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Comparison of Bohr and Hulthén Hydrogen Atomic Energy Levels Using the Time-Independent Solution of Schrödinger's Equation and Confluent Hypergeometric Function

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Abstract. The energy for each level of the hydrogen atom was triggered by Neils Bohr, where the amount of energy decreases at every level of orbit. The value of energy depends on the principal quantum number which only applies to atoms with the s subshell of an atom with the same characteristics as the hydrogen atom. With the advancement of science, specifically in quantum physics, many potential equations aimed to solve the time-independent Schrödinger equation with the solution of the estimated value of energy. One of the applicable potential equations is the Hulthén potential which is explained about the potential at a small distance and only applies to atoms and micro-scale objects in physics and only has a solution at the azimuth quantum number value $\ell=0$ or groups of atoms subshell s. Using the confluent hypergeometric function, the combination of the Hulthén potential and time-independent Schrödinger equation generates the estimated energy value of the hydrogen atom level, which can be used as a comparison with the estimated energy value of Bohr's hydrogen atom. This study found that the comparison between Hulthén and Bohr energy level lies in the same ratio 1:1

THEORETICAL OVERVIEW

Bohr Theory

The Bohr's model is the atomic model proposed by Niels Bohr in 1913.This model describes the atom as a small and positively charged nucleus surrounded by electrons moving in orbits around the nucleus like the solar system [1], but the role of force gravity is replaced by electrostatic forces. This Bohr model is also a primitive model of the hydrogen atom. As a theory, the Bohr's model can be thought of as a first-order approximation of the hydrogen atom using the more general and accurate quantum mechanics [2].

In the early 20th century, experiments by Ernest Rutherford show that atoms consist of a diffuse cloud of negatively charged electrons surrounding a small, dense, positively charged nucleus. Based on these experimental data, it is only natural that physicists would then imagine a model of a planetary system applied to atoms. The Rutherford model of 1911, with electrons orbiting the nucleus like planets orbit the sun [2], [3]. However, the planetary system model for the atom encountered several difficulties. For example, the laws of classical mechanics (Newtonian) predict that electrons will give off electromagnetic radiation while orbiting the nucleus. Because the electron loses energy during this loss, over time it will fall in a spiral towards the nucleus. To overcome this and other difficulties in explaining the motion of electrons in atoms, Niels Bohr proposed, in 1913, what is now called the Bohr atomic model [3], [4], [5], [12].

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TABLE 1. *Bohr's Idea of Electron Orbit*

No	Idea
1.	Electrons move in orbits and have quantized angular momentum, and thus quantized energy. This means that not every orbit, but only a few specific orbits is possible to exist at a specific distance from the nucleus.
2.	The electrons will not lose energy slowly as they move in orbit, but will remain stable in an orbit that does not decay.

The significance of this model lies in the statement that the laws of classical mechanics do not apply to the motion of electrons around the nucleus. Bohr proposed that a new form of mechanics, or quantum mechanics, describes the motion of electrons around a nucleus. When an electron jumps into a lower orbit, it will produce an energy beam, this energy difference is carried by particles called photons which have the same energy as the energy difference between the two orbits [5], [6]. The permissible orbits depend on the quantized (discrete) values of the orbital angular momentum :

$$L = \frac{nh}{2\pi} \tag{1}$$

Where n = 1,2,3,… and is called the principal quantum number, and h is the Planck's constant. There are 3 simple assumptions in Bohr's theory

- Mechanical energy (Hamiltonian)
- Discrete angular momentum
- The electrons in orbit are affected by the Coulomb force and the centripetal force

These three assumptions produce the following mathematical formula for the Bohr energy equation

$$E_n = -\frac{m_e{}^2 e^4}{2k^2\hbar^2}\frac{1}{n^2} = -\frac{E}{n^2} \tag{2}$$

Useful Equation and Concept Overview

Time Independent Schrödinger Equation

Schrödinger's equation is an equation that represents a wave with a certain change in energy in a potential where this energy does not change with time explicitly, but the energy of the wave will change as position changes. The Schrödinger equation is formulated as follows

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dr^2} + V\psi = E\psi \tag{3}$$

Hulthén Potential and Relation to Schrödinger Equation

This potential is called Hulthén after the name of its discoverer, Lamek Hulthén, a theoretical physicist from Sweden. This potential speaks of a potential over a small distance and only applies to atoms / micro-scale objects in physics. Hulthén potential is a potential in the form of the equation: [10], [11]

$$V_{ot}(r) = -Vo\frac{e^{-\frac{r}{a}}}{1-e^{-\frac{r}{a}}} \tag{4}$$

This potential can only be solved through the time-independent Schrödinger equation with azimuth value ℓ = 0 or atoms in the s subshell such as hydrogen [7].

Classical Electron Radius

The classical electron radius is a constant which concerning the distance of an electron from the nucleus, where the value of this classical electron ring differs for different atoms, for example, the classical electron radius of an atom whose valence is in the s subshell will be different from that in the p subshell and so on. The classical electron radius also determined as the well below the quantum-classical transition scale [13].The value of this classical electron radius is $3{,}53 \times 10^{-16}$ m [8].

