.

In this Chapter, we shall calculate the energy eigen-values for the ground state (*l*=0) for the confined H-atom for different values of N and S, and then we shall express the results in graphs. Remember that the ground state corresponds to the largest root x_n (smallest value of λ).

With the help of the following formulae, mathematica software version 5.0 will be used to locate the roots of the wave functions of the confined H-atom in its ground state for given values of S, and N.

Here, we shall consider only the largest root, which corresponds to the smallest value of λ, taking into consideration that the wave function might have more than one root.

The following formulas are needed to perform the calculations,

$$R_{\lambda L}(\rho) = A' \rho^{l} e^{\left(-\frac{\rho}{2}\right)} {}_1F_1\left(l+\frac{N-1}{2}-\frac{2S}{\rho a_0}; 2l+N-1; \rho\right) \quad (3.1)$$

$$\rho = \frac{2S}{\lambda a_0} \quad (3.\ 2)$$

$$\lambda = \frac{2S}{\rho a_0} = \frac{2S}{x_n a_0} \quad (3.3)$$

and thus,

$$E_{\mathrm{n}} = -\frac{\hbar^2}{2\mu}\frac{X_{\lambda l}{}^2}{4S^2} = \left(\frac{X_{\lambda \mathrm{L}}{}^2}{4S^2}a_0{}^2\right)E_0 = \frac{-13.6}{\lambda^2} \qquad (3.4)$$

Now,

For $l = 0,\ {}_1F_1\left(l + \frac{N-1}{2} - \frac{2S}{\rho a_0};\ 2l + N - 1;\ \rho\right)$ becomes, (3.5)

$${}_1F_1\left(\frac{N-1}{2} - \frac{2S}{\rho a_0};\ N - 1;\ \rho\right) \qquad (3.6)$$

For the free hydrogen atom,

$$E_n = (-\mu e^4/2\hbar^2)\ \frac{1}{(n + \frac{N-3}{2})^2} = \frac{-13.6}{(n + \frac{N-3}{2})^2}\ (eV) \qquad (3.7)$$

In table (1) the suggested values of S, the radius of the cavity, are listed in columns as well as the calculated ground state energies for $l = 0$, and for spatial dimensions from 3 to 10.

One column for the largest x_n is presented for N = 3 only, while for the other spatial dimensions the calculated energy eigen values are presented without showing the corresponding $x_n's$.

The chosen cavity radii are in terms of the Bohr radius a_0. Therefore they were referred to as S x a_0 in the tables and they are expressed in meters, while the energies are expressed in (eV) with accuracy of ten decimal numbers or less.

The listed $x_n's$ are read with accuracy of six decimal numbers or less too.

Table (1): The Energy eigen-values for different values of S, and for specific values of N, when l=0.

N=3			N=4		N=5	
$S \times a_0$ (m)	E(eV)	x_n	$S \times a_0$ (m)	E(eV)	$S \times a_0$ (m)	E(eV)
14.00000	-13.59999903	27.999999	13.0000	-6.042119818	13.00000	-3.34789349
13.00000	-13.59999895	25.999999	12.0000	-6.044444444	12.00000	-3.34356944
12.00000	-13.59998867	23.999990	11.0000	-6.030714876	11.00000	-3.27748760
9.000000	-13.59984889	17.999900	10.0000	-6.014260000	10.00000	-3.19906000
6.000000	-13.58028715	11.991300	9.00000	-5.944123457	9.000000	-3.10449383
4.000000	-13.14487281	7.8650000	8.00000	-5.912945312	8.000000	-2.83103125
3.000000	-11.53190278	5.5250000	7.00000	-5.809316327	7.000000	-2.34226000
2.000000	-3.400000000	2.0000000	6.00000	-5.455111111	6.000000	-1.51111111
1.950000	-2.467091385	1.6662000	5.00000	-4.814740000	5.500000	-0.80727802
1.900000	-1.470288384	1.2494400	4.00000	-3.068500000	5.300000	-0.43695265
1.850000	-0.352170619	0.5954000	3.50000	-1.110204082	5.100000	-0.02647059
1.845000	-0.233969341	0.4839900	3.40000	-0.430617647	5.090000	-0.00188976
1.840000	-0.114611142	0.3378250	3.33000	-0.312775838	5.088500	-0.00041728
1.837500	-0.054474543	0.2325866	3.30000	-0.019513314	5.088350	-0.00009218
1.836500	-0.030333814	0.1734663	3.29950	-0.016092901	5.088340	-0.00008207
1.835500	-0.006139872	0.0780000	3.29850	-0.010124904	5.088330	-0.00004494
1.835250	-0.000089113	0.0093850	3.29750	-0.004502687	5.088329	-0.00004445
1.835247	-0.000016232	0.0040100	3.29700	-0.001088792	5.088328	-0.00004446
			3.29690	-0.000548072	5.088327	-0.00004350
			3.29685	-0.000165477	5.088308	-0.00004255
			3.29683	-.0000175958		

Table (2): The Energy eigen values for different values of S, and for specific values of N, when *l*=0.

N=6		N=7		N=8	
S × a_0 (m)	E(eV)	S × a_0 (m)	E(eV)	S × a_0 (m)	E(eV)
23.0000	-2.17491	35.000000	-1.51104	54.000	-1.11042
21.0000	-2.17263	30.000000	-1.51036	37.000	-1.10571
19.0000	-2.16608	26.000000	-1.50687	36.000	-1.09714
17.0000	-2.14412	23.000000	-1.49081	32.000	-1.08777
14.0000	-2.06099	20.000000	-1.48110	27.000	-1.07776
13.0000	-2.01183	17.000000	-1.37224	20.000	-0.97317
12.0000	-1.91675	16.000000	-1.35482	17.800	-0.85000
11.0000	-1.75367	15.000000	-1.27900	17.000	-0.79106
10.0000	-1.54913	14.000000	-1.16641	16.000	-0.68850
9.00000	-1.24677	13.000000	-1.10285	15.000	-0.58087
8.00000	-0.72728	12.000000	-0.85000	14.000	-0.39139
7.50000	-0.29255	11.000000	-0.58172	13.500	-0.30152
7.35000	-0.15121	10.000000	-0.19580	12.500	-0.09596
7.25000	-0.05475	9.7500000	-0.07010	12.400	-0.01872
7.23500	-0.03752	9.6500000	-0.01688	12.385	-0.01384
7.22500	-0.02585	9.6350000	-0.00916	12.380	-0.01182
7.21500	-0.01976	9.6250000	-0.00376	12.370	-0.00910
7.20500	-0.00802	9.6200000	-0.00140	12.355	-0.00451
7.20250	-0.00443	9.6175000	-7.2E-05	12.351	-0.00305
7.20125	-0.00347	9.6174000	-1.7E-05	12.350	-0.00273
7.20050	-0.00289	9.6173750	-4.9E-06		
7.20025	-0.00213	9.6173700	-2.2E-06		
7.20025	-0.00213	9.6173680	-7.8E-07		
		9.6173670	-5.0E-07		
		9.6173665	-2.5E-07		

Table (3): The Energy eigen values for different values of S, and for specific values of N, when *l*=0.

N=9		N=10	
$S \times a_0$ (m)	E (eV)	$S \times a_0$ (m)	E (eV)
44.0000	-0.84923	77.500	-0.671595
40.0000	-0.84152	54.000	-0.671168
26.0000	-0.79845	42.000	-0.659666
20.0000	-0.54400	31.000	-0.597919
18.0000	-0.37778	25.000	-0.460442
16.0000	-0.11402	23.000	-0.361531
15.5000	-0.02503	20.000	-0.146391
15.4000	-0.00703	19.000	-0.039580
15.3800	-0.00345	18.900	-0.026864
15.3750	-0.00208	18.700	-0.002335
15.3740	-0.00200	18.685	-0.000429
15.3700	-0.00125	18.684	-0.000265
15.3690	-0.00109	18.682	-.0000477
15.3650	-0.00030		
15.3640	-0.00010		
15.3635	-9.7E-06		

The following graphs represent these results. The plots were made using Excel 2007.

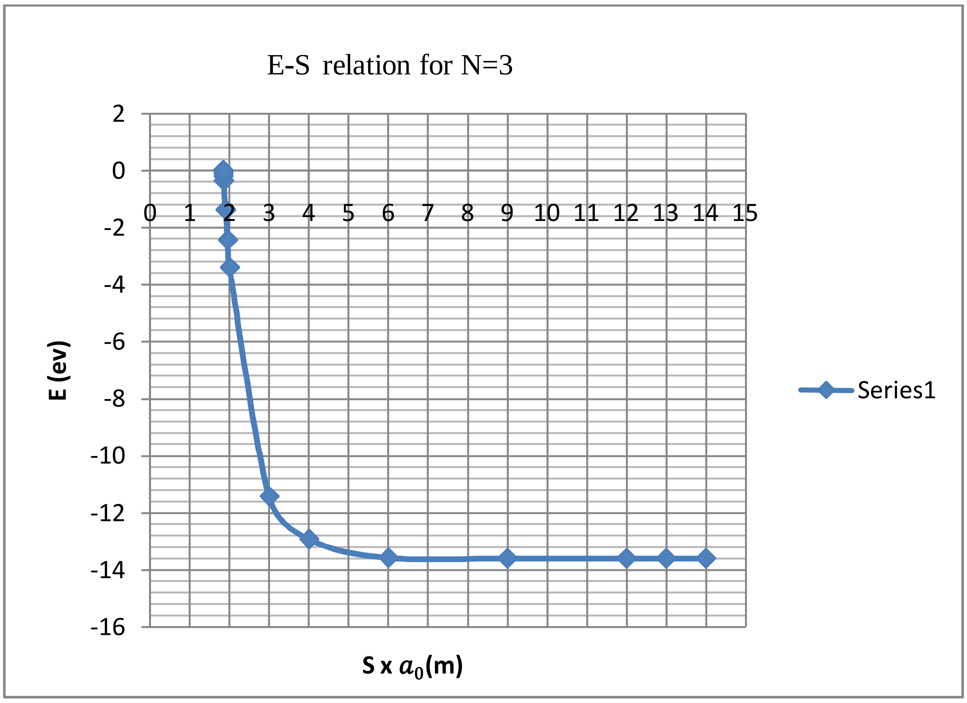

Fig.(3): Relation between the ground state energy eigen values of a confined H-atom, and the radius of the cavity for N=3&*l*=0.

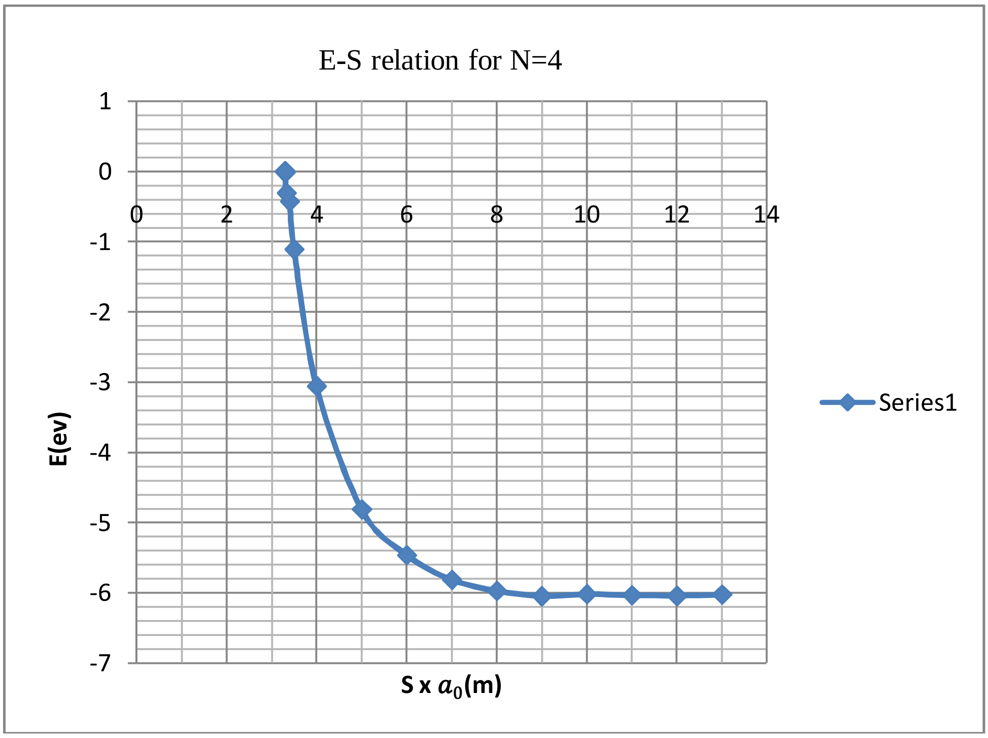

Fig.(4): Relation between the ground state energy eigen values of a confined H-atom, and the radius of the cavity for N=4&*l*=0.

