The quantum states for Hydrogen atom: spherical harmonics and the orbitals geometrical representation

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***Abstract**: Our work utilizes the quantum model of the hydrogen atom which is based on the Schrödinger equation with Coulomb potential. Specifically, we concentrate on the angular components of the wave eigenfunctions derived from this model. We consider the quantum states with $n \leq 4$. In order to visualize the orbital shapes of these states, we built in the spherical coordinates system their 3D geometric representations. Furthermore, we use the corresponding spherical harmonics, to calculate the θ nodal values that describe the configurations of these orbital states.*

***Key Words**: spherical harmonics, stellar oscillations modes, quantum states, orbitals 3D visualization*

1. INTRODUCTION

Through their works of early twentieth century, Planck, Schrödinger (1926), Bohr, Pauli and others developed Quantum Mechanics. This allows the study of physical phenomena on an atomic and subatomic scale. It also complements areas such as Acoustics and Optics, and facilitates the development of Field Theory along with Quantum Electrodynamics, Nuclear Physics and the Standard Model. Some books allow the application of Quantum Physics [1] in areas as Astrophysics [2] and Stellar Atmosphere [3].

In our preoccupations [4-6], we focus on the harmonic components of the wave functions generated by the physical model of hydrogen atom.

In addition to various theoretical aspects, the angular components of wave functions complement the purely mathematical and topological studies relating to the spherical harmonics, which are also found in the pulsation modes of stars [7].

The paper structure is as follows: in Section 2, we briefly present the basic equations and formulas for our atomic model; in Section 3, for a fixed ***n*** less than 5, we consider the spherical harmonics and compute the corresponding θ nodal values. We then construct 3D representations of orbital states and describe them using these nodal values.

Finally, we underline the importance of visualizing orbitals in 3D using spherical harmonics corresponding to the atomic shells and sub-shells.

2. BASIC EQUATIONS FOR THE HYDROGEN ATOMIC QUANTUM MODEL

In the fine structure atomic model, for an atemporal potential like Coulomb potential,

$V = V(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$, Schrödinger equation becomes [1]:

$$\left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(r)\right] \cdot \psi_{nlm}(r,\theta,\varphi) = E_{nl} \cdot \psi_{nlm}(r,\theta,\varphi) \tag{1}$$

where $r > 0$, $\theta \in (0, \pi)$, $\varphi \in [0, 2\pi)$ are the spherical coordinates, μ the reduce mass, e is the electron charge and ε_0 is the permittivity of vacuum.

This potential has also spherical symmetry [4], so we can write Laplace's operator:

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

Solving the Schrödinger equation using the variables separation method, we find the space components of wave functions:

$$\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r) \cdot Y_l^m(\theta,\varphi) \tag{3}$$

and the following quantum states (n, ℓ, m) characterized by n =1,2,3 … the principal quantum number which quantifies the total energy of the electron ℓ = 0, 1, 2, …, n-1, the quantum number of the orbital angular momentum and m = - ℓ, ... 0, ...ℓ, the magnetic quantum number. Further, the radial components are:

$$R_{n\ell}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)}{2n[(n+l)!]^3}}\, e^{-\frac{r}{a_0}} \left(\frac{2r}{na_0}\right)^{\ell} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right) \tag{4}$$

with their associated Laguerre's polynomials and the first Bohr's radius a_0.

Also, the harmonic components are:

$$Y_\ell^m(\theta,\varphi) = (-1)^m \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\, P_\ell^m(\cos\theta)e^{im\varphi}, \qquad m \geq 0 \tag{5}$$

and:

$$Y_\ell^{-m}(\theta,\varphi) = (-1)^m Y_\ell^m(\theta,\varphi), m < 0 \tag{6}$$

with their associated Legendre's polynomials.

From physical reasons we compute a useful quantum expression namely the electron localization probability density function by formula

$$|\psi_{nlm}(r,\theta,\varphi)|^2 \tag{7}$$

Since in eq. (6) the spherical harmonics expressions Y_ℓ^m m show quasi-symmetric in relation to the index m, in this paper we work in the convention $m = |m|$.

3. THE 2D AND 3D REPRESENTATION OF THE ATOMIC ORBITALS

In the system of spherical coordinates in colatitude $\theta \in (0, \pi)$ and azimuth $\varphi \in [0, 2\pi)$, and based on the formulas (5) - (7), we build and describe the orbital shapes associated with the quantum states of the hydrogen atom excited with $n \leq 4$.

For a fixed n, their sub-shells are used to compute the spherical expressions [5] via the formula (5) up to the degree $\ell = 3$ and $m = 0\ldots\ell$. Then, we compute the θ nodal values for each sub-shell and obtain the following results:

For $\ell = 1$:

$Y_1^0(\theta,\varphi)$ generates the θ nodal value: $\frac{\pi}{2}$.

