

The Hydrogen-like atom: geometric representation of its orbital types

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Abstract. In the atomic physics, the Rydberg states of an atom or molecule denote electronically excited states with energies that follow the hydrogen-like atom theory. They represent an important direction in the Spectrum analysis and also in the quantum information processing techniques.

In this paper, considering the Schrödinger equation in the stationary case with Coulomb potential in the frame of two-body problem, we evaluate the wave functions with the principal quantum numbers $n = 1..5$. Further, we plot the effective potential of the Rydberg states with $\ell = 0..4$ and also obtain the 2D representation of the $s p d f g$ - electron systems and 3D visualization of the S, P orbitals type.

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Key words: visualisation of the Rydberg atom; Lyman hydrogen radiation; ultra-cold plasma.

1 Introduction

The Rydberg states describe systems that have electronic structure roughly similar to atomic hydrogen and they are important to study the cold plasma and condensed matter.

The Rydberg atoms are produced by excitation of hydrogen like atoms [1] or the ions species X^+ [2]. In astrophysics fields, an interesting topic is about Lyman Hydrogen emission spectra [3].

It is noteworthy that these orbitals play an essential role for a better understanding of how these states intervene in the ionization and crystallization processes [4].

In this paper, we plot the effective potential for the orbital quantum number $\ell = 0..4$ and also obtain the 2D representation of Rydberg atomic orbitals for $\ell = n - 1$ and the principal quantum number $n = 2..5$ and 3D representation of S and P orbitals type.

2 The wave functions of the Rydberg atom

In the frame of two-body problem and considering natural units, we use a physical model based on the Schrödinger equation in the stationary case:

$$(2.1) \quad \left[-\frac{1}{2\mu} \nabla^2 + V(r) \right] \cdot \psi_{n\ell m}(r, \theta, \varphi) = E_{n\ell} \cdot \psi_{n\ell m}(r, \theta, \varphi)$$

with the electron reduce mass μ , the Coulomb potential $V(r) = \frac{A}{r}$, the energy eigenvalues $E_{n\ell}$, and the wave eigenfunctions $\psi_{n\ell m}(r, \theta, \varphi)$.

The complete form of the solution is: [5]

$$(2.2) \quad \Psi_{n\ell m}(r, \theta, \varphi, t) = R_{n\ell}(r) \cdot Y_{\ell m}(\theta, \varphi) \cdot e^{-i \cdot E \cdot t}$$

where

$$(2.3) \quad R_{n\ell}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \cdot \frac{(n-\ell-1)!}{2n[(n+1)!]^3}} \cdot e^{-\frac{r}{na_0}} \left(\frac{2r}{na_0}\right)^\ell \cdot L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right)$$

is the radial component which contains the associated Laguerre polynomials, the Bohr's radius a_0 , and

$$(2.4) \quad Y_{\ell m}(\theta, \varphi) = (-1)^m \cdot \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}} \cdot P_\ell^m(\cos(\theta)) \cdot e^{i \cdot m \cdot \varphi}, m \geq 0$$

$$(2.5) \quad Y_{\ell(-m)}(\theta, \varphi) = (-1)^m \cdot Y_{\ell m}^*(\theta, \varphi), m < 0$$

is the angular component which contains the associated Legendre polynomials.

3 Results and discussion

In Rydberg states we must consider the effective potential, because it is influenced by high angular momenta through the centrifugal term.

Figure 1 depicts the effective potential associated to the Coulomb potential [5]

$$(3.1) \quad V_{eff}(r) = V(r) + \frac{\ell(\ell+1)}{2\mu r^2}.$$

Taking into account the above formula of wave functions we compute the density of local probability:

$$(3.2) \quad |\Psi_{n\ell m}(r, \theta, \varphi)|^2$$

such that, we are able to locate the electrons on the *s p d f g* orbitals.

Figure 1: The superposition of the effective Coulomb potential for $\ell = 0..4$ starting from bottom to the upper of the graphic

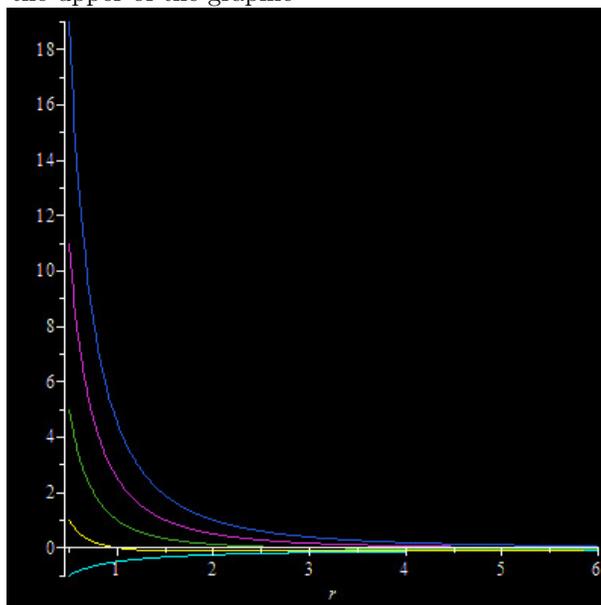


Figure 2: The 2D representation of hydrogen-like orbitals using the usual spectral notation $1s$ $2pz$ $3dz$ $4fz$ $5gz$

