

Electron Orbit's Shape for Hydrogen and Helium Atoms

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Abstract- This paper is a continuous work of some facts about the electrons in the first orbit of H and He atoms. Position of electron according to angle around the nucleus, the shapes of the first orbit, as well as the electron intensity from De Broglie equation are all illustrated.

Keywords- Orbit shape; intensity of electron.

I. INTRODUCTION

Atomic orbitals can be the hydrogen-like “orbitals” which are exact solutions to the Schrödinger equation for a hydrogen-like “atom” (i.e., an atom with one electron).

Alternatively, atomic orbitals refer to functions that depend on the coordinates of one electron (i.e., orbitals) but are used as starting points for approximating wave functions that depend on the simultaneous coordinates of all electrons in an atom or molecule. The coordinate systems chosen for atomic orbitals are usually cylindrical coordinates (r, θ, z) in atoms and Cartesians (x, y, z) in a polyatomic molecules.[1]

II. METHOD

At θ_i and $|v_i|$ there is two components of velocity; we can find them as the following:

$$v_{x,i} \text{ and } v_{y,i}, \text{ and } v_{x,i} = |v_i| \cos \theta_i$$

$$v_{y,i} = |v_i| \sin \theta_i$$

And the time at each () point can be given from:

$$\tan \theta_i = \frac{y_i}{x_i}$$

$$y_i = x_i \tan \theta_i$$

$$y_i = \frac{\sin \theta_i}{\cos \theta_i} \cdot x_i$$

$$y_i \cos \theta_i = x_i \sin \theta_i$$

And the distance is:

$$(y_i = v_{y,i} \cdot t_i) \text{ and } (x_i = v_{x,i} \cdot t_i)$$

$$\text{So, } t_i = \frac{x_i \sin \theta_i}{v_{y,i} \cos \theta_i} \text{ or } t_i = \frac{y_i \cos \theta_i}{v_{x,i} \sin \theta_i}$$

From above if we know the velocity of electron and the angle we can be certain about the location of electron at any instant. Also, this equation helps us to find the electron since we know the whole orbit diagram.

In other words

$$t_i = \frac{x_i \tan \theta_i}{v_{y,i}}$$

or

$$t_i = \frac{y_i}{v_{x,i} \tan \theta_i}$$

Now, we have to convert from the Cartesian coordinate system () to the cylindrical coordinate system (). Notice we ignore z component in the Cartesian coordinate system and in the cylindrical coordinate system.

$$r_i^2 = x_i^2 + y_i^2$$

And since,

$$y_i = x_i \tan \theta_i$$

So,

$$r_i^2 = x_i^2 + x_i^2 \tan^2(\theta_i)$$

Now, we can find values of x_i and y_i from the following relations:

$$x_i = \sqrt{\frac{r_i^2}{1 + \tan^2(\theta_i)}}$$

And

$$y_i = x_i \tan \theta_i$$

The radius of atom's orbit is from the following:

$$r_1 = \frac{n^2 a_0}{Z}$$

Where n is the orbit number and z is the atomic number of the atom. While $a_0 = 0.0529 \times 10^{-9} \text{ nm}$

By comparing with Pauli's figure:[2]

III. RESULTS

When the angle θ_i is changing from 0 to 360 degrees and the $\Delta\theta = 0.1$ degree; we find the orbit shape of H atom and He atom by EXCEL; as the following:

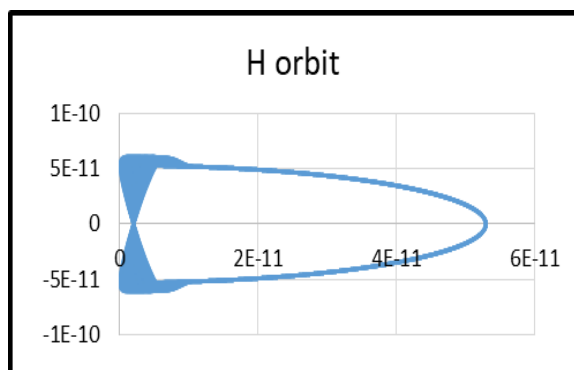


Fig 1. Electron orbit shape in Hydrogen atom.