$Y_1^1(\theta,\varphi)$ generates the θ nodal value: 0, π.

For $\ell = 2$:

$Y_2^0(\theta,\varphi)$ generates the θ nodal values: $arccos\sqrt{\frac{1}{3}}, \pi - arccos\sqrt{\frac{1}{3}}$.

$Y_2^1(\theta,\varphi)$ generates the θ nodal value: 0, $\frac{\pi}{2}$, π.

$Y_2^2(\theta,\varphi)$ generates the θ nodal value: 0, π.

For $\ell = 3$:

$Y_3^0(\theta,\varphi)$ generates the θ nodal values: $\frac{\pi}{2}, arccos\sqrt{\frac{3}{5}}, \pi - arccos\sqrt{\frac{3}{5}}$.

$Y_3^1(\theta,\varphi)$ generates the θ nodal values: 0, π, $arccos\sqrt{\frac{1}{5}}, \pi - arccos\sqrt{\frac{1}{5}}$.

$Y_3^1(\theta,\varphi)$ generates the θ nodal value: 0, $\frac{\pi}{2}$, π.

$Y_3^2(\theta,\varphi)$ generates the θ nodal value: 0, π.

In Figure 1, we make the 2D representation of the sub-shells corresponded to the quantum states (4 ℓ = 0..3 0).

Further, we build the 3D representation of the sub-shells, including of the special quantum states [6], as follows:

The sub-shell ℓ= 0 contains only the state (4 0 0) (Fig. 2).

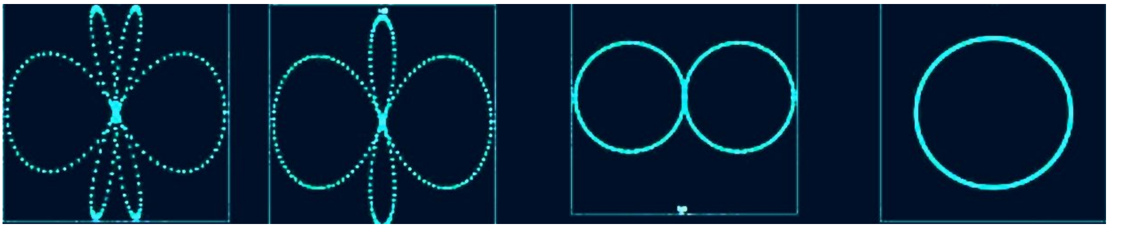

Fig. 1 – The 2D representation of states (4 ℓ = 0..3 0) beginning from the left panel for the orbital S with ℓ = 0 to the right panel for orbital F with ℓ = 3, respectively

Remark: According to formula (5) and also from Fig. 2 we obtain that the state (4 0 0) does not display any nodal angle and we can generalize this remark to S-type orbitals.

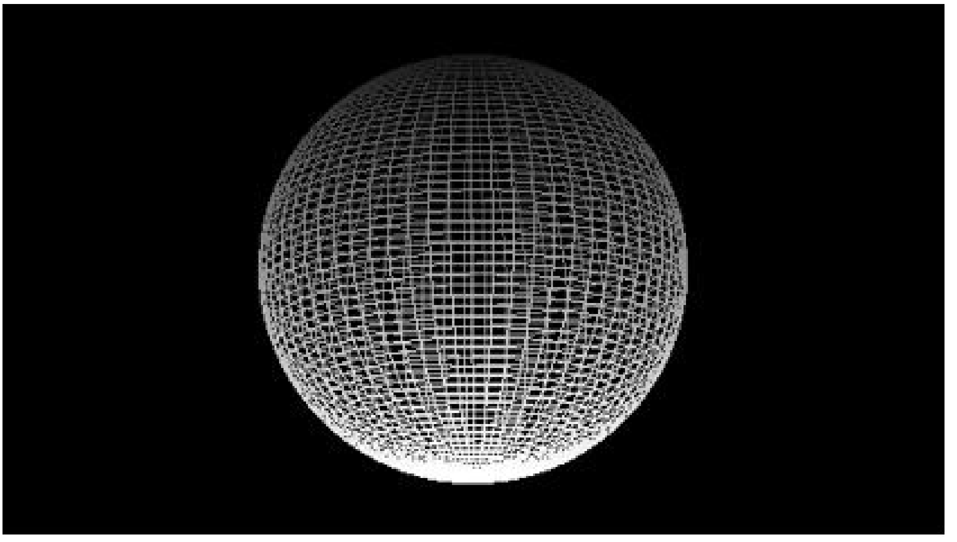

Fig. 2 – The 3D representation of state (4 0 0).

Inside the shell $n = 4$, we construct the geometric representations in spherical coordinates (θ, φ) for each sub-shell, namely for each fixed ℓ.