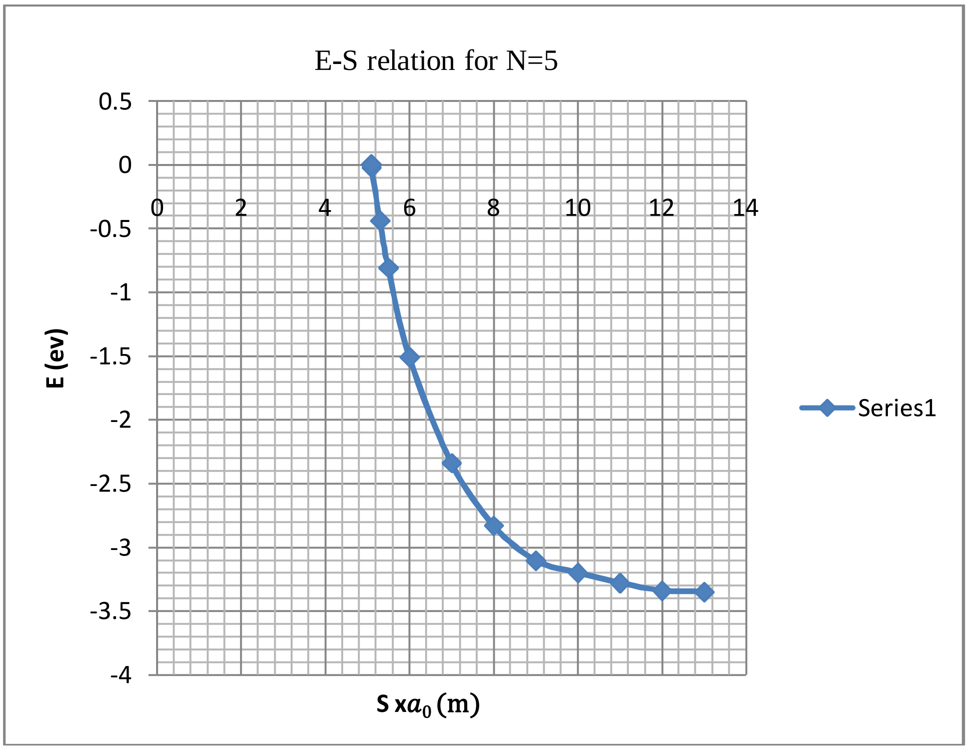

Fig.(5): Relation between the ground state energy eigen values of a confined H-atom and the radius of the cavity for N=5&*l*=0.

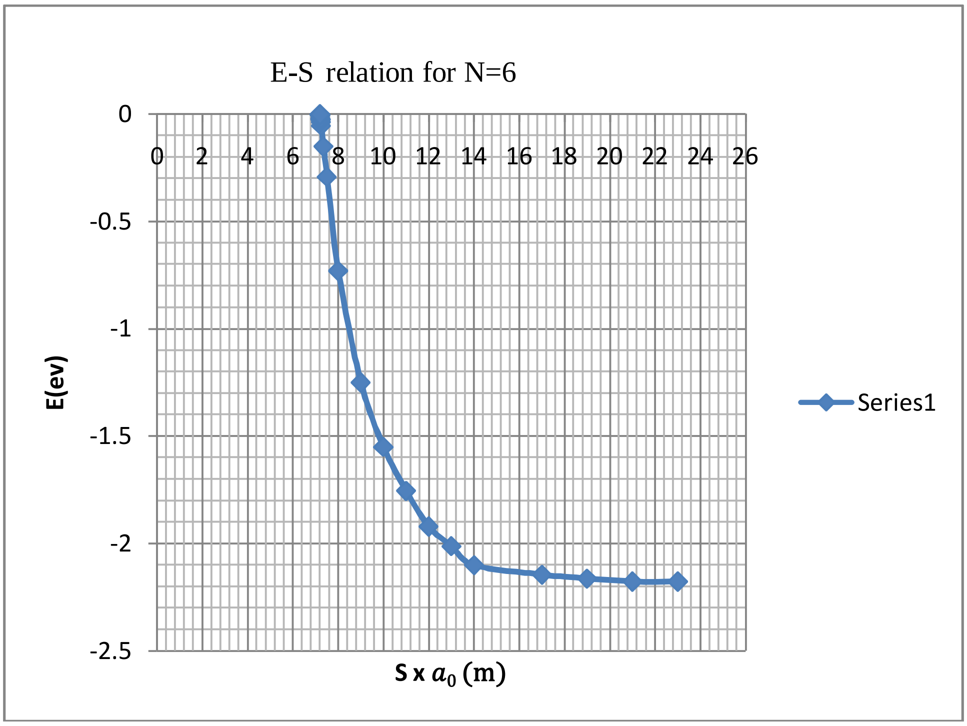

Fig.(6): Relation between the ground state energy eigen values of a confined H-atom and the radius of the cavity for N=6&*l*=0.

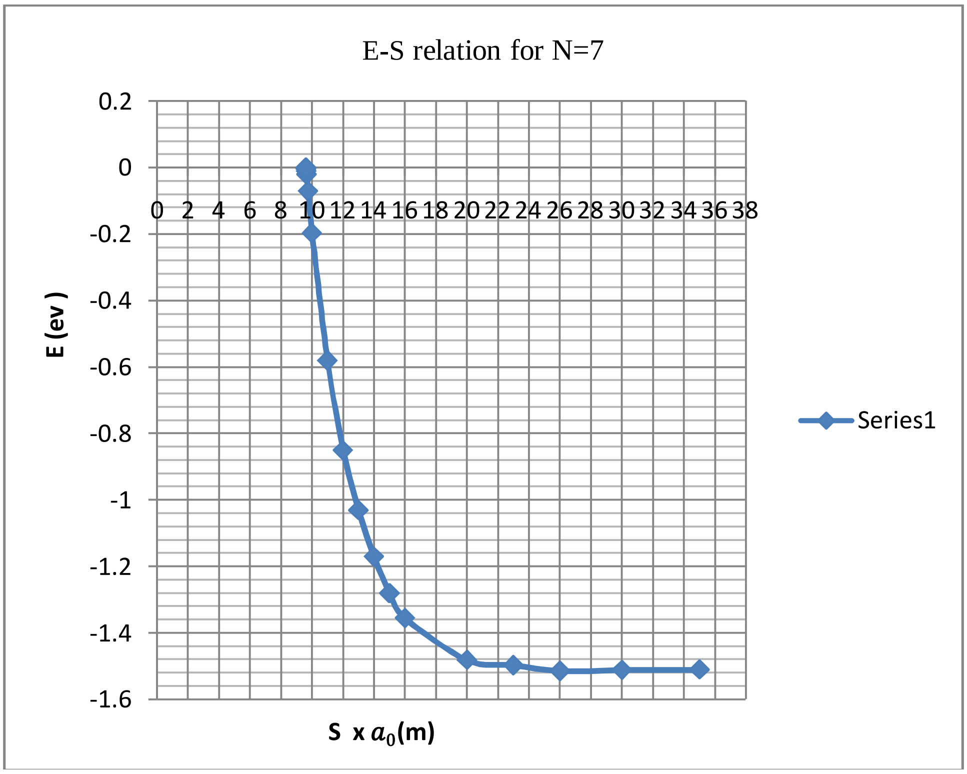

Fig.(7): Relation between the ground state energy eigen valuesof a confined H-atom and the radius of the cavity for N=7&*l*=0.

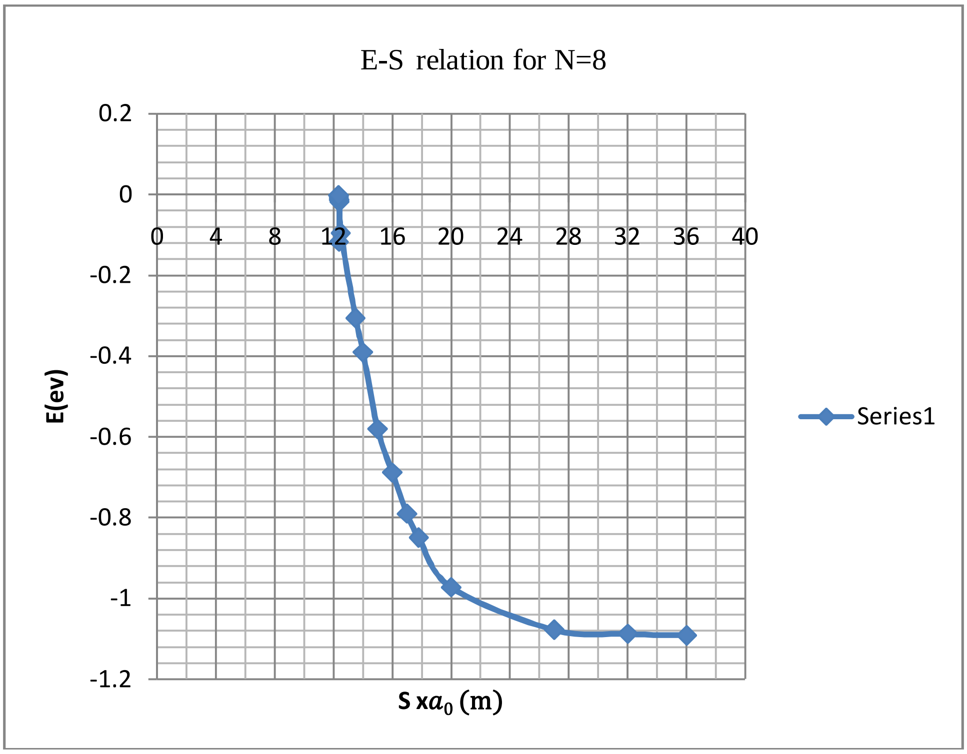

Fig.(8): Relation between the ground state energy eigen values of a confined H-atom and the radius of the cavity for N=8&*l*=0.

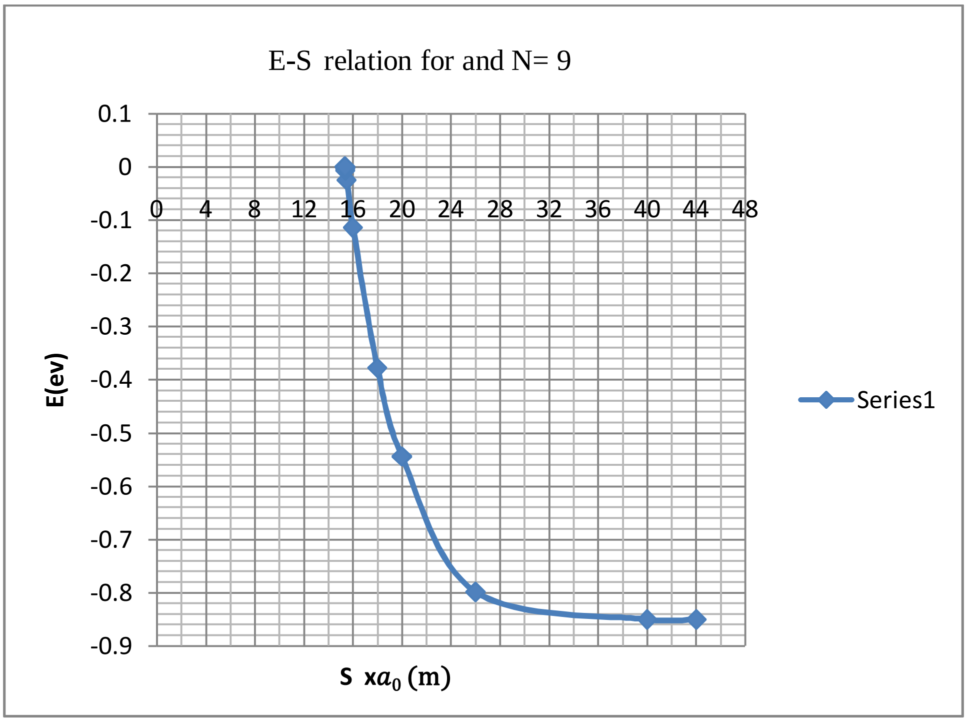

Fig.(9): Relation between the ground state energy eigen values of a confined H-atom and the radius of the cavity for N=9&*l*=0.

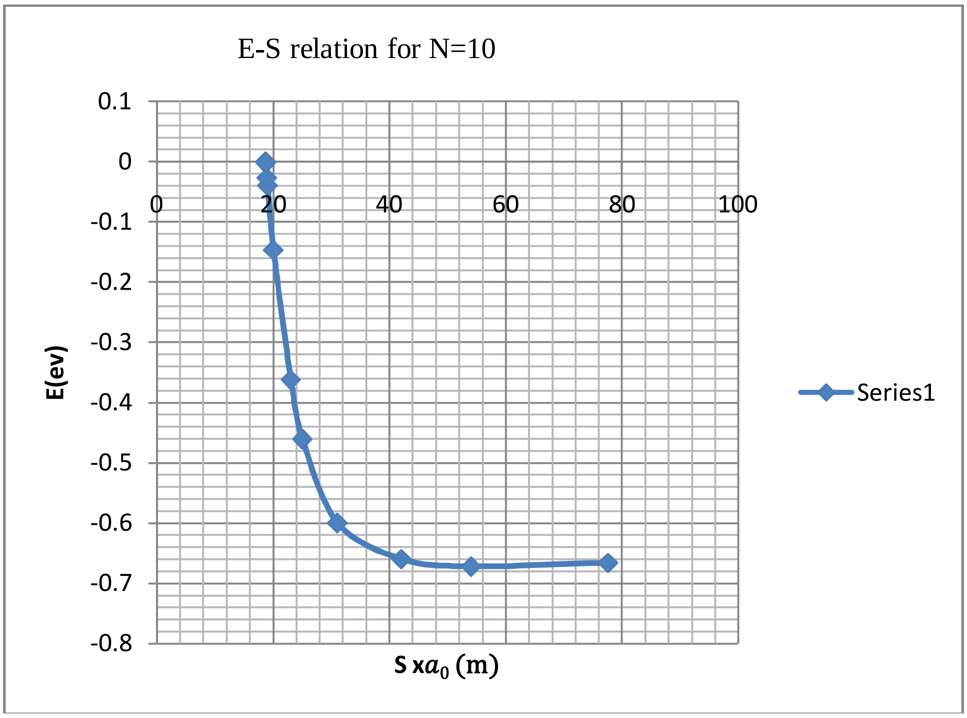

Fig.(10): Relation between the ground state energy eigen values of a confined H-atom and the radius of the cavity for N=10&*l*=0.

