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Calculating The Position Of Electrons Around The Nucleus And Demonstrating The Orbital Shape Of Hydrogen Atom And Helium Atom

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Introduction:[1]

In atomic theory and quantum mechanics, an atomic orbital is a mathematical function describing the location and wave-like behavior of an electron in an atom. This function can be used to calculate the probability of finding any electron of an atom in any specific region around the atom's nucleus. The term atomic orbital may also refer to the physical region or space where the electron can be calculated to be present, as predicted by a particular mathematical form of the orbital. Atomic orbitals are the basic building blocks of the atomic orbital model (alternatively known as electron cloud or wave mechanics model), a modern framework for visualizing the submicroscopic behavior of electrons in matter. In this model the electron cloud of a multi-electron atom may be seen as being built up (in approximation) in an electron configuration that is a product of simpler hydrogen-like atomic orbitals.[1]

With the development of quantum mechanics and experimental findings (such as the two slit diffraction of electrons), it was found that the orbiting electrons around a nucleus could not be fully described as particles, but needed to be explained by the wave particle duality. In this sense, the electrons have the following properties [1]:

A. Wave-like properties:[1]

- 1) The electrons do not orbit the nucleus in the manner of a planet orbiting the sun, but instead exist as standing waves. Thus, the lowest possible energy an electron can take is similar to the fundamental frequency of a wave on a string. Higher energy states are similar to harmonics of the fundamental frequency.
- 2) The electrons are never in a single point location, although the probability of interacting with the electron at a single point can be found from the wave function of the electron. The charge on the electron acts like it is smeared proportional at any point to the squared magnitude of the electron's wave function.

B. Particle-like properties:[1]

- 1) The number of electrons orbiting the nucleus can only be an integer.
- 2) Electrons jump between orbitals like particles.

The electrons retain particle-like properties such as; each wave state has the same electrical charge as its electron particle. Each wave state has a single discrete spin (spin up or spin down) depending on its superposition. Thus, electrons Cannot be described simply as solid particles.[1]

An analogy might be that of a large and often oddly shaped “atmosphere” (the electron), distributed around a relatively tiny planet (the atomic nucleus). Atomic orbitals exactly describe the shape of this “atmosphere” only when a single electron is present in an atom.[1]

When more electrons are added to a single atom, the additional electrons tend to more evenly fill in a volume of space around the nucleus so that the resulting collection (sometimes termed the atom’s “electron cloud”) tends toward a generally spherical zone of probability describing the electrons location, because of the uncertainty principle.[1]

Types of orbitals[1]:

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 spherical coordinates (r, θ, z) in atoms and Cartesians (x, y, z) in polyatomic molecules.[1]

Method:

At θ_i and $|v_i|$ there is two components of velocity; $v_{x,i}$ and $v_{y,i}$, and we can find them as the following:

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

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

And the time t_i at each (x_i, y_i) 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: ($y_i = v_{y,i} \cdot t_i$) 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.

$$\text{In other words } t_i = \frac{x_i \tan \theta_i}{v_{y,i}} \text{ or } t_i = \frac{y_i}{v_{x,i} \tan \theta_i}$$

Now, we have to convert from the Cartesian coordinate system (x_i, y_i) to the Spherical coordinate system (r_i, θ_i). Notice we ignore z component in the Cartesian coordinate system and in the Spherical 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:

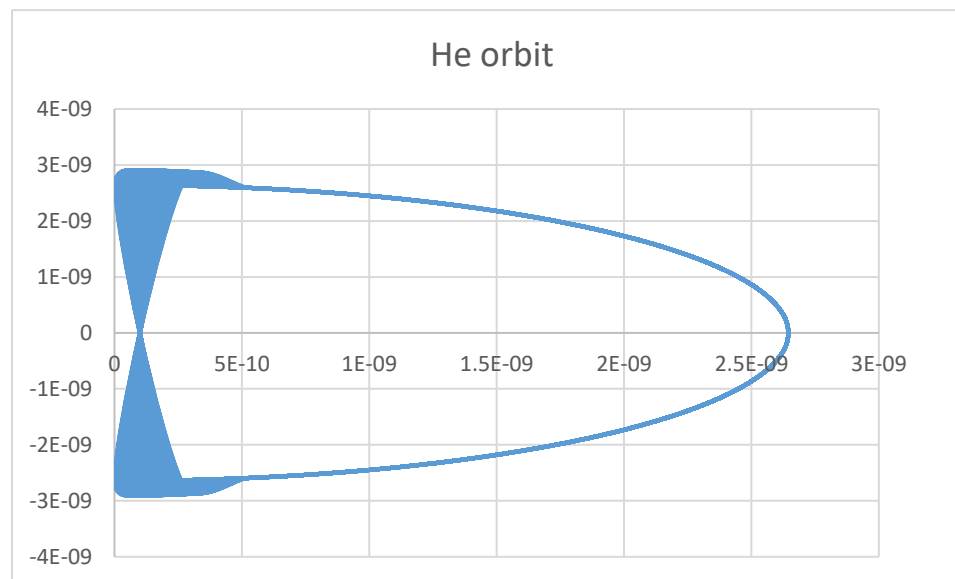
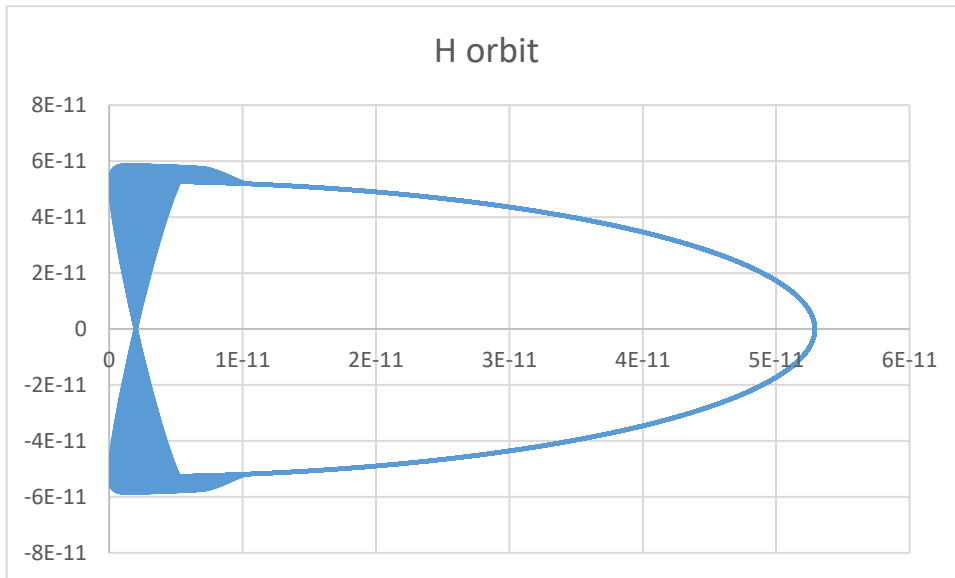
$$x_i = \sqrt{\frac{r_i^2}{1 + \tan^2(\theta_i)}} \quad \text{and} \quad y_i = x_i \tan \theta_i$$

The radius of atom's orbit is from the following: $r_i = \frac{n^2 a_o}{Z}$

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

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:



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

$$t_i = \frac{x_i \sin \theta_i}{v_{y,i} \cos \theta_i} = \frac{x_i \tan \theta}{v_{y,i}} \quad \text{and} \quad t_i = \frac{y_i \cos \theta_i}{v_{x,i} \sin \theta_i} = \frac{y_i}{v_{x,i} \tan \theta}$$

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

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

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

$$v^2 = v_{x,i}^2 + v_{y,i}^2$$

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

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

$$v^2 t_i^2 = y_i^2 \left(1 + \frac{y_i^2}{x_i^2 + \tan(\theta)^4} \right)$$

$$v^2 = \frac{y_i^2}{t_i^2} \left(1 + \frac{y_i^2}{x_i^2 + \tan(\theta)^4} \right)$$

$$v^2 = v_{y,i}^2 \left(1 + \frac{y_i^2}{x_i^2 + \tan(\theta)^4} \right)$$

$$v_{x,i}^2 = v_{y,i}^2 \left(1 + \frac{y_i^2}{x_i^2 + \tan(\theta)^4} \right) - v_{y,i}^2$$