Thus, we obtain 3D orbital visualizations from all three harmonic pulsation modes: namely, for $m = 0$, $m = \ell$ and for the rest of orbital states [2].

In Figures 3, 4 and 5, we represent the modes with $m = 0$ corresponding to the orbital states (4 1 0), (4 2 0), (4 3 0).

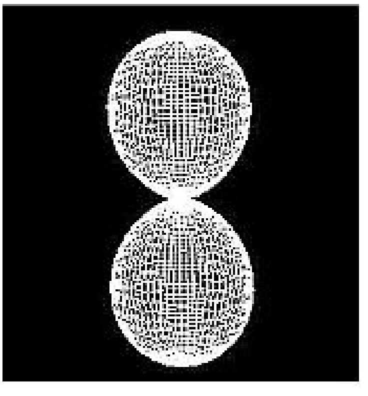

Fig. 3 – The 3D representation of state (4 1 0)

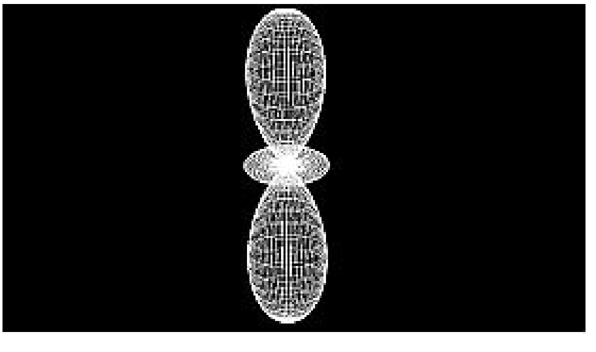

Fig. 4 – The 3D representation of state (4 2 0)

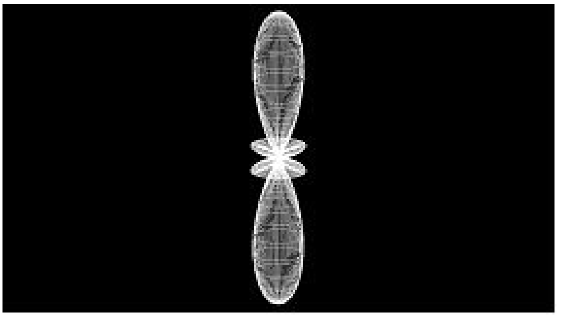

Fig. 5 – The 3D representation of state (4 3 0)

In Figures 6, 7 and 8, we represent the modes with $m = \ell$ corresponding to the orbital states (4 1 1), (4 2 2), (4 3 3).

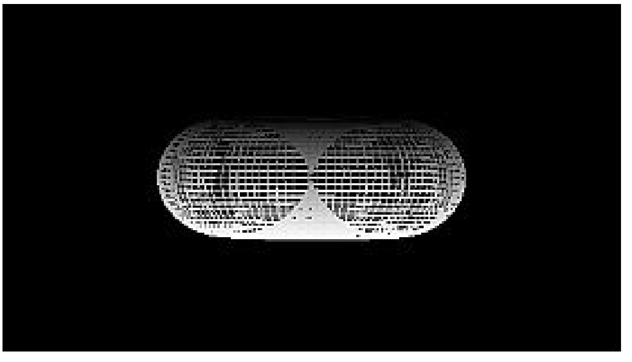

Fig. 6 – The 3D representation of state (4 1 1)

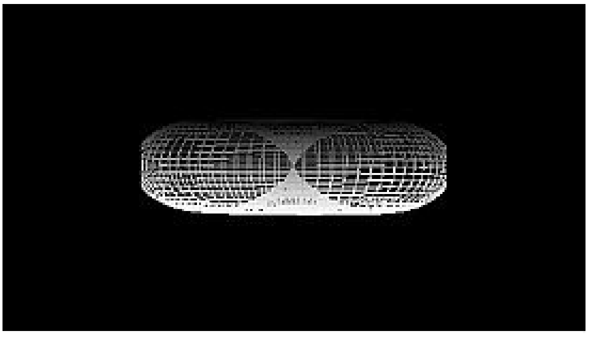

Fig. 7 – The 3D representation of state (4 2 2)

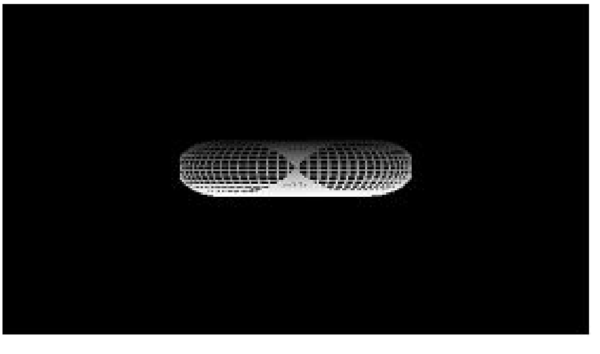

Fig. 8 – The 3D representation of state (4 3 3)

In Figures 9, 10 and 11, we built the pulsating modes for the rest quantum states, namely (4 2 1), (4 3 1), (4 3 2).