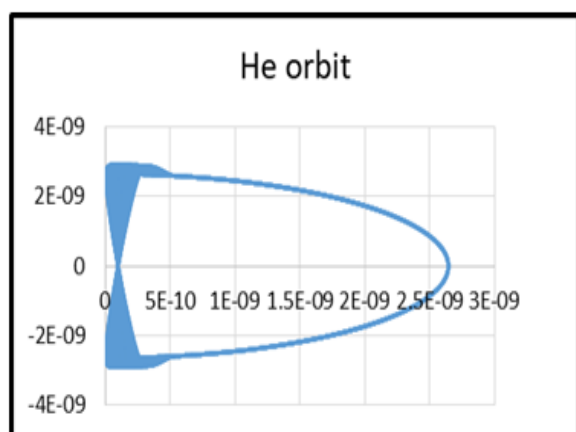


Fig 2. Electron orbit shape in Helium atom.

When the angle θ_i is changing from 0 to 360 degrees and the $\Delta\theta = 1$ degree; we find the orbit shape of H atom and He atom by EXCEL; as the following:

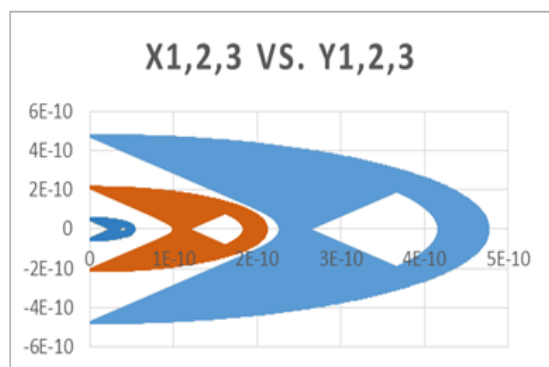


Fig 3. The shapes of first orbit in Hydrogen atom, and first and second orbits in Helium.

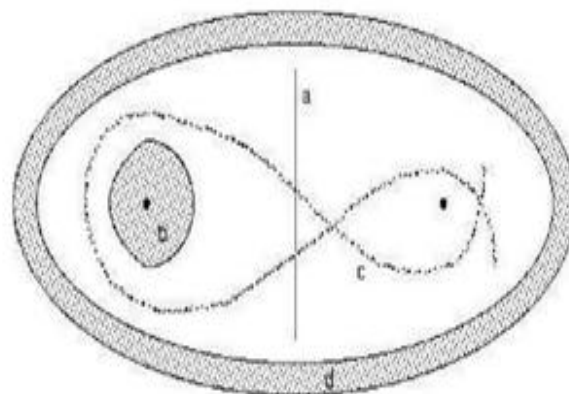


Fig 4. Pauli's classification of planar electron orbits in the hydrogen molecule ion, H_2^+ : (a) pendulum orbit, (b) satellite orbit.

In comparison with the following figure of Dying Star:

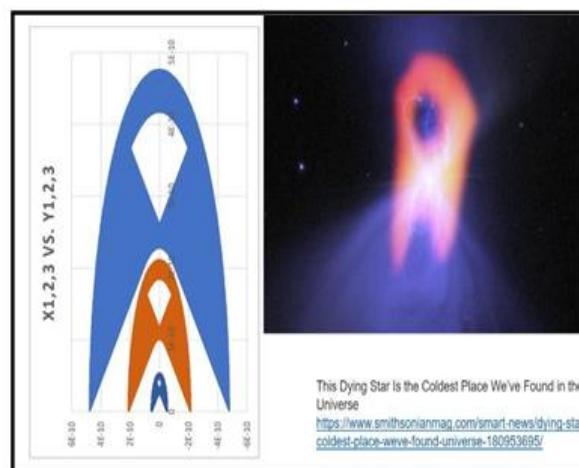


Fig 5. It shows how dying star looks like one electron's orbit shape.

And to figure out the second electron in the orbit by giving (-x) values and find the y, we get the following shape:

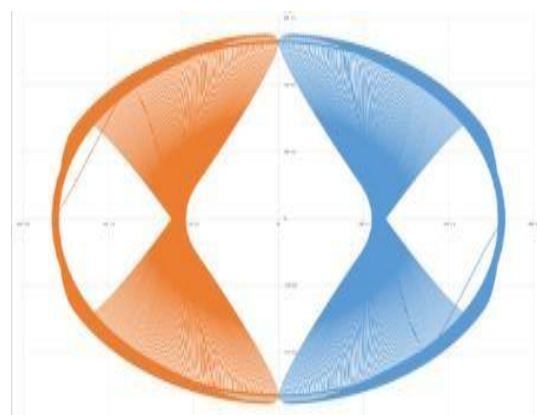


Fig 6. Two electrons orbiting the atom at the first orbit.