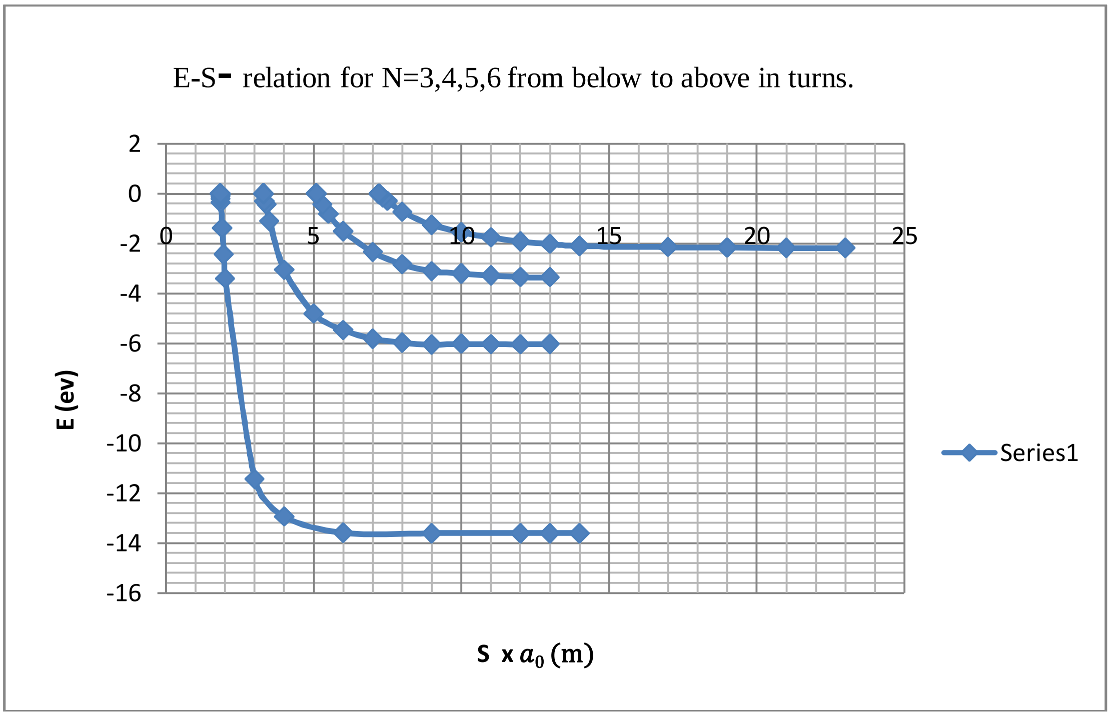

Fig. (11): Relation between ground state energy eigen values of a confined H-atom and the radius of the cavity for given space dimensions when *l*=0 For N=3, 4, 5, 6 from below to above.

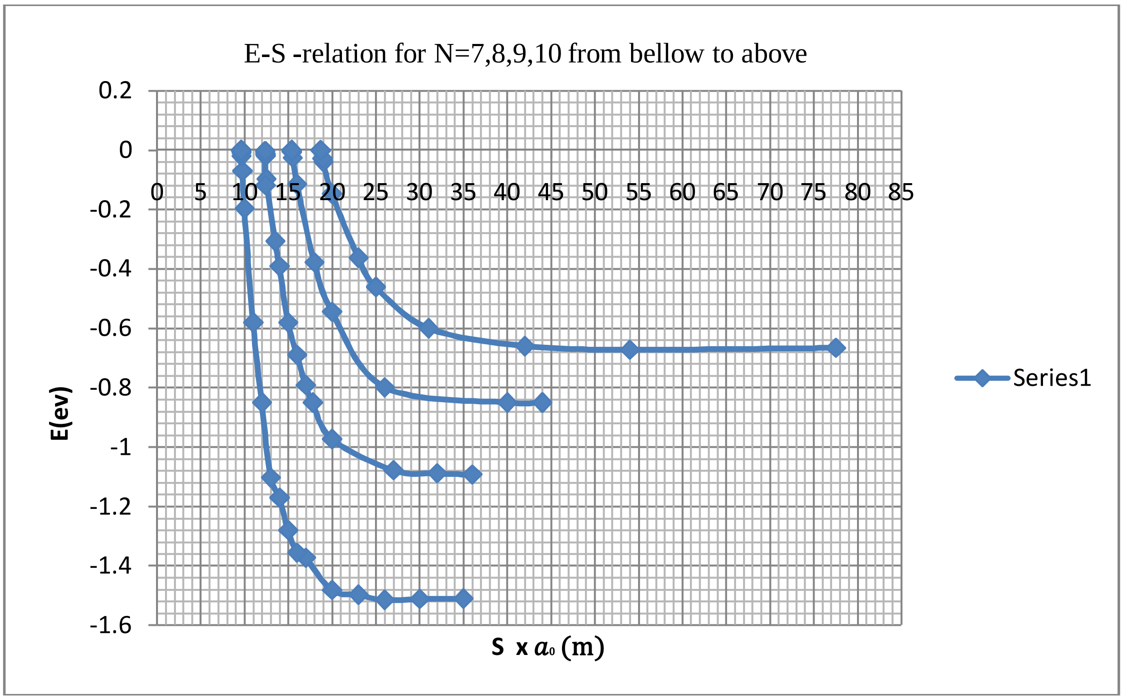

Fig. (12): Relation between ground state energy eigen values of a confined H-atom and the radius of the cavity for given space dimensions when *l*=0, for N= 7, 8, 9, 10 from below to above.

Studying the data in the tables and studying the graphs, one can figure out the effect of the radius of the cavity on the ground state energy of the confined H- atom. As the radius of the cavity increases, the energy of the confined H- atom decreases and its limiting value becomes equal to that for the free H- atom in that dimension which can be easily calculated from eqn. (3.7), which means that the effect of the cavity becomes negligible for large values of S.

Meanwhile, as the radius of the cavity decreases the ground state energy increases for a given N, this is so because as the cavity becomes smaller, then the confined atom will suffer many collisions with the walls of the cavity which will increase its kinetic energy (which is positive), and thus the total energy, then, increases, hence the particle is less bound. Alternatively, as the cavity radius decreases the surface gets closer to the position where the electron radial distribution function

$$D_{\lambda l}(\mathrm{r}) = r^{N-1}|R_{\lambda l}\,(\mathrm{r})|^2 \qquad (3.8)$$

is maximum, and hence the confinement effect is expected to become more profound.

A distribution function gives the probability of finding the particle a distance r in space from a certain reference point.

One more observation about our results is that the confinement effects become more profound in higher dimensions. For example, for a given cavity radius S, we can calculate from tables above the percentage difference from the ground state energy of the free hydrogen atom, or

$$\text{The percentage difference} = \frac{E_{free-}\,E_{confined}}{E_{free}} \times 100\% \qquad (3.9)$$

Lets choose S= $14a_0$ then the corresponding percentage differences for N=3, 4,5,6,7 are 8.33×10^{-5} %, 0%, 1.66% 11.9%, 77.8%.

It is easy to see in Figurs. (11), (12) that when N increases, the limiting value of the energy increases, which is due to the additional repulsive term in the effective potential term where

$$V_{eff} = V(r) + [l(l+N-2) + \frac{(N-1)(N-3)}{4}]\frac{1}{r^2} \qquad (3.10)$$

The total energy is kinetic energy plus potential energy, here V_{eff} becomes more positive with increasing N, thus the total energy is more positive too, in other words it increases.

3.2: Critical cage radius:

An important point to discuss is to find the minimum cavity size that allows a bound state. Our previous results show that: As the cavity radius decrease the binding energy diminishes and therefore, there is a critical value. S_c for the cavity radius at which the binding energy becomes zero. This critical value is called the critical cage radius. The critical cage radius of hydrogen atom is relevant to the ionization of its ground state. Here we search for the smallest cavity radius, for a given dimension N, at which the bound state energy approaches zero. We carry the calculations for N = 2 to 10, and present our results in Table (4). For the N=3, our results give S_c = $1.835247\times a_0$ in meters.

Sommerfield and Welker [12] obtained a critical cage radius = $1.835\times a_0$ in meters. Our results show that the value of the critical cage increases as the space dimension N decreases. This is so because as the dimension increases the particle is repelled further away from the nucleus which is due to the extra repulsive term in the effective potential.

The results are displayed in the following table and in Fig (13).

Table (4): Critical cage radius of the cavity S_c in different space dimension N for l=0.

N	$S_c \times a_0$(m)
2	0.722890
3	1.835247
4	3.296850
5	5.088327
6	7.200250
7	9.617367
8	12.35000
9	15.36350
10	18.68200

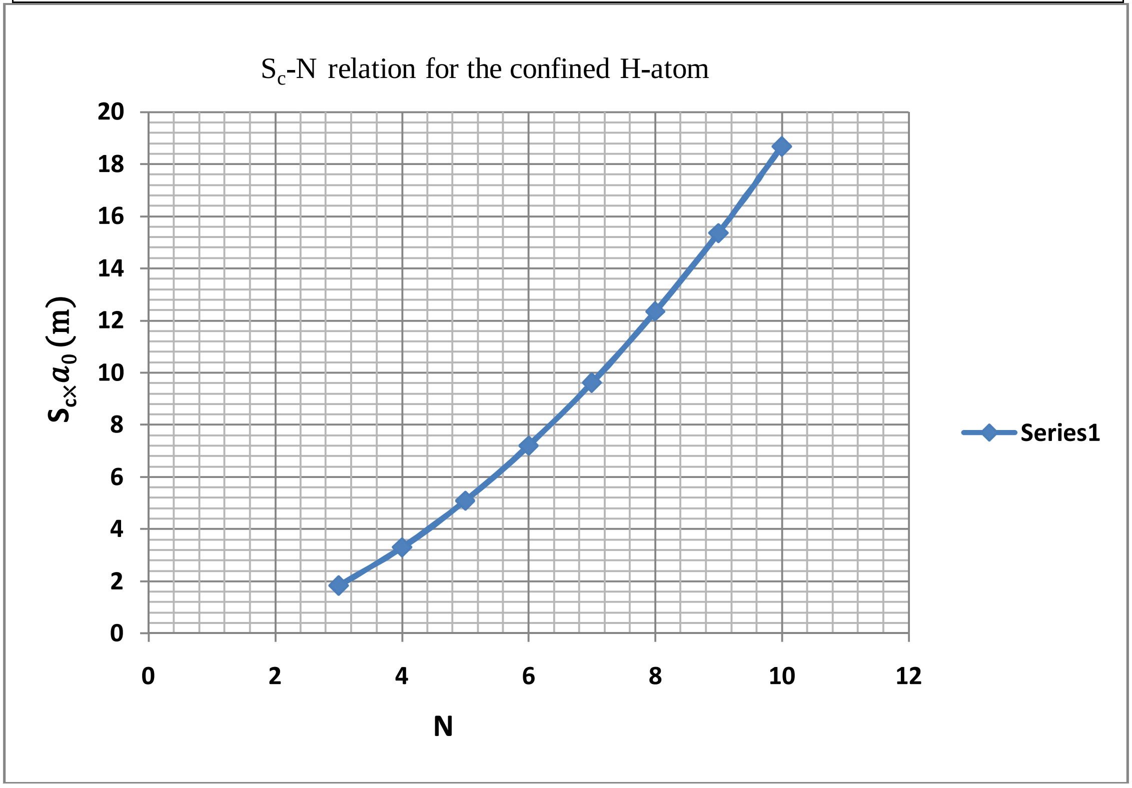

Fig.(13): Relation between the critical radius of the cavity and the dimension N for the ground state of the confined H-atom for l = 0.

Table (5): Values of E vs. N (the dimensionality of space) at S=12a_0, when *l*= 0.

N	E (ev)
3	-13.59998867
4	-6.044444444
5	-3.343570000
6	-1.916750000
7	-0.850000000
8	…

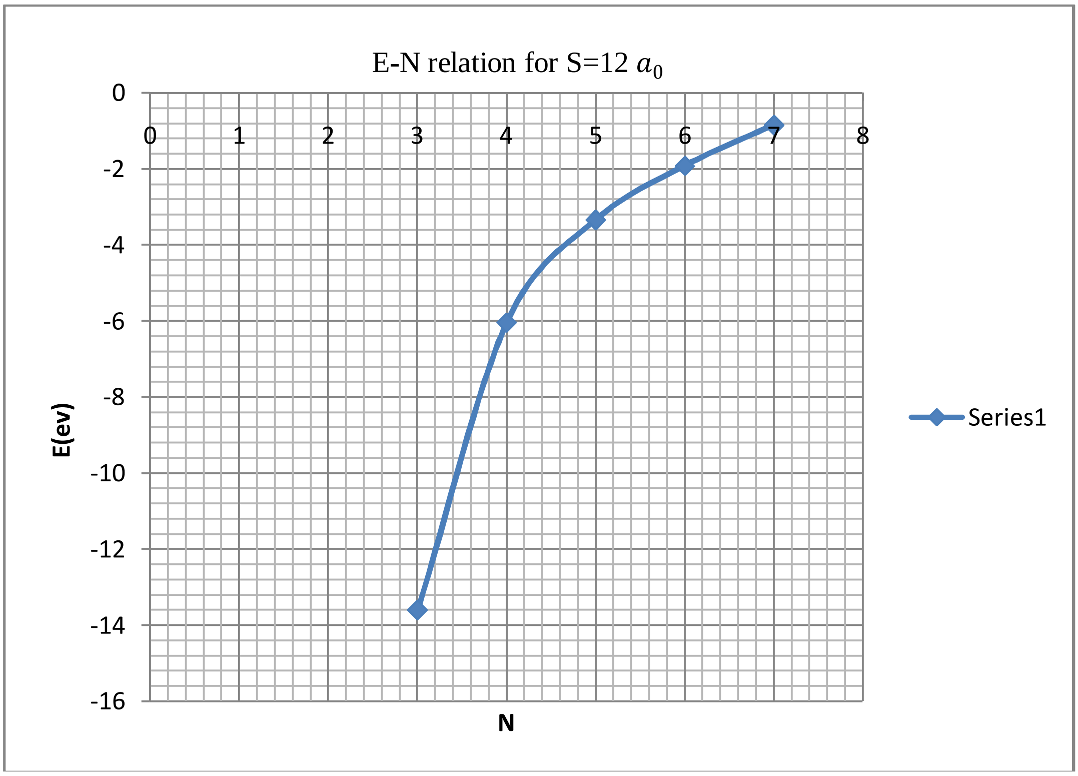

Fig. (14): Relation between energy eigen-values and N for the confined H-atom for S=12a_0 and for *l*=0.