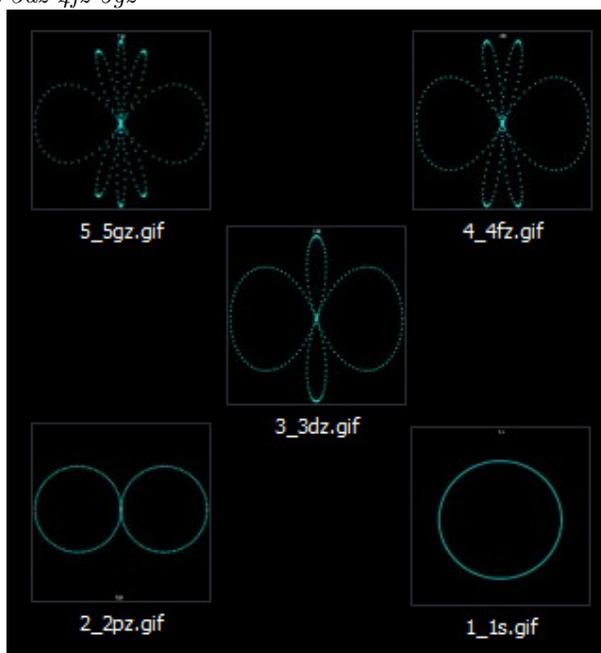


Figure 3: The 3D representation of S orbital type

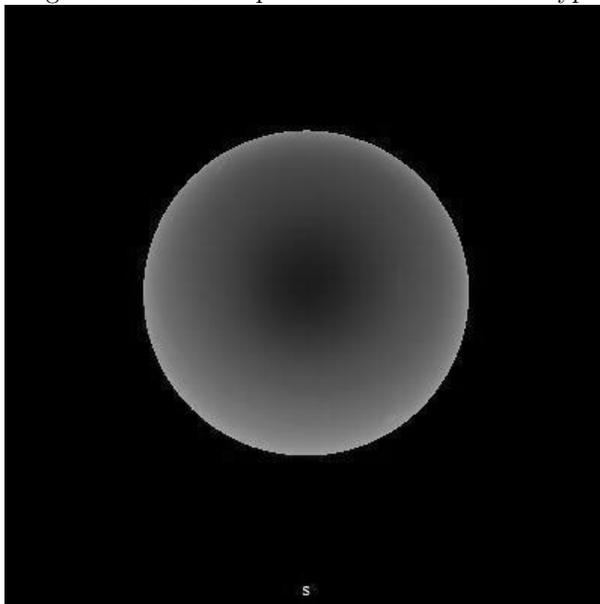
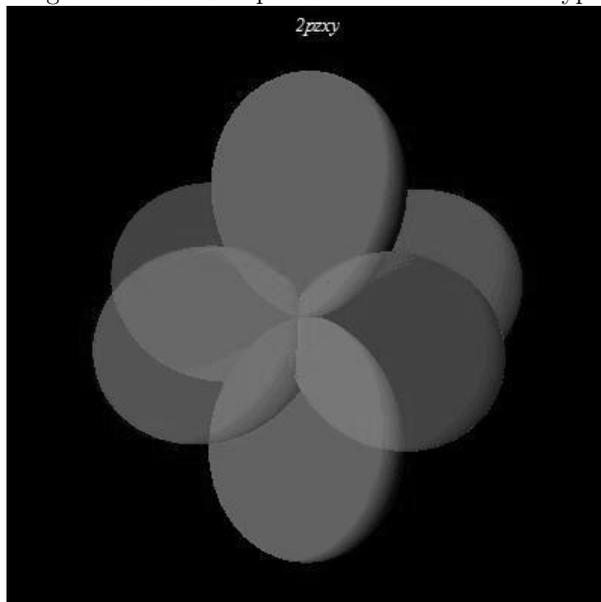


Figure 4: The 3D representation of P orbital type



In the figure 2, we show the 2D space representation of Rydberg atomic orbitals for $\ell = n - 1$ and $m=0$, with $n = 1..5$.

In Figure 3 and in Figure 4, we obtain the 3D representation of S and P orbitals.

Consequently, we obtain of a spatial representation of Rydberg orbitals, offering a good 2D and 3D view of them. It is noteworthy that these orbitals are suitable to study the atomic species including the lanthanide and actinide (e.g., Cerium).

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