From the De Broglie assumption:

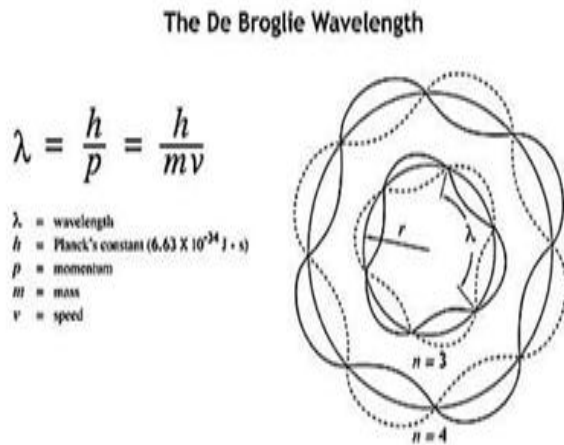


Fig 7. De Broglie wavelength equation.

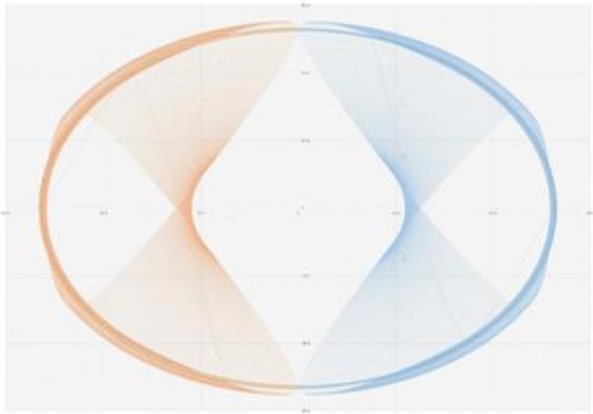


Fig 8. Elarged figure to see how the electron orbits the atom.

Now, to calculate the velocity, we find its value from the following steps;

$$v^2 = v_{y,i}^2 \left(1 + \frac{y_i^2}{x_i^2 + \tan^2(\theta)} \right)$$

$$v_{x,i}^2 = v_{y,i}^2 \left(1 + \frac{y_i^2}{x_i^2 + \tan^2(\theta)} \right) - v_{y,i}^2$$

$$v_{x,i}^2 = v_{y,i}^2 \left(\frac{y_i^2}{x_i^2 + \tan^2(\theta)} \right)$$

$$v_{x,i} = \frac{v_{y,i} y_i}{x_i \tan(\theta)}$$

$$v_{x,i} t_i = \frac{v_{y,i} y_i}{x_i \tan(\theta)} t_i$$

$$y_i t_i = x_i \tan \theta \rightarrow v_{x,i} t_i = \frac{y_i v_{y,i}}{v_{y,i} t_i \tan \theta}$$

$$v_{x,i} = \frac{y_i}{t_i^2 \tan \theta}$$

$$v_{x,i} t_i = \frac{y_i}{\tan \theta}$$

$$v_{x,i} = \frac{y_i}{t_i^2 \tan \theta} = \frac{y_i v_{x,i}^2 \tan^2(\theta)}{y_i^2 \tan \theta}$$

$$v_{x,i} = \frac{y_i^2}{\tan \theta}$$

$$v_{x,i} = \frac{y_i^2}{\tan \theta}$$

$$v_{y,i} = \frac{v_{x,i} x_i \tan(\theta)^2}{y_i} = \frac{y_i^2 x_i \tan(\theta)^2}{\tan \theta y_i}$$

$$v_{y,i} = y_i x_i \tan \theta$$

So, $v_{x,i} = \frac{y_i^2}{\tan \theta}$, $v_{y,i} = y_i x_i \tan \theta$, and $v = \sqrt{v_{x,i}^2 + v_{y,i}^2}$

The following graph shows the speed versus positions and velocities respectively of the electron in Hydrogen atom:

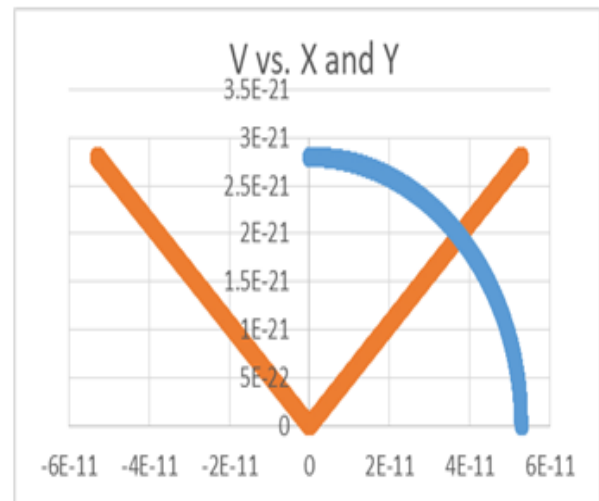


Fig 9. Total velocity against x-axis and y-axis velocities.