Table (6): Values of E vs. N for specific values of S, when *l* = 0.

N	E(ev)	E(ev)	E(ev)	E(ev)	E(ev)	E(ev)
	S=3a_0	S=6a_0	S=9a_0	S=12a_0	S=16a_0	S=20a_0
3	-11.532	-13.58029	-13.59985	-13.59999	-13.5999	-13.9999
4		-5.455111	-5.944123	-6.044444	-6.04444	-6.10500
5		-1.511111	-3.104490	-3.343570	-3.39703	-3.39949
6			-1.246770	-1.916750	-2.08000	-2.17600
7				-0.850000	-1.35482	-1.48110
8					-0.68850	-0.97317
9					-0.11402	-0.54400
10						-0.14639

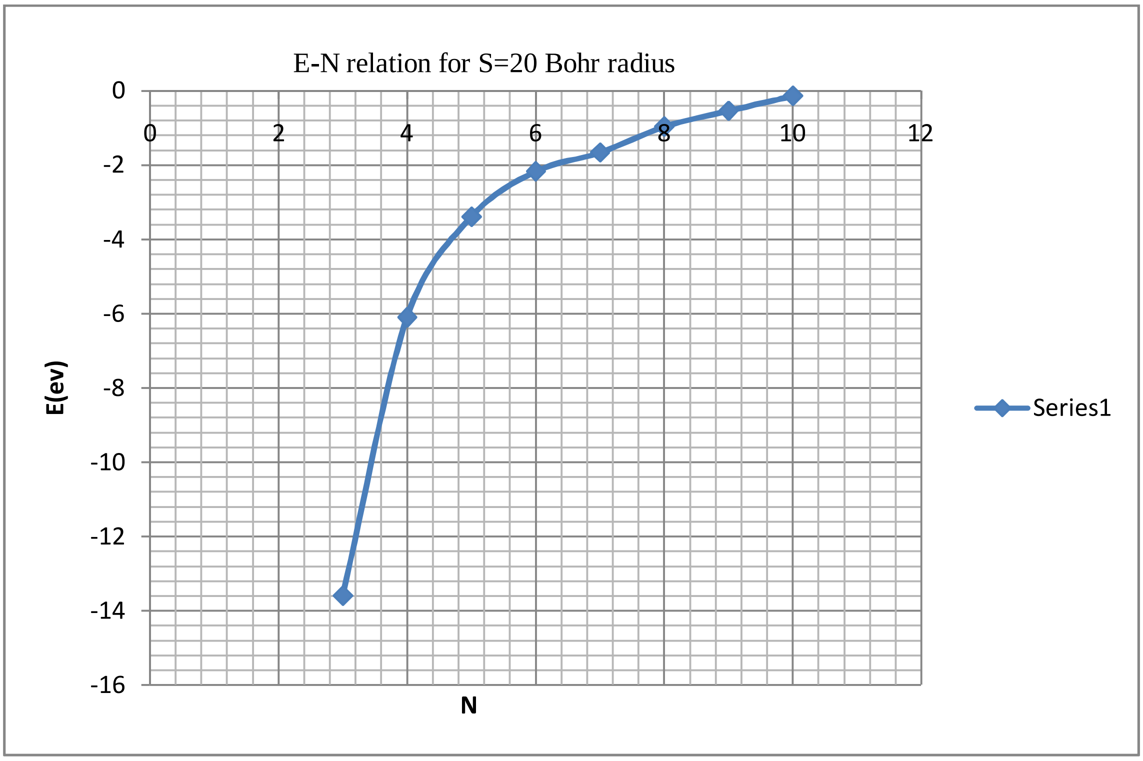

Fig. (15): Relation between energy eigen-values of a confined H-atom and N when S=20a_0 &*l*=0.

The idea of the critical cage can be noticed from the plots in Figures (14), (15), and Tables (5), (6) where in the case of equal radii of cavities, as N increases the energy of the confined hydrogen atom increases, but one can see that there are no bound states for dimensions higher than 7 for S= 12a_0, this manifests the idea of the critical cage radius. Going back to Table (5) above, we can find that S = $12a_0$ is less than S_c for N=8, 9, 10. That is to say_for dimensions higher than 7, and for radius =$12a_0$ there are no bound states for the confined H-atom when l=0.

That is because, when N increases, the energy increases as we have shown before, at the same time the energy increases when the radius of the cavity decreases, in another words the kinetic energy increases up to a certain value at which the total energy equals zero as S decreases.

We can see from Table (6) that the Energy is quantized, (i.e. for certain values of S & N there are specific values of bound states of the energy.

Again don't forget that the energy is calculated corresponding to the largest zero of ${}_1F_1\,(l+\frac{N-1}{2}-\lambda;\,2l+N-1;\,\rho)$ which means lowest value of λ, which corresponds to the ground state energies.

3.3. Bound states:

Now, let's consider the effect of the confinement and dimensionality of space on the number of bound states of the confined H-atom. To that end, we choose two values for the cavity radius (S= $22a_0$ & $44a_0$). The number of bound states is determined by the number of zeros or roots of the confluent hyper-geometric function which we search for using mathematica software version 5.0.

As before, once the zeros are located, the bound state energies are calculated using equation (3.4), the lowest bound state energy is the ground state say (n=1), and the next ones are exited states (n=2, 3, 4,….).These calculations are carried out for dimensions N=3 to 10. It is tempting to compare these energy values with those for the free N-dimensional H-atom. Our results for *l*=0, are shown in Tables (7), & (8) for S= $22a_0$, S=$44a_0$ respectively. The results are also presented into graphs (14, 15).

The results in tables (7) & (8) show interesting features: Firstly, for a given S the number of bound states decreases as N increases, and this is due the extra repulsive term in the effective potential which reduces the effect of the negative potential energy, which means that the total energy of the atom will approach zero faster which stops having additional bound states.

Secondly, the larger the cavity radius the higher the number of the bound states for a given N, since the confinement effect is small for large confining cavity, and because increasing the radius of the cavity leads to decreasing the energy of the confined hydrogen atom which allows more bound states.

Thirdly, upon comparing the bound-state energies of the confined case, here we chose S=22a_0, with those corresponding states of the free one, we note that while the ground state energies are very close, the excited-state energies have a difference which increases as we go to higher excited states. This is explained by the fact that the radial distribution function has a maximum at a point that gets closer to the cavity surface as we go to higher excited states and thus the confinement effects become profound.

It is of great importance to consider the special case $\propto$ = -1. Here, eqn. (2) in Appendix B implies that ${}_1F_1(\propto;\gamma;x)$ has only one zero, (i.e. the series terminates when the power of x is 1), whose value $x=\gamma$ as eqn. (2) in Appendix B shows, and thus we have only one bound state. Therefore, for $l=0$, and for ${}_1F_1(l+\frac{N-1}{2}-\lambda;2l+N-1;\rho)={}_1F_1(\propto;\gamma;\rho)$, we get $\rho=\gamma=(N\text{-}1)$, and thus eqns. (3.3) and (3.6) yield the cavity radius and eqn. (3.7) yield the binding energy, namely

$$\text{S} = \frac{N^2-1}{4}a_0 \tag{3.11}$$

$$\text{E} = \frac{4}{(N+1)^2}E_0 \tag{3.12}$$

It is interesting to note that the above state energy coincides with the energy of the first exited state (n=2) for the free hydrogen atom as can easily be checked using eqn. (3.7). One can also observe that in the infinite dimensional space (N⟶∞) the binding energy vanishes and the cavity radius becomes infinite which means that the H-atom isn’t anymore confined. This implies that we can’t confine a H-atom in the infinite dimensional space.

Table (7): Bound state energies for confined and free H-atom in different dimensions for l=0 and S=22a_0.

N	n	$E_{n\ \mathrm{confined}}$ (eV)	$E_{n\ \mathrm{free}}$ (eV)
3	1	-13.5994	-13.60000
3	2	-3.39938	-3.400000
3	3	-1.42647	-1.511111
4	1	-5.98962	-6.044444
4	2	-2.16365	-2.176000
4	3	-0.78931	-1.110204
5	1	-3.39938	-3.400000
5	2	-1.46274	-1.511110
5	3	-0.12629	-0.850000
6	1	-2.15134	-2.176000
6	2	-0.89700	-1.110204
7	1	-1.47696	-1.511111
7	2	-0.37435	-0.085000
8	1	-1.02850	-1.110204
9	1	-0.64740	-0.850000
10	1	-0.30600	-0.671605

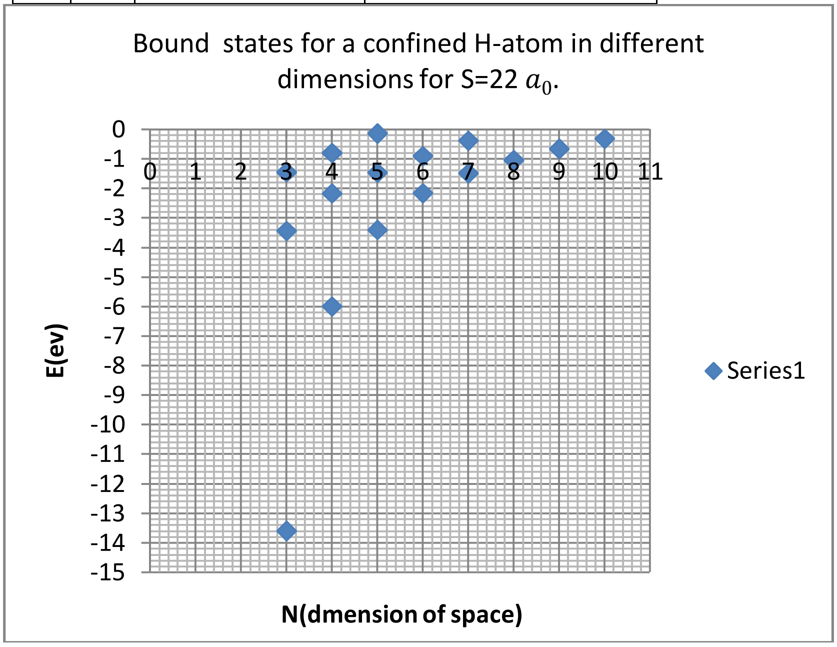

Fig. (16): Bound states for of a confined H-atom in different dimensions for S=22a_0&l=0.

Table (8): Bound state energies for confined and free H-atom in different dimensions for l=0 and S=44a_0.