$$v_{x,i}^2 = v_{y,i}^2 \left(\frac{y_i^2}{x_i^2 + \tan(\theta)^4} \right)$$

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

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

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

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

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

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

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

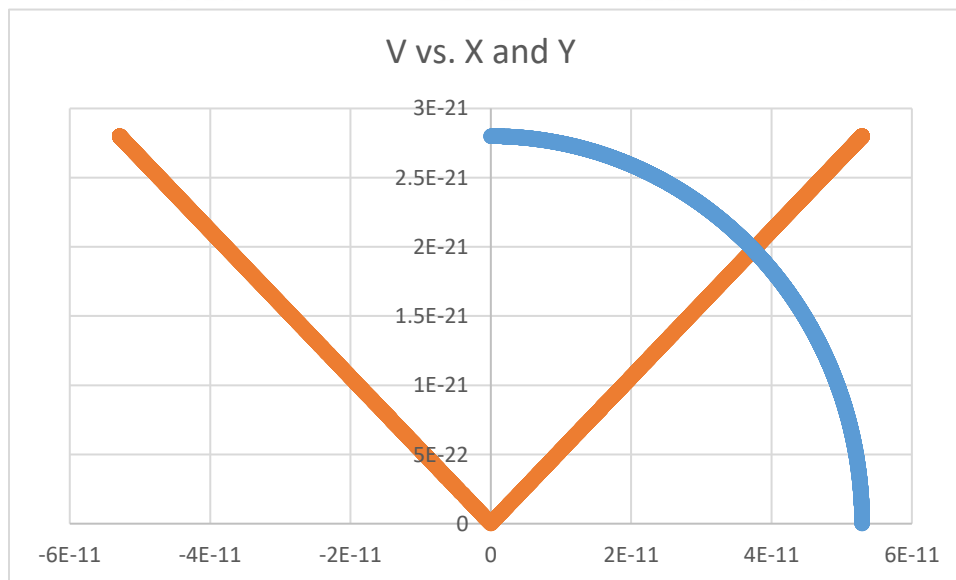
$$v_{x,i} = \frac{y_i^2}{\tan \theta}$$

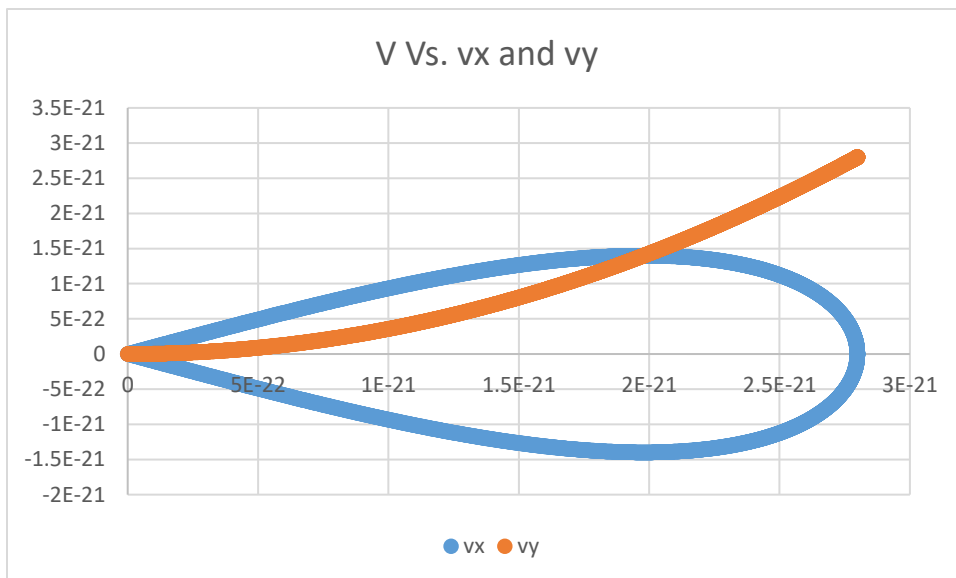
$$v_{y,i} = \frac{v_{x,i}x_i \tan(\theta)^2}{y_i} = \frac{y_i^2}{\tan \theta} \frac{x_i \tan(\theta)^2}{y_i}$$

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

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:



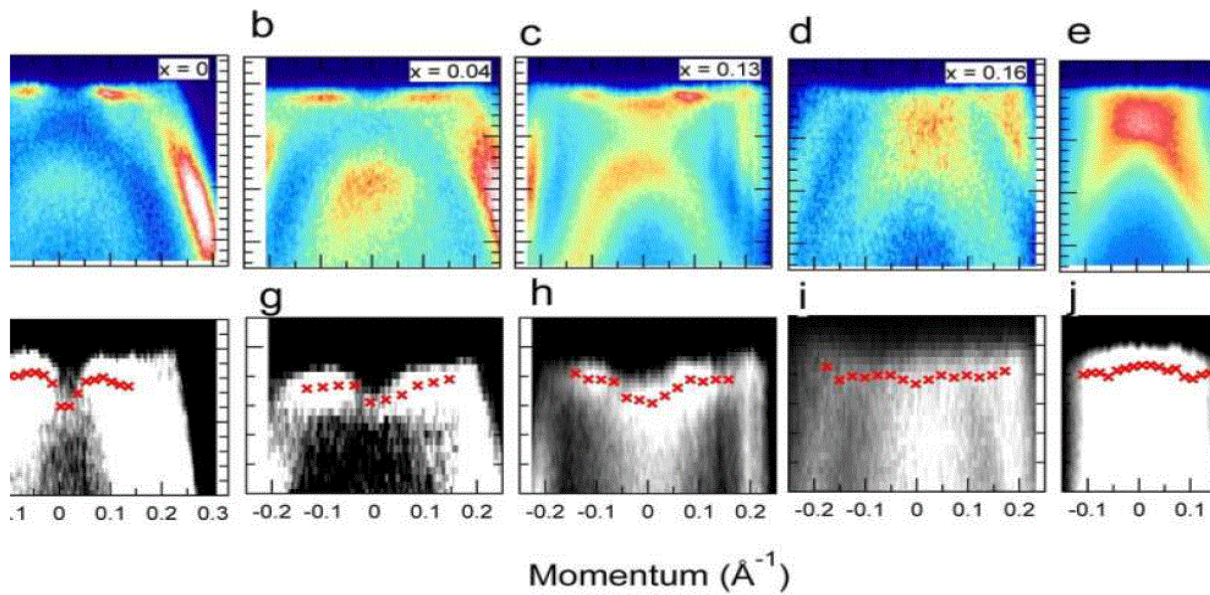


Comparing With Others [2]:

By university of Tokyo;

Superconductivity is a phenomenon in which electric circuit loses its resistance and becomes extremely efficient under certain conditions. Okazaki and his team used the method of ultralow-temperature and high-energy resolution laser-based photoemission spectroscopy to observe the way electrons behaved during a material's transition from The Bardeen-Cooper-Shrieffer (BCS) to Bose-Einstein

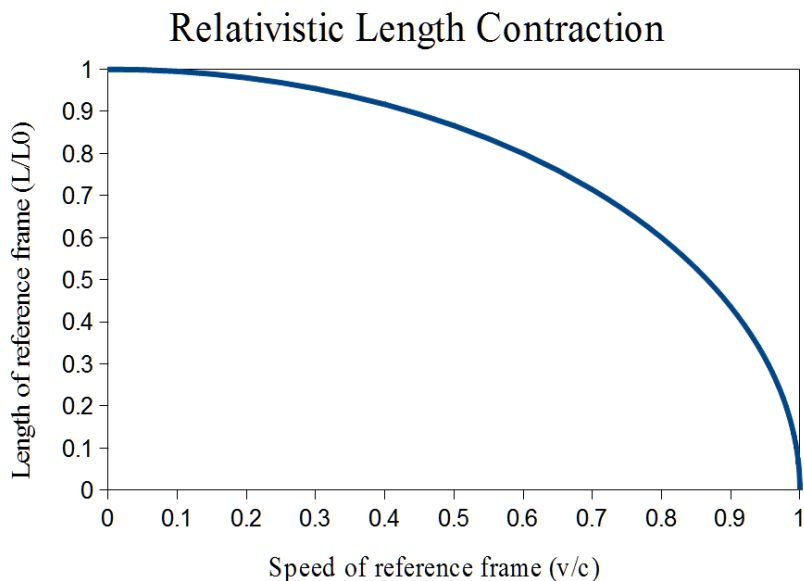
condensate (BEC). Electrons behave differently in the two regimes and the change between them helps fill some gaps in the bigger picture of superconduction.[2]



Polarized light images show researchers how electrons, represented by red crosses, in their test samples behave under different circumstances. Credit: © 2020 Okazaki et al.

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Also, you can compare the velocities with modern physics;[3]



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- [3] Science Questions with Surprising Answers. 2020. *Why Is Time Frozen From Light's Perspective?*. [online] Available at: <<https://www.wtamu.edu/~cbaird/sq/2014/11/03/why-is-time-frozen-from-lights-perspective/>> [Accessed 16 November 2020].