Now, the aim is to find the intensity of electron: From De Broglie:

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

We find wavelength from $v_{x,i}$ and $v_{y,i}$ from then we take the square root to get the values of λ and v .

$$\lambda = \frac{6.63 \times 10^{-34}}{9.109 \times 10^{-31} \times v}$$

Then, finding the temperature from Wien's law:

$$T = \frac{2.898 \times 10^{-3}}{\lambda_{max}}$$

Finally, we apply the intensity law:

$$S_{\lambda_{max}} = \frac{8\pi v h}{\lambda_{max}^5} \times \frac{1}{e^{hv/\lambda_{max} K_B T} - 1}$$

Where K_B equals to 1.38×10^{-23} (m²Kg s⁻² K⁻¹).

The following graph illustrates the relationship between intensity and temperature.

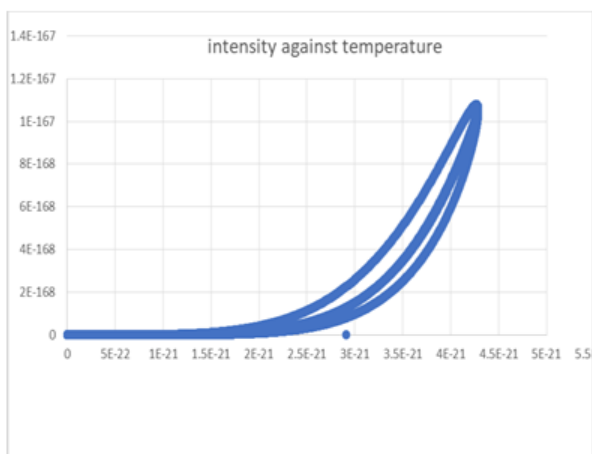


Fig 10. The relationship between intensity and temperature.

In similar way, applying the following law to find the frequency:

$$f = \frac{v}{\lambda}$$

And we can get the following results:

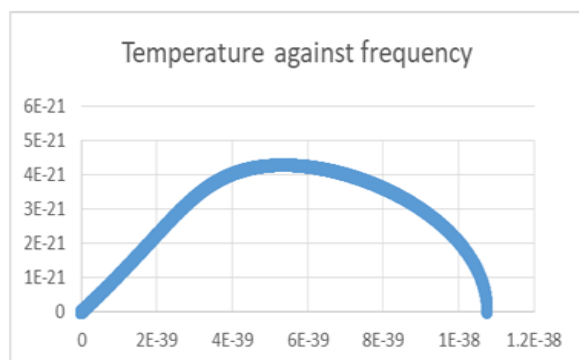


Fig 11. Temperature in vertical axis against the frequency in the horizontal axis.

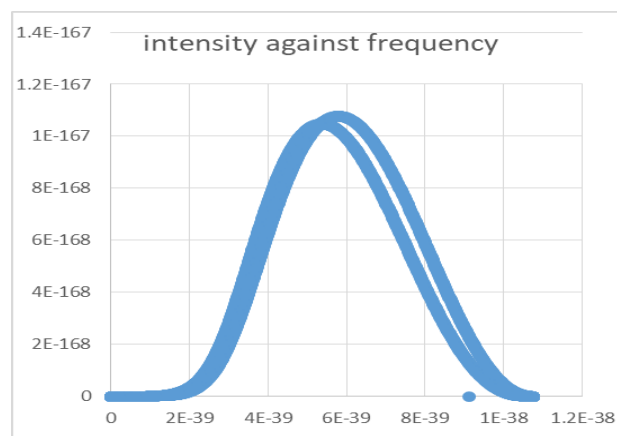


Fig 12. Intensity in the vertical axis against frequency in the horizontal axis.

REFERENCES

- [1] Wikipedia contributors. (2021, March 21). Atomic orbital. Wikipedia. https://en.wikipedia.org/wiki/Atomic_orbital
- [2] www.researchgate.net/publication/1910478_Rise_and_fall_of_the_old_quantum_theory/figures.