N	n	$E_{n\ \text{confined}}$	$E_{n\ \text{free}}$	N	n	$E_{n\ \text{confined}}$	$E_{n\ \text{free}}$
3	1	-13.59999	-13.6000	6	1	-2.15134	-2.17600
3	2	-3.399985	-3.40000	6	2	-1.11526	-1.11020
3	3	-1.48717	-1.51111	6	3	-0.64068	-0.67161
3	4	-0.84320	-0.85000	6	4	-0.20107	-0.45959
3	5	-0.40043	-0.54400	7	1	-1.50768	-1.51111
4	1	-6.03072	-6.04444	7	2	-0.85774	-0.85000
4	2	-2.21325	-2.17600	7	3	-0.45522	-0.54444
4	3	-1.09762	-1.11020	8	1	-1.09762	-1.11111
4	4	-0.64068	-0.67161	8	2	-0.64741	-0.67161
4	5	-0.14864	-0.44959	8	3	-0.27441	-0.44959
5	1	-3.40000	-3.40000	9	1	-0.84927	-0.85000
5	2	-1.50768	-1.51111	9	2	-0.43565	-0.54444
5	3	-0.84479	-0.85000	9	3	-0.07193	-0.37777
5	4	-0.42193	-0.54400	10	1	-0.65417	-0.67161
				10	2	-0.34421	-0.44959

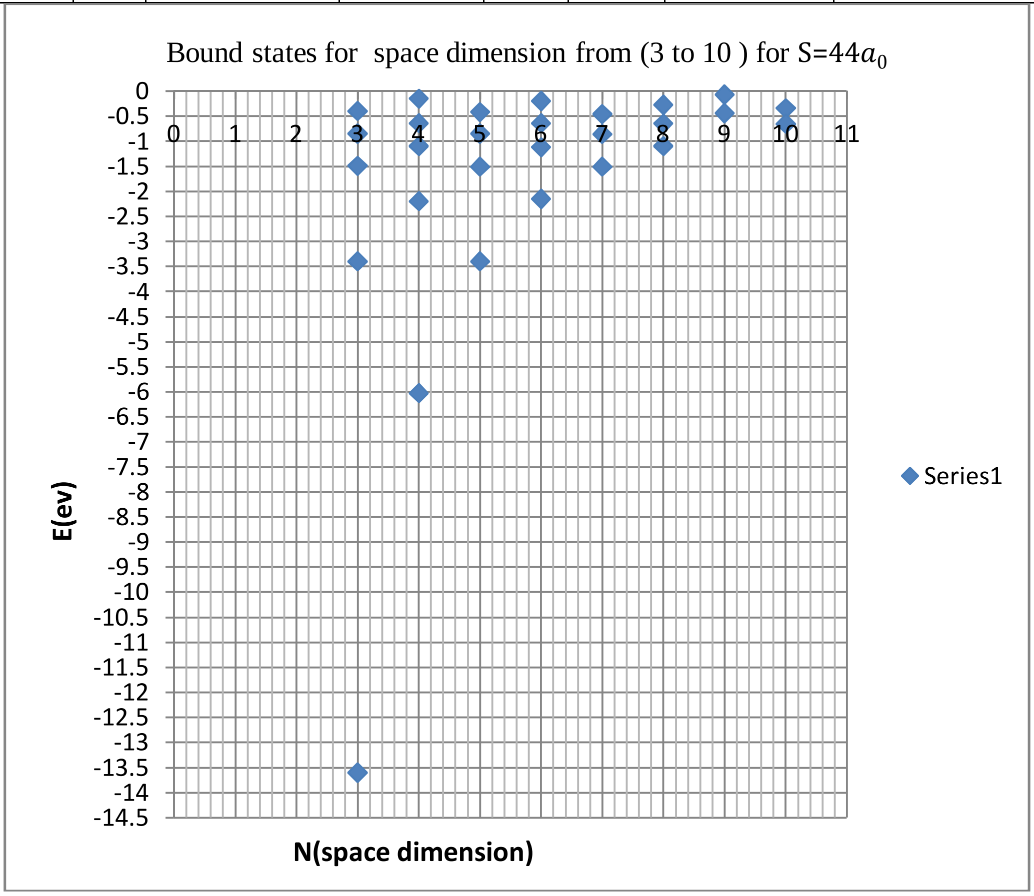

Fig. (17): Bound states of a confined H- atom in different dimensions for S=44a_0 &l=0

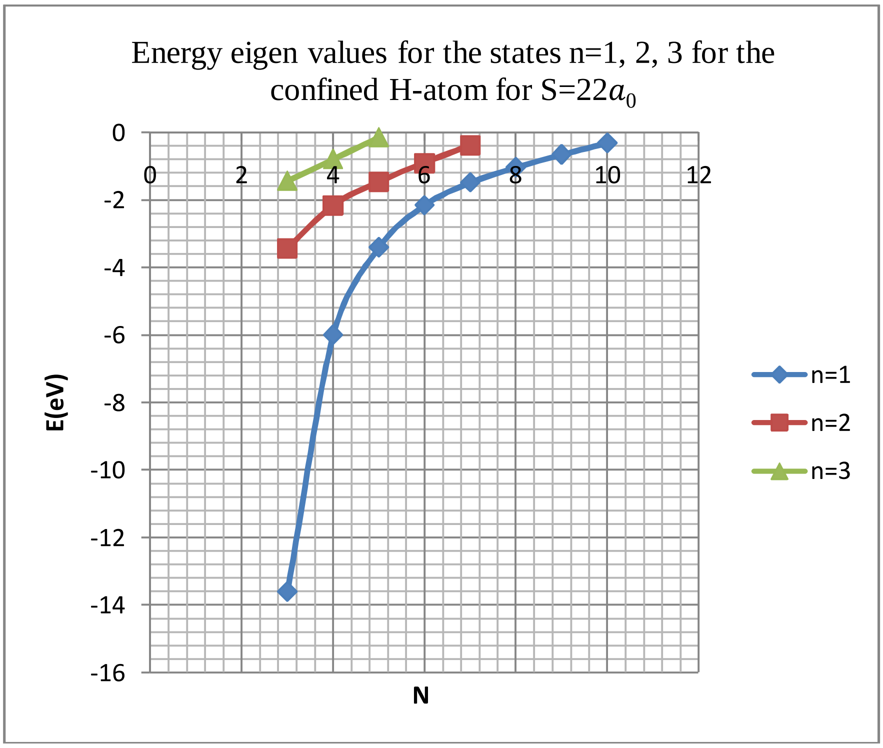

Fig.(18): The energy eigen values of states (n=1, 2, 3) of
a confined H-atom as a function of N for *l*=0, and for S=22a_0.

This shows that the energy eigen-values for the excited states of the confined H-atom for *l*=0 behaves like those of its ground state energy eigen-values, in other words E increases as N increases for the excited states also.

3.4. Pressure calculations and graphs:

In chapter two, we have derived an equation that relates the pressure exerted on a confined H-atom with the radius of the cavity and the spatial dimension N. The dependence can be written as:

$$P_N = \frac{\left(\frac{N}{2}-1\right)!}{\pi^{N/2}} \frac{{X_{\lambda l}}^2 {a_0}^2}{4S^{N+2}} E_0 \ . \qquad (3.13)$$

For N=3, $P_{N=3} = \frac{1}{8\pi} \frac{{X_{\lambda l}}^2 {a_0}^2}{S^5} E_0 = \frac{13.6 \, {X_{\lambda l}}^2}{8\pi \, d^5} \left(\frac{eV}{{a_0}^3}\right)$, where S= d$a_0$, and

0 < d < ∞, or simply S is a multiple of Bohr radius.

The calculated pressure as a function of N&S are presented in Tables (9) - (16) and graphs (19) – (26). All these calculations are expressed in terms of $eV/\,{a_0}^N$.

Table (9): Relation between pressures exerted on a confined hydrogen atom and the radius of the cavity when *l*=0,N=3.

S× a_0 (m)	P(eV/a_0^3)
14.00000	0.0007889
13.00000	0.0009852
12.00000	0.0012526
9.000000	0.0029691
6.000000	0.0100064
5.000000	0.0172469
4.000000	0.0326881
3.000000	0.0679767
2.500000	0.0930108
2.400000	0.0945503
2.000000	0.0676413
1.950000	0.0532823
1.900000	0.0341165
1.850000	0.0088524
1.845000	0.0059292
1.840000	0.0029282
1.837500	0.0013974
1.836500	0.0007794
1.835500	0.0001502
1.835250	0.0000022
1.835200	0.0000016
1.835175	0.0000079
1.835170	0.0000079

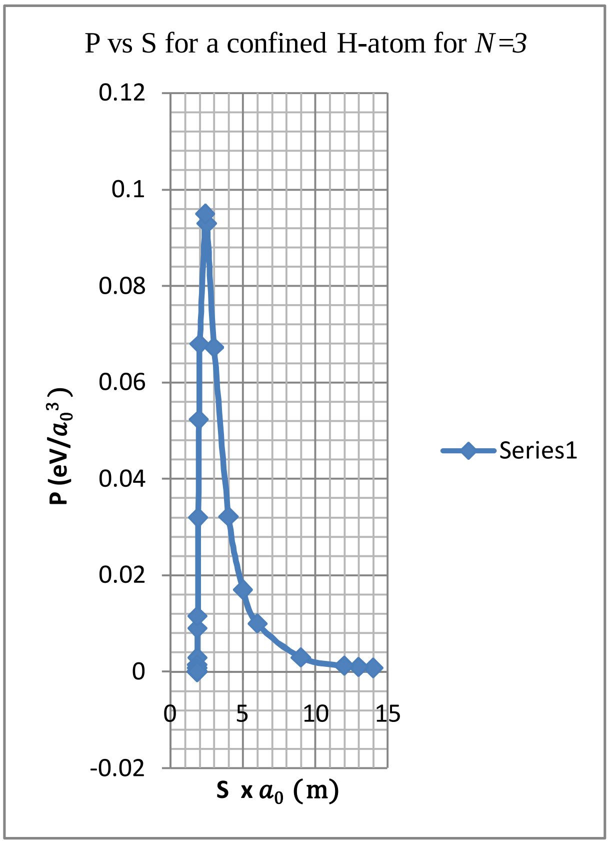

Fig.(19): Relation between the pressure exerted on the confined H-atom in a cavity and its radius for *l* = 0 and N=3.

One can notice here that the pressure is maximum at S=2.4a_0.

Table (10): Relation between pressures
Exerted on a confined hydrogen atom
and the radius of the cavity when *l*=0,N=4.

S× a_0 (m)	P(eV/$a_0{}^4$)
13.0000	0.000022
12.0000	0.000026
11.0000	.0000422
10.0000	0.000061
9.00000	0.000094
8.00000	0.000150
7.00000	0.000245
6.00000	0.000430
5.00000	0.000781
4.00000	0.001210
3.50000	0.000750
3.40000	0.000330
3.35000	0.000250
3.30000	0.000170
3.29950	0.000014
3.29850	8.7E-06
3.29750	3.81E-06
3.29700	9.34E-07
3.29690	4.3E-07
3.29685	1.4E-07

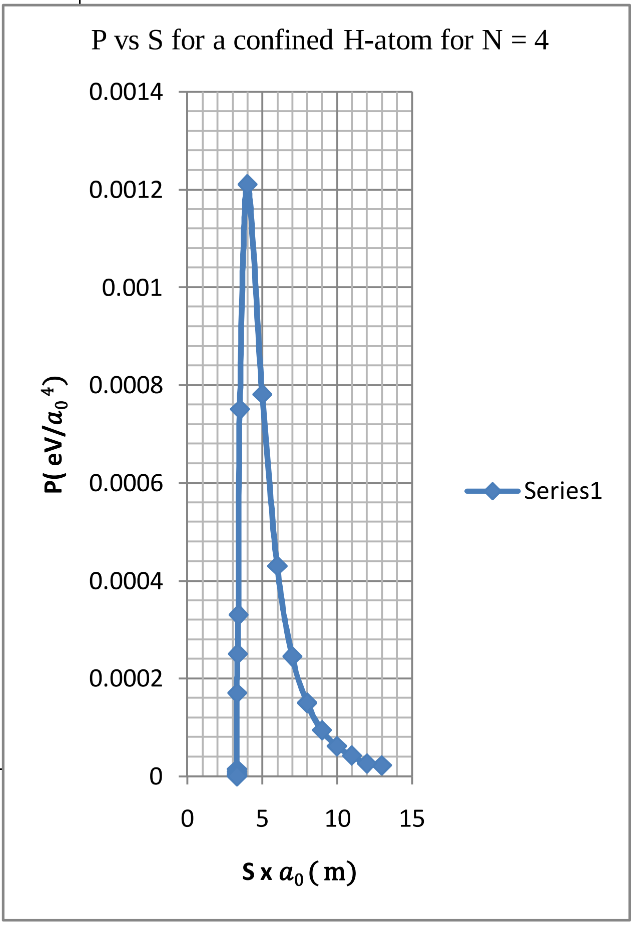

Fig.(20): Relation between the pressure exerted on a confined H-atom and the radius of the cavity when *l* = 0 for N=4.

Table (11): Relation between pressures
Exerted on a confined hydrogen atom
and the radius of the cavity when *l*=0,N=5.

$S \times a_0$ (m)	P (eV/$a_0{}^5$)
13.00000	0.00000046
12.00000	0.00000068
11.00000	0.00000103
10.00000	0.00000162
9.000000	0.00000270
8.000000	0.00000440
7.000000	0.00000706
6.000000	0.00000985
5.500000	0.00000813
5.300000	0.00000520
5.100000	0.00000311
5.090000	0.00000003
5.088500	5.25E-08
5.088350	1.4E-09
5.088340	1.22E-09
5.088330	6.7E-10
5.088329	6.61E-10
5.088328	6.46E-10
5.088327	6.3E-10

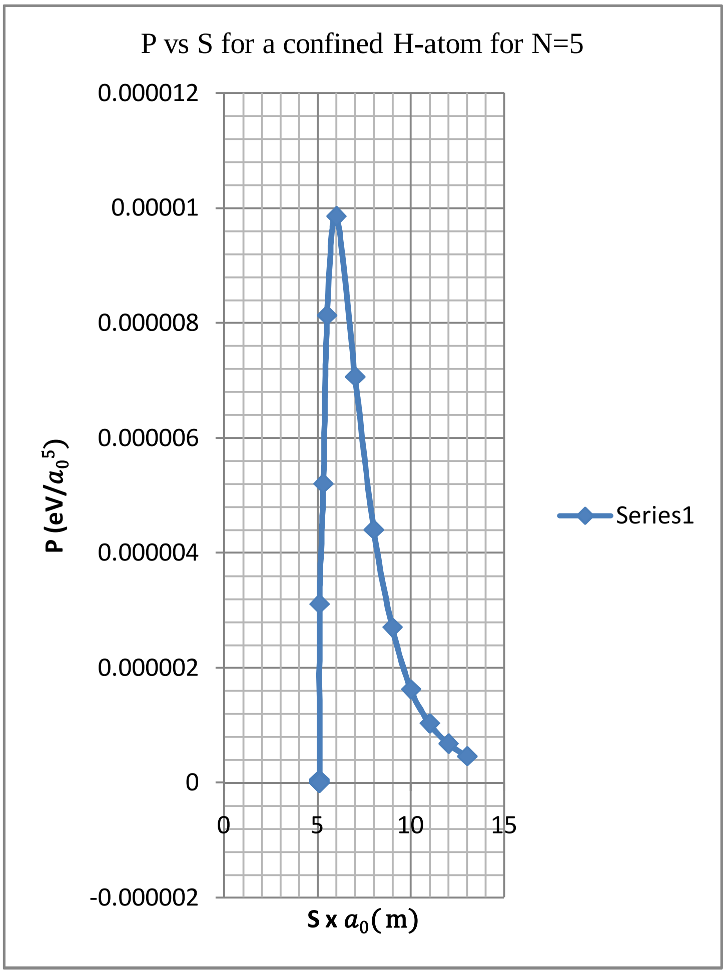

Fig. (21): Relation between the pressures exerted on a confined H-atom and the radius of the cavity when *l* = 0, N=5.