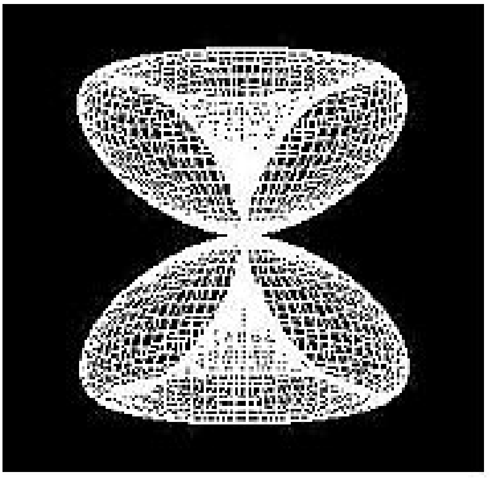

Fig. 9– The 3D representation of state (4 2 1)

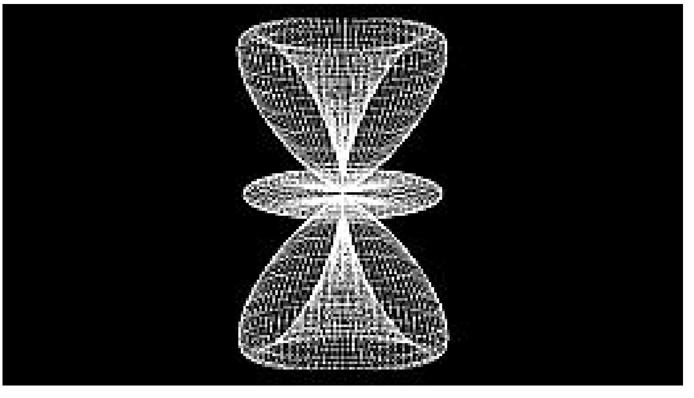

Fig. 10 – The 3D representation of state (4 3 1)

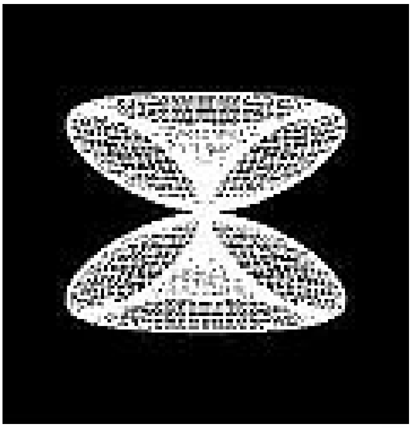

Fig. 11– The 3D representation of state (4 3 2)

In Fig. 12, we make a synthesis of the spherical harmonic types to illustrate the connection with the sub-shells with n = 4 of the hydrogen atom.

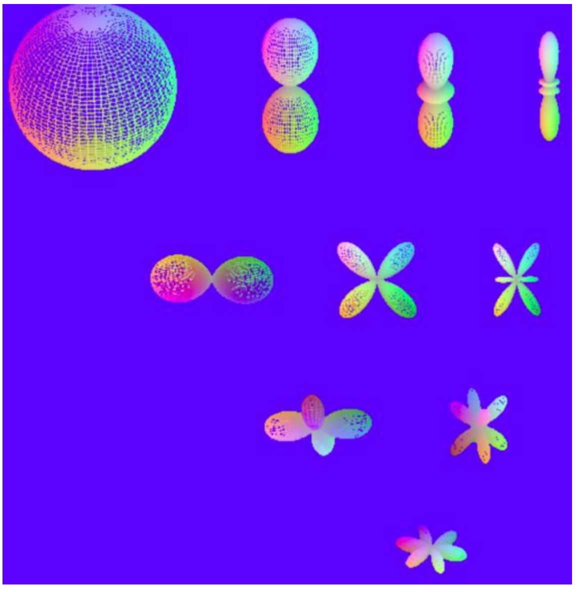

Fig. 12 – The 3D representation of states (4 ℓ m) using the real part of harmonic components

4. CONCLUSIONS

In our work, we have constructed 3D geometric representations and given an analysis for the shapes of the hydrogen atomic orbitals associated with the states for a fixed n less than 5 (the 10 states and their description in Section 3). We chose this case, because it contains at least one representative orbital for each of the three types of harmonics that we have found both in purely mathematical, topological studies and in the pulsation modes of stars [7]. We then, highlighted the role of observables such as θ nodal values, which are useful in the analysis and description of atomic orbital configurations in both 2D and 3D – representations.

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