Table (12): Relation between pressures exerted on a confined hydrogen atom and the radius of the cavity for *l*=0,N=6.

S× a_0	P x 10^{-8}(eV/$a_0{}^6$)
23.0000	0.0095
21.0000	0.0160
19.0000	0.0297
17.0000	0.0573
14.0000	1.7656
13.0000	2.6885
12.0000	4.1406
11.0000	6.3852
10.0000	9.9923
9.00000	15.133
8.00000	17.895
7.50000	10.603
7.35000	6.1862
7.25000	2.4318
7.23500	1.6909
7.22500	1.1723
7.21500	0.9035
7.20500	0.3670
7.20250	0.2050
7.20125	0.1605
7.20050	0.0134
7.20025	0.0098

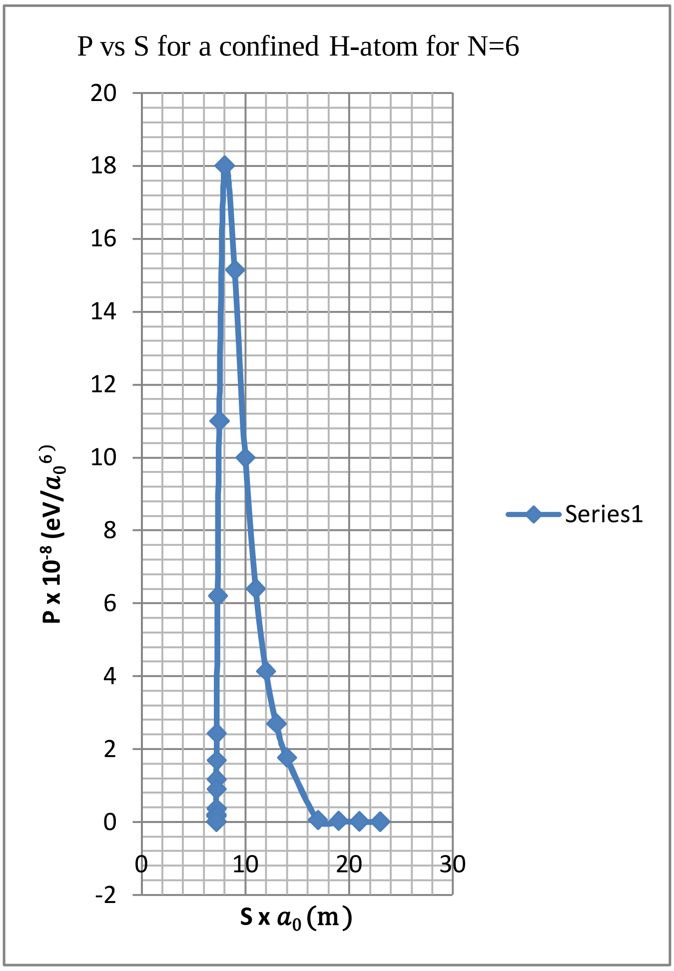

Fig (22): Relation between the pressures exerted on a confined H-atom and the radius of the cavity when *l* = 0, N=6.

Table (13): Relation between Pressures exerted on a confined hydrogen atom and the radius of the cavity for *l*=0,N=7.

S × a_0 (m)	P × 10^{-10}(eV/$a_0{}^7$)
35.00000	0.01420
30.00000	0.04176
26.00000	0.11451
23.00000	0.26477
20.00000	0.69968
17.00000	2.02222
16.00000	3.05201
15.00000	4.52666
14.00000	6.69111
13.00000	9.91163
12.00000	14.3448
11.00000	18.0514
10.00000	11.8433
9.750000	5.06102
9.650000	1.31007
9.635000	0.71827
9.625000	0.29697
9.620000	0.11079
9.617500	0.00565
9.617400	0.00066
9.617375	0.00039
9.617370	0.00018
9.617368	0.00006
9.617367	0.00004
9.617367	0.00002

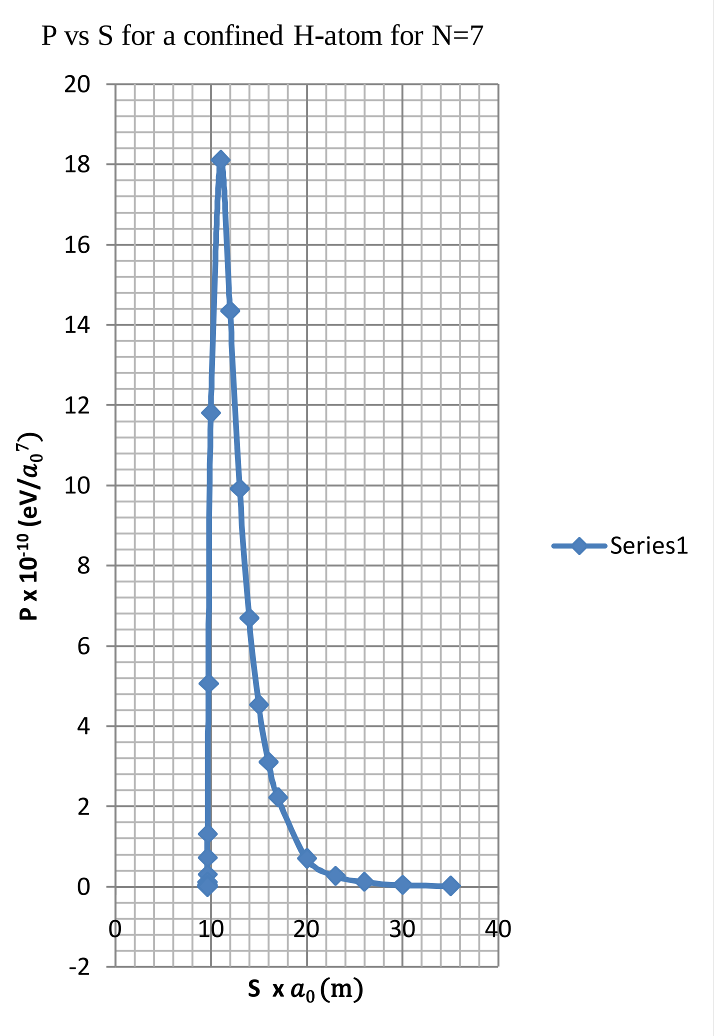

Fig (23): Relation between the pressures exerted on a confined H-atom and the radius of the cavity when *l* = 0, N=7.

Table (14): Relation between pressures exerted on a confined hydrogen atom and the radius of the cavity for *l*=0,N=8.

$S \times a_0$ (m)	$P \times 10^{-12} (\mathrm{eV}/{a_0}^8)$
54.00	0.00096
37.00	0.01940
36.00	0.02396
32.00	0.06094
27.00	0.23501
20.00	2.34156
17.80	5.19539
17.00	6.98518
16.00	9.87425
15.00	13.9608
14.00	16.3360
13.50	17.1085
12.500	9.91693
12.400	2.06252
12.385	1.53933
12.380	1.31971
12.370	1.02259
12.355	0.05120
12.351	0.03452
12.350	0.03110

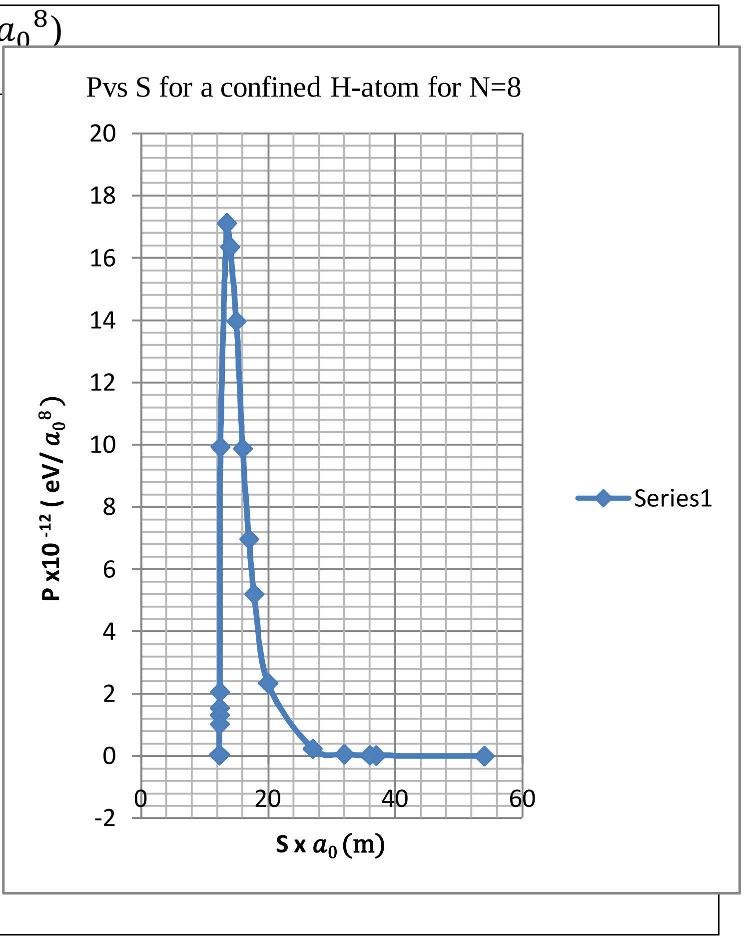

Fig (24): Relation between the pressure exerted on a confined H-atom in a cavity and the radius of the cavity when *l* = 0, N=8.

Table (15): Relation between Pressures exerted on a confined hydrogen atom and the radius of the cavity for *l*=0,N=9.

S× a_0 (m)	P × 10^{-16}(eV/$a_0{}^9$)
65.0000	0.0069
46.0000	0.1553
44.0000	0.2316
40.0000	0.5469
30.0000	6.8913
29.0000	9.3323
26.0000	24.772
23.0000	63.767
20.0000	178.97
18.0000	320.80
17.0000	377.03
16.0000	279.47
15.5000	81.655
15.4000	24.288
15.3800	12.073
15.3750	7.2867
15.3740	7.0257
15.3700	4.4072
15.3690	3.8326
15.3650	1.0686
15.3640	0.3675
15.3635	0.0344

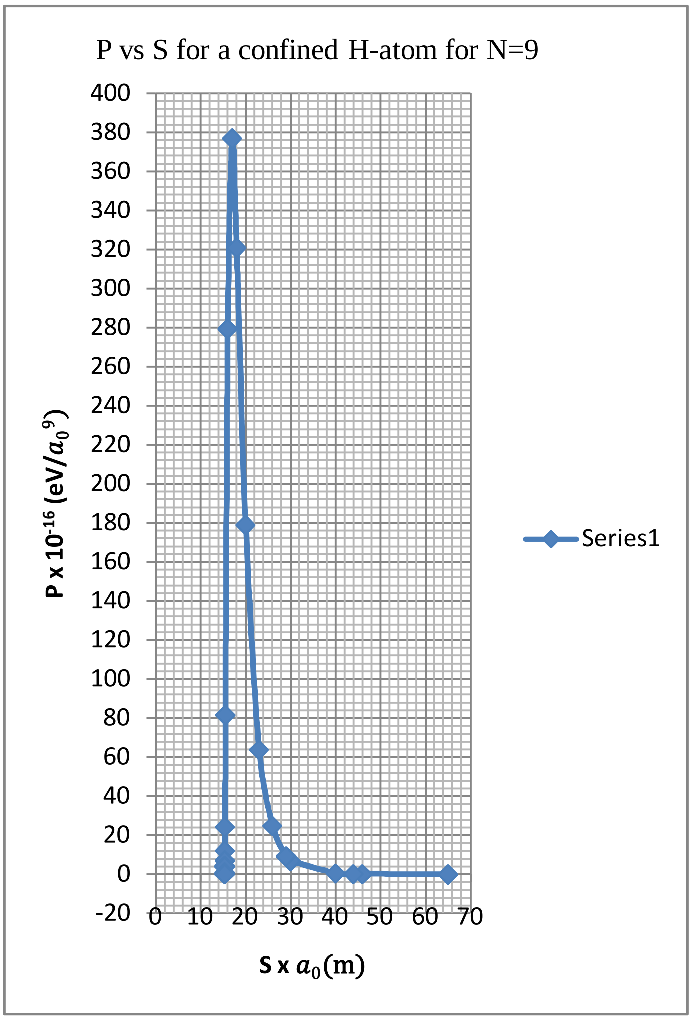

Fig.(25): Relation between the pressure exerted on a confined H- atom in a cavity and the radius of the cavity when *l* = 0, N=9.

Table (16): Relation between Pressures exerted on a confined hydrogen atom and the radius of the cavity for *l*=0,N=10.

S× a_0 (m)	P× 10^{-18}(eV/${a_0}^{10}$)
77.500	0.00668
54.000	0.24983
42.000	3.02896
31.000	57.2121
25.000	378.649
23.000	683.432
20.000	1121.19
19.000	506.298
18.900	362.258
18.700	35.0134
18.685	6.49326
18.684	4.01117
18.682	0.72287

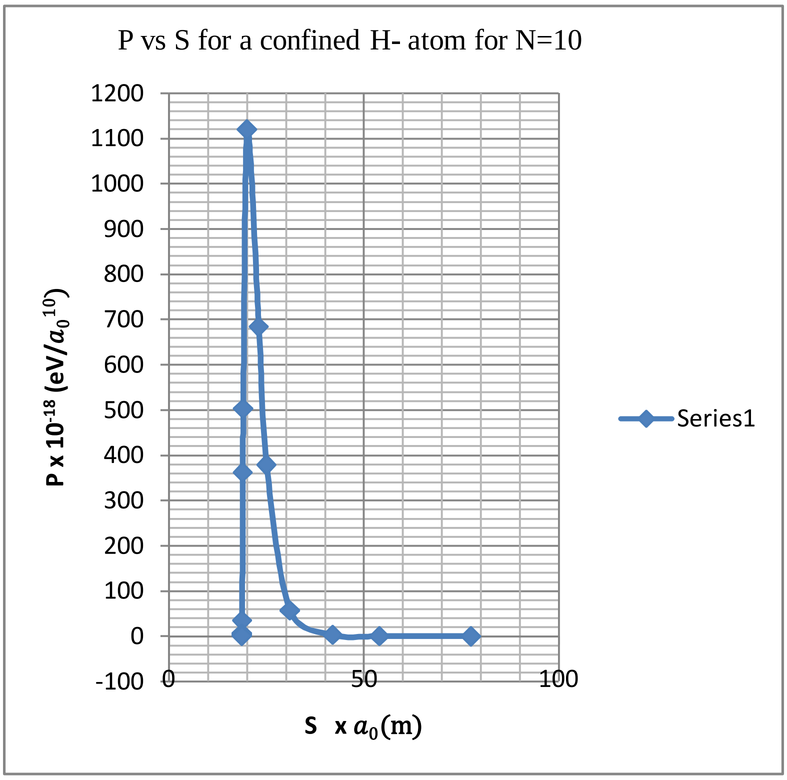

Fig.(26): Relation between the pressures exerted on a confined H-atom in a cavity and the radius of the cavity for *l* = 0, N=10.

In this part of the study, we represent the relation between the pressures exerted on the H-atom due to change of radius of the cavity for each value of N from 3 to 10 in graphs as shown above from Fig (19) to Fig. (26).

This relation is interesting, where it is noticed that when the radius of the cavity is increased the pressure decreases and approaches zero as S is large, which implies that the cavity effect becomes negligible and the H-atom acts like a free one. While when the radius of the cavity decreases the pressure increases gradually up to a certain maximum value, for each value of N, this maximum occures at a certain value of the cavity radius which we call $S_{p\ max}$. If the radius of the cavity becomes less than $S_{p\ max}$, the pressure will decrease rapidly until it approaches zero again within a very short range of S. We suggest that this is because as S decreases, one is moving away from maximum distribution function, and the probability of finding the H-atom within this region becomes small. (Radial distribution function gives the probability of finding the particle in a distance **r** from a certain point in space),

Table (17): Relation between the values of S, where the pressure is maximum and N.

$S_{P\ max} \times a_0$ (m)	N
2.4	3
4.0	4
6.0	5
8.0	6
11.0	7
13.5	8
17.0	9
20.0	10

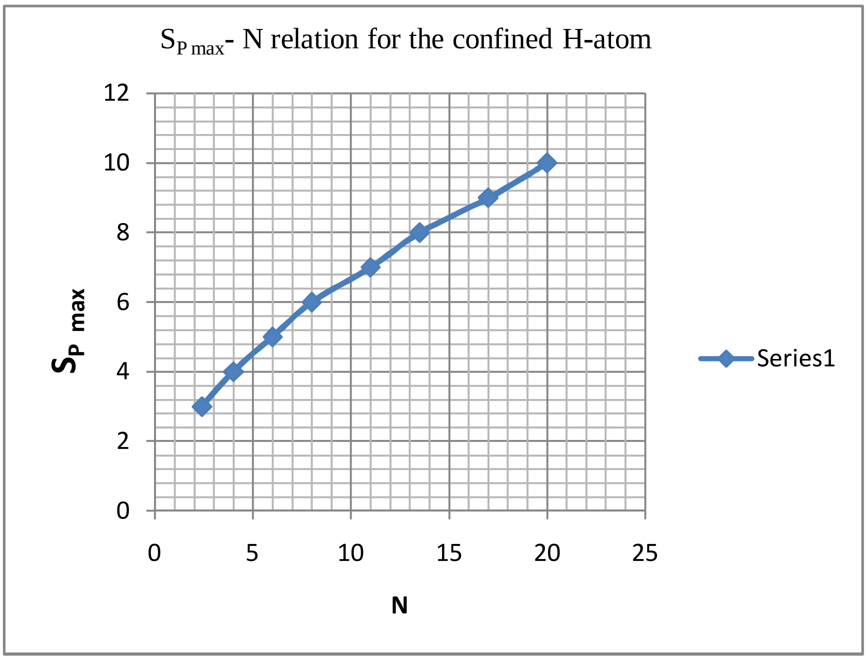

Fig. (27): Relation between the radius of the cavity at which the pressure has a maximum value, and N for the ground state of a confined H-atom.

We examined the relation between the radius at which pressure is maximum, $S_{p\ max}$, and N, see Fig. (27) above, we found that as N increases $S_{p\ max}$ increases which is due to the dependence of the radial distribution function on space dimension N.

Chapter 4

Conclusions and Future Work

Chapter four

Conclusions:

After completing this study, the following conclusions can be drawn:

1- In this study the Schrödinger equation for the confined H-atom in a spherical cavity has been solved, in N-dimensions. It has been shown that the wave functions are dimension-dependent and having the same form as those of the free H-atom in N- dimensions.

2- The ground state energy eigen-values for the confined H-atom in a spherical cavity, for $l=0$ have been evaluated for spatial dimensions from 3 to 10. We found that the energy eigen-values are quantized and dimension-dependent. That is for a certain dimension and for a given radius of the cavity there are a certain number of zeros, these zeros represent the solutions of the Schrödinger equation and the largest zero coincides with the boundary conditions for this problem, and the corresponding eigen-values represent the bound states for these N & S. The largest value of the zeros corresponds to the smallest λ which, here, corresponds to the smallest value of energy of the confined H-atom, in other words indicates the ground state energy.

It has been noticed that the energy of the confined H-atom, increases as the radius of the cavity decreases until it approaches zero where the kinetic energy equals the potential energy at a value of the radius of the cavity called the critical cage radius. It has been shown that as the size of the cavity is lowered, there ultimately exists a point where the electron becomes delocalized (its binding energy becomes zero) and it behaves like a particle in a sphere.

As a definition, the critical cage radius means the minimum radius of a cavity where the total energy of the confined electron becomes zero, or not bound.

Critical cage radius has been calculated for space dimensions N (2-10).Our results show that the critical cage increases as N increases. This is because the particle is repelled further away from the nucleus, due to the extra repulsive potential in the effective term. According to our calculations, for N=3, the value of $S_c = 1.835247 \times a_0$ where it was found by Sommerfeled and Welker that $S_c = 1.835 \times a_0$. The critical cage radii for different values of N are calculated and listed in Table (4).

Also the energy of the confined H-atom decreases as the radius of the cavity increases, down to the free limiting value where the radius of the cavity becomes large enough so that the confined H-atom acts like a free one, and thus the value of its energy approaches that of the free H-atom in that dimension.

The dependence of the energy on the dimension N has also been investigated, it has been noticed that the energy increases as N increases.

In other words, the effect of space dimension on the ground-state energy becomes more profound as N increases.

Our results revealed that the number of bound states decreases either as the cavity size decreases for given N or as the space dimension N increases for a given cavity radius.

An interesting case ($\propto = -1$) in the hyper geometric part of the wave function $R_{\lambda l}(\rho)$, shows that there is only one bound state, for a given dimension, whose energy coincides with the first exited-state energy (n=2) for the free H-atom in that dimension. It has also been shown that in the limit of infinite dimension ($N \longrightarrow \infty$) the cavity radius becomes infinite and thus the hydrogen atom becomes a free one.

A comparison between the ground state energy of the free H- atom and a confined one for given N reveals that the percentage difference between these energies is more profound for large values of N, go back to Tables (7), (8).

3- The pressure exerted on the wall of the cavity due to enclosing the H-atom inside a cavity of radius S, depends on N and S, it is found that for a given N, the pressure increases with decreasing radius up to a certain value and then starts to decrease, this value of P is a maximum. The value of this pressure increases with increasing N, and the value of the radius of the cavity at which the pressure is maximum increases as N increases.

4- As I mentioned before this study is only for the ground-state energy (l=0). As a future study I am looking forward to extend this work for different values of l, *to* examine the effect of confinement, for $l > 0$, on physical properties of the confined H-atom.

Appendix A

Theoretical background

In the 20th century, some natural phenomena that classical physics couldn't explain were noticed. One of these phenomena is the photoelectric effect, another one is the diffraction pattern of the electrons from crystals, and the phenomenon of the black body radiation, and the stability of atoms, and all of these phenomena were questions with no answers. These simulate the need for a new theory which is based on new assumptions that build a new model in physics. This new model is called the quantum theory which was originated by Max Planck in the year 1901. The model has been used by Einstein, and Bohr to explain photoelectric effect and the spectrum of the H- atom for its simplicity. Afterwards, de Broglie proposed the wave nature of particles; and proposed a formula for the wave length that is accompanied by the moving particle, namely,

$$\lambda = \frac{h}{p} \tag{A.1}$$

Where h is the Planck's constant and p is the linear momentum of the moving particle. This wave aspect of particles was proved experimentally through the Davison and Germer experimental confirmation, where the electrons were diffracted from the crystal like waves.

But the de Broglie theory was unsatisfactory, because it depends on the classical basics of uniquely momenta and uniquely defined wave lengths.

The new model shows uncertainty in locating the position of the particle or indicating its momentum that is shown by the Heisenberg uncertainty principle.

The mathematical aspects of nonrelativistic quantum mechanics are determined by solutions to Schrödinger equation.

The time independent Schrödinger equation for a particle of mass m, with potential energy V(x) in one dimension is,

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \qquad \text{(A.2)}$$

This has a complete solution including the time dependence given in this form, $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$ (A.3)

While in 3-dimensions by using spherical coordinates, the Schrodinger equation is,

$$\frac{-\hbar^2}{2m}\nabla^2\psi(r,\theta,\varphi) + V(r)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi) \qquad \text{(A.4)}$$

$\psi(r,\theta,\varphi)$ is the Schrödinger wave function which is a mathematical description of the wave packet which describes the particle, and it is composed of a collection of waves representing a range of momentum. The particle is localized in a region of space defined by its wave packet, that contains all of the information that are available about the particle, and hence (particle ≡ wave packet).

For $\psi(r,\theta,\varphi)$ to be acceptable as a wave function, it must be normalizable, and any solution of the Schrödinger equation which allows $\psi(r,\theta,\varphi)$ becoming infinite must be discarded.

Then $\psi(r,\theta,\varphi)$ as well as its first derivative across any boundary must be continuous exept when the potential has an infinite jump where $\frac{d\psi}{dx}$ is discontinuous. Finally, it must be orthonormalized.

Now, we are concerned in finding the radial part of $\psi(r,\theta,\varphi)$, that is

ψ(r) . Thus knowing ψ(r) of a particle enables us to calculate many of its properties,

∇^2 operator in 3 dimensions is given by,

$$\nabla^2 = \frac{\partial^2\psi(r,\theta,\varphi)}{\partial r^2} + \frac{2}{r}\frac{\partial\psi(r,\theta,\varphi)}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\psi(r,\theta,\varphi)}{\partial\theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial^2\psi(r,\theta,\varphi)}{\partial\varphi^2} \tag{A.5}$$

Now, in N dimensional space, the laplacian operator in polar coordinates (r,θ_1, θ_2, θ_3, θ_4, θ_5, … … … …, θ_{N-2}, φ) , of R^N.

$$\nabla^2 = \mathrm{r}^{(1-\mathrm{N})}\frac{\partial}{\partial \mathrm{r}}\left(\mathrm{r}^{(\mathrm{N}-1)}\frac{\partial}{\partial \mathrm{r}}\right) + \frac{1}{r^2}\Lambda^2 \tag{A.6}$$

Λ^2 is a partial differential operator on the unit sphere S^{N-1}, which also is the square of the angular momentum operator [1].

Making separation of variables in eqn. (A.8) yields a radial equation and angular equation.

The radial Schrodinger equation is written in different references as follows[1],

$$r^{1-N}\frac{d}{dr}\left(r^{N-1)}\frac{dR}{dr}\right)-\frac{\beta}{r^2}R+\frac{2m}{\hbar^2}(V(r)-E)\,R=0 \qquad \text{(A.7)}$$

Here β is the separation constant which also are the eigen values of $\wedge^2$, and

$$\beta = l(l+N-2\,) \qquad \text{(A.8)}$$

It worths here to write down the relation between the polar coordinates in N- dimensional Euclidian space (r, θ_{N-2}, …., θ_1, φ). Where $0\leq \varphi \leq 2\pi$, and $0 \leq \theta_i \leq \pi$, and the Cartesian coordinates ($x_{1,}x_{2,}$….,x_n) [21].

$$x_1 = \mathrm{r}\cos\varphi\ sin\ \theta_1 sin\ \theta_2 \ldots\ldots\ldots\ldots sin\ \theta_{n-2}$$

$$x_2 = \mathrm{r}\sin\varphi\ sin\ \theta_1 sin\ \theta_2 \ldots\ldots\ldots\ldots sin\ \theta_{n-2}$$

$$x_3 = \mathrm{r}\cos\theta_1\ \sin\theta_2 \ldots\ldots\ldots\ldots\ldots\ldots \sin\theta_{n-2}$$

.

.

$$x_i = \mathrm{r}\cos\theta_{\ i-2}\ \sin\theta_{\mathrm{i}-1}\ \ldots\ldots\ldots\ \sin\theta_{\mathrm{n}-2}$$

.

.

$$x_n = \mathrm{r}\ \cos\theta_{n-2} \qquad \text{(A.9)}$$

Where the length element is given by [19],

$$ds^2 = \sum_{i,j=1}^{n} g_{ij}\, du^i du^j \qquad \text{(A.10)}$$

where $u^1 = r,\ u^2 = \theta_{\mathrm{n-2}}, \ldots\ldots\ldots u^{n-1} = \theta_1,\ u^n = \varphi$, And the metric tensor in N-dimensional polar coordinates is,

$$\begin{pmatrix} 1 & 0 & 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & 0 \\ 0 & r^2 & 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots & 0 \\ 0 & 0 & r^2 sin\theta_{n-2} & \ldots\ldots\ldots\ldots\ldots & 0 \\ 0 & 0 & 0 & \ldots\ldots\ldots\ldots\ldots\ldots\ldots & 0 \\ . & . & . & \ldots\ldots\ldots\ldots\ldots\ldots\ldots & 0 \\ . & . & . & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ \ldots\ldots & r^2 \sin^2\theta_{\mathrm{n-2}} \ldots \sin^2\theta_1 \end{pmatrix}$$

(A.11)

Let g = det g_{ij} = $r^{2(n-1)} sin^{2(n-2)}\theta_{(n-2)} \ldots sin^2\theta_1$

(A.12)

Then the $\nabla^2 = \frac{1}{\sqrt{g}} \sum_{i,j=1}^{n} \frac{\partial}{\partial u^i} \left(\sqrt{g}\ \frac{1}{g_{ij}} \frac{\partial}{\partial u^j} \right)$ (A.13)

Since we are interested in the radial part, then

$$\nabla^2 = \frac{1}{r^{N-1}} \frac{d}{dr} \left(r^{N-1} \frac{d}{dr} \right) = \frac{d^2}{dr^2} + \frac{N-1}{r} \frac{d}{dr} \qquad \text{(A.14)}$$

The Hamiltonian for a particle of mass m with potential *V(r)* is,

$$H = \frac{-\hbar^2}{2m} \nabla^2 + V(r) = \frac{-\hbar^2}{2m} \left[\frac{d^2}{dr^2} + \frac{N-1}{r} \frac{d}{dr} + \text{‘angular momentum term’} \right] + V(r) \qquad \text{(A.15)}$$

As soon as the Laplacian and the Hamiltonian operators are written, the Schrödinger equation can be easily written as,

$$\frac{-\hbar^2}{2m}\,\nabla^{2}R(\mathrm{r}) + V_{eff}\,R(\mathrm{r}) - E\,R(\mathrm{r}) = 0 \qquad \text{(A.16)}$$

Or

$$\left[\frac{d^2}{dr^2} + \frac{N-1}{r}\frac{d}{dr} - \frac{l(l+N-2)}{r^2} + \frac{2m}{\hbar^2}\frac{e^2}{4\pi\varepsilon_0 r} + \frac{2m}{\hbar^2}E\right] R(r) = 0 \qquad \text{(A.17)}$$

This equation is very important in this research, whose solution will be used to find the eigen functions and the eigen values for the confined H-atom in a spherical cavity.

Appendix B

The confluent hyper-geometric function [22].

The confluent hyper geometric differential equation is,

$$x\frac{d^2u}{dx^2} + (\gamma - x)\frac{du}{dx} - \propto x = 0 \tag{B.1}$$

This equation has a solution called the Kummer confluent hyper-geometric functions $u(x) = {}_1F_1(\propto ; \gamma ; x) = \frac{\sum_{n=0}^{\infty}(\propto)_n x^n}{(\gamma)_n n!}$.

$$u(x) = 1 + \frac{\propto}{\gamma}\frac{x}{1!} + \frac{\propto(\propto+1)}{\gamma(\gamma+1)}\frac{x^2}{2!} + \ldots\ldots\ldots\ldots\ldots\ldots \tag{B.2}$$

$\gamma \neq 0,-1,-2,\ldots\ldots\ldots\ldots\ldots$

If $\propto$ is zero or negative number then ${}_1F_1(\propto; \gamma; x)$ becomes a polynomial.

The Pochhammer symbol $(\propto)_n$ is defined as,

$$(\propto)_n = \propto(\propto+1)(\propto+2)\ldots\ldots\ldots\ldots(\propto+n-2)(\propto+n-1) \tag{B.3}$$

$$= \frac{(\propto+n-1)!}{(\propto-1)!} = \frac{\Gamma(\propto+n)}{\Gamma(\propto)} \quad n \geq 1 \tag{B.4}$$

Notice that $(\propto)_0 = 1$, $\propto \neq 0$, and $\Gamma(n+1) = n!$

The Lagurrre polynomials $L_{\propto}^{\gamma}(x)$ are related to the confluent hyper geometric functions as follows,

$$L_{\propto}^{\gamma}(x) = \frac{(\propto+\gamma)!}{\propto!\gamma!}{}_1F_1(-\propto;\gamma+1;x) = \frac{\Gamma(\propto+\gamma+1)}{\propto!\Gamma(\gamma+1)}{}_1F_1(-\propto;\gamma+1;x) \tag{B.5}$$

Therefore if $R_{\lambda l}\ (\rho) = \ A\ \rho^{l+1}\ e^{\ (-\frac{\rho}{2})}\ L_{\propto}^{\gamma}\ (\rho)$ then we can write it equivalently using the confluent hyper-geometric function as,

$$R_{\lambda l}(\rho)\ =\ A\ \rho^{l+1}\ e^{\ (-\frac{\rho}{2})}\ \frac{(\propto+\gamma)!}{\propto!\gamma!}\ {}_1F_1\ (-\propto;\gamma\ +1;\rho)$$

$$= A'\ \rho^{l+1}\ e^{\ (-\frac{\rho}{2})}\ {}_1F_1\ (-\propto;\gamma\ +1;\rho) \qquad \text{(B.6)}$$

$$A' = A\,\frac{(\propto+\gamma)!}{\propto!\gamma!} \qquad \text{(B.7)}$$

with $\propto = l + \frac{N-1}{2} - \lambda$ (B.8)

$$\gamma = 2l + N - 1 \qquad \text{(B.9)}$$

then $R_{\lambda l}(\rho) = A\ \rho^{l+1}\ e^{\ (-\frac{\rho}{2})}\ \frac{\left(\lambda+l+\frac{N-3}{2}\right)!}{\left(l+\frac{N-1}{2}-\lambda\right)!(2l+N-2)\,!}\ {}_1F_1\ (-\propto;\gamma\ +1;\rho)$ (B.10)

where $A\ \frac{\left(\lambda+l+\frac{N-3}{2}\right)!}{\left(\lambda-l-\frac{N-1}{2}\right)!(2l+N-2)\,!}\ =\ A'$ (B.11)

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جامعة النجاح الوطنية

كلية الدراسات العليا

ذرة الهيدروجين المحصورة في فجوة كروية في فضاء متعدد الأبعاد

اعداد

مزين عبد الحميد علي شقور

اشراف

أ.د. سامي الجبر

قدمت هذه الأطروحة استكمالاً لمتطلبات درجة الماجستير في الفيزياء بكلية الدراسات العليا في جامعة النجاح الوطنية في نابلس - فلسطين.

2009

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الملخص

في هذا البحث تم حل معادلة شرودنجر لذرة الهيدروجين المحصورة في فجوة كروية وفي فضاء متعدد الأبعاد $N \geq 3$، حيث تم ايجاد الاقترانات الموجية التي تمثل ذرة الهيدروجين تلك. كما تم ايجاد صيغة لحساب قيم الطاقة التي يمكن لها أن تمتلكها.

ومن اللافت للنظر في حل هذه المسألة أن معادلة شرودنغر تحت هذه الظروف لها نفس صيغة معادلة شرودنغر في حالة ذرة الهيدروجين الحرة وفي الفضاء متعدد الأبعاد ولذلك كان لها نفس صيغة الحل (الاقتران) والتي تنطبق عندها شروط تحقيق الحل؛ في حين تختلف قيم الطاقة في حالة ذرة الهيدروجين الحرة عن تلك في حالة ذرة الهيدروجين المحصورة في فجوة كروية مغلقة، حيث أن الصيغة التي تستخدم لحساب قيم الطاقة في حال كونها حرة هي معادلة(3.7)، في حين أن الصيغة التي تستخدم لحساب قيم الطاقة في حال كونها محصورة تعطى بمعادلة (3.4).وكانت صيغة اقتران الحل هي:

Confluent Hyper geometric function

أي

$$R_{\lambda l}(\rho) = A' \rho^{l} e^{\left(-\frac{\rho}{2}\right)} {}_1F_1\left(l+\frac{N-1}{2}-\lambda;\ 2l+N-1;\ \rho\right)$$

وهذا الحل يحقق ظروف المسألة عند حدود الفجوة، حيث تكون قيمة الاقتران تساوي صفرا عندما r تساوي نصف قطر الفجوة حيث $\rho = \frac{2}{a_0\,\lambda}\; r|_{r=S}$، ولهذا نحتاج لايجاد قيم النقاط التي تكون عندها قيمة الاقتران تساوي صفرا وهذه النقاط تسمى أصفار الاقتران، وللحصول على أدنى قيمة للطاقة نختار أكبر قيمة من قيم هذه الأصفار، ولقد تم استخدام Mathematica (5.0) لايجاد أصفار الاقتران $_1F_1\,(l+\frac{N-1}{2}-\lambda;\, 2l+N-1;\, \rho)$ والتي يتحقق عندها الحل والتي تستخدم لتحديد قيم الطاقة التي يمكن لذرة الهيدروجين امتلاكها في أي مستوى حسب العلاقة $E_n = \frac{a_0^2}{4}\frac{{x_n}^2}{S^2}E_0$.

حيث E_0 هي طاقة ذرة الهيدروجين الحرة وهي في أدنى مستوى للطاقة، أما a_0 فهي نصف قطر مستوى الطاقة الاول لذرة الهيدروجين ويسمى نصف قطر بور، أما S فهي نصف قطر الفجوة.

ولقد تم استنتاج ان قيم الطاقة لذرة الهيدروجين تحت هذه الظروف تعتمد على N (عدد الأبعاد التي تمثل الفضاء الذي يحتوي ذرة الهيدروجين) ، كما وتعتمد على نصف قطر الفجوة التي تحتوي على ذرة الهيدروجين.

ففي هذه الدراسة حسبت قيم الطاقة في المستوى الأدنى لذرة الهيدروجين المحصوره في فجوة كروية عندما $l=0$ حيث وجد أنه كلما زادت N زادت E_n أيضا، وكلما زادت S قلت E_n. ويفسر هذا بالأعتماد على قيمة الجهد الفعال والذي يعطى بالعلاقة:

$$V_{eff} = V(r) + [l\,(l+N\text{-}2) + \frac{(N-1)(N-3)}{4}]\frac{1}{r^2}$$

والتي منها نستطيع أن نستنتج أن قيمة الجهد الفعال تزداد بزيادة N وتصبح أقل سلبية وعندها تكون قيمة الطاقة الحركية للالكترون والتي تستطيع الغاءها أ قل، وعندها تكون الطاقة الكلية للالكترون صفرا.

أما نصف قطر الفجوة التي تصبح عندها ألطاقة الكلية للالكترون تساوي صفرا فيسمى نصف القطر الحرج للفجوة S_c وعند هذه القيمة لا يعود الالكترون مقيدا.

ولقد حسبت قيم نصف القطر الحرج في هذا البحث، للأبعاد من 2 – 10 ودونت في جدول رقم (4)، حيث وجد أنه بزيادة N تزداد قيمة S_C وهذا يعود لتأثير الجزء الاضافي في الجهد الفعال $l(l+N-2)+\frac{(N-1)(N-3)}{4}$ والذي يعمل على طرد الالكترون بعيدا عن النواة والذي يزداد بزيادة N.

كما وتمت دراسة مستويات الطاقة التي يمتلك فيها الالكترون طاقة سلبية ووجد أن عددها يزداد كلما نقصت قيمة N وكلما زادت قيمة S، حيث أن زيادة S ونقصان N ينقص من قيمة الطاقة الكلية للالكترون.

وعند اجراء مقارنة بين قيم الطاقة التي تمتلكها ذرة الهيدروجين الموجودة في الفجوة ذات أبعاد معينة عندما l=0 مع قيم الطاقة التي تمتلكها هذه الذرة وهي حرة في نفس البعد للفضاء التي توجد فيه، تبين أن التباعد بين قيم الطاقة في الحالتين يكون ملحوظا أكثر كلما زادت قيمة N.

كما ودرست العلاقة بين نصف قطر الفجوة والضغط الذي يحدثه تغيير نصف قطرها، حيث وجد ان انقاص نصف القطر يزيد الضغط الى قيمة قصوى نسمي عندها نصف قطر الفجوة $S_{p\ max}$ واذا تناقص نصف القطر أكثر تتناقص بعدها قيمة الضغط حتى تؤول الى الصفر.