Cofluent Hypergeometric Function

General equation

$$y(y-1)w''(y) - \big((a+b+1)y-(c)\big)w'(y) - (ab)w(y) = 0 \tag{5}$$

Solution

$$w(y) = A\,{}_2F_1(a,b,c;y) + By^{1-c}\,{}_2F_1(a-c+1,(b-c+1),(2-c);y) \tag{6}$$

CALCULATION AND MATHEMATICAL OPERATION

Using substitution, elimination and some assumptions with α and β, we have

$$\frac{d^2\psi}{dx^2} + \left[-\alpha^2 + \beta^2\left(\frac{e^{-x}}{1-e^{-x}}\right)\right]\psi = 0 \tag{7}$$

Equation (7) transforms to hypergeometric coffluent with some substitution

$$y^2\nabla^2\psi + y\nabla\psi + \left[-\alpha^2 + \beta^2\left(\frac{y}{1-y}\right)\right]\psi = 0 \tag{8}$$

Equation (8) divided into three differents term, and the result of each term are

$$y^2\frac{d^2\psi}{dy^2} = (\alpha(\alpha-1)y^{\alpha} - \alpha(\alpha+1)y^{\alpha+1})w(y) + 2(\alpha y^{\alpha+1} - (\alpha+1)y^{\alpha+2})w'(y) + (y^{\alpha+2} - y^{\alpha+3})\,w''(y) \tag{9}$$

$$y\frac{d\psi}{dy} = (\alpha y^{\alpha} - (\alpha+1)y^{\alpha+1})w(y) + (y^{\alpha+1} - y^{\alpha+2})\,w'(y) \tag{10}$$

$$\left[-\alpha^2 + \beta^2\left(\frac{y}{1-y}\right)\right]\psi = ((y^{\alpha+1} - y^{\alpha})\alpha^2 + y^{\alpha+1}\beta^2)\,w(y) \tag{11}$$

Following the result of each term, the final cofluent hypergeometric equation is

$$y(y-1)w''(y) - \big((2\alpha+3)y - (2\alpha+1)\big)w'(y) - (\beta^2 - 2\alpha - 1)w(y) = 0 \tag{12}$$

General Solution of Cofluent Hypergeometric Function

To find the proper solution of the cofluent hypergeometric function, we have to set the first boundary term with y=0 and using the identity of the hypergeometric equation which is defined as [9], [11]: ${}_2F_1(a,b,c;y)$

$$= \left[\frac{\Gamma(2\alpha+1)\Gamma(\varepsilon-1)}{\Gamma(\alpha-\gamma+\varepsilon)\Gamma(\alpha+\gamma+\varepsilon)}\,{}_2F_1(\alpha+1+\gamma,\alpha+1-\gamma,2\alpha+1;1-y)\right]$$

$$+(1-y)^{\varepsilon-1}\left[\frac{\Gamma(2\alpha+1)\Gamma(1-\varepsilon)}{\Gamma(\alpha+1+\gamma)\Gamma(\alpha+1-\gamma)}\,{}_2F_1(\alpha-\gamma+\varepsilon,\alpha+\gamma+\varepsilon,\varepsilon;1-y)\right] \tag{13}$$

With

$${}_2F_1(a,b,c;1-y) = 1 + \frac{ab}{c}(1-y) + \cdots + \tag{14}$$

Then, limit the solution of equation hypergeometric confluence to find the possible energy values. Put the second boundary condition when the value of y = 1 and the limit condition ε → 0 so that the value of equation (13) when viewed from equation (14) is

$$\lim_{\varepsilon\to 0}\frac{\Gamma(2\alpha+1)\Gamma(\varepsilon-1)}{\Gamma(\alpha-\gamma+\varepsilon)\Gamma(\alpha+\gamma+\varepsilon)} = \frac{\Gamma(2\alpha+1)}{\Gamma(\alpha+\gamma+\varepsilon)}\lim_{\varepsilon\to 0}\frac{\Gamma(\varepsilon-1)}{\Gamma(\alpha-\gamma+\varepsilon)} \tag{15}$$

Equation (15) only has a value if and only if

$$E_n = -Vo\frac{\alpha^2}{\beta^2} = -Vo\left(\frac{\beta^2-n^2}{2n\beta}\right)^2 \tag{16}$$

Final Equation of Energy Value using Classical Electron Radius

The final result of mathematical operation shows on the equation below

$$E_n = -9{,}07\ 10^{-5}\left(\frac{\frac{2mVo}{\hbar^2}{a^2}^2 - n^2}{4n\frac{mVo}{\hbar^2}a^2}\right)^2 \tag{17}$$

TABLE 2. *Result of Hulthén's Energy*

n value	Result
1	$E_1 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (1)^2}{\left[4(1)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -13{,}601\ \text{eV}$
2	$E_2 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (2)^2}{\left[4(2)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -3{,}400\ \text{eV}$
3	$E_3 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (3)^2}{\left[4(3)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -1{,}511\ \text{eV}$
4	$E_4 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (4)^2}{\left[4(4)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -0{,}850\ \text{eV}$
5	$E_5 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (5)^2}{\left[4(5)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -0{,}544\ \text{eV}$
6	$E_6 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (6)^2}{\left[4(6)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -0{,}378\ \text{eV}$
7	$E_7 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (7)^2}{\left[4(7)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -0{,}278\ \text{eV}$
8	$E_8 = -9{,}07\ 10^{-5}\left(\frac{\left[\frac{2(0{,}511)(9{,}07\ 10^{-5})}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]^2 - (8)^2}{\left[4(8)\frac{(0{,}511)9{,}07\ 10^{-5}}{(6{,}58\ 10^{-16})^2}(5{,}29\ 10^{-11})^2\right]}\right)^2 = -0{,}212\ \text{eV}$

CONCLUSION

In terms of energy level, Bohr Energy and Hulthén Energy for hydrogen atom has the similarity. The estimated value of the Hulthén energy level is identical to the Bohr energy.

TABLE 3. *Comparison of Bohr and Hulthén Energy Levels of Hydrogen Atom*

No	Bohr Energy (eV)	Hulthén Energy (eV)
1	-13,600	-13,600
2	-3,400	-3,400
3	-1,511	-1,511
4	-0,850	-0,850
5	-0,544	-0,544
6	-0,377	-0,377
7	-0,277	-0,277
8	-0,212	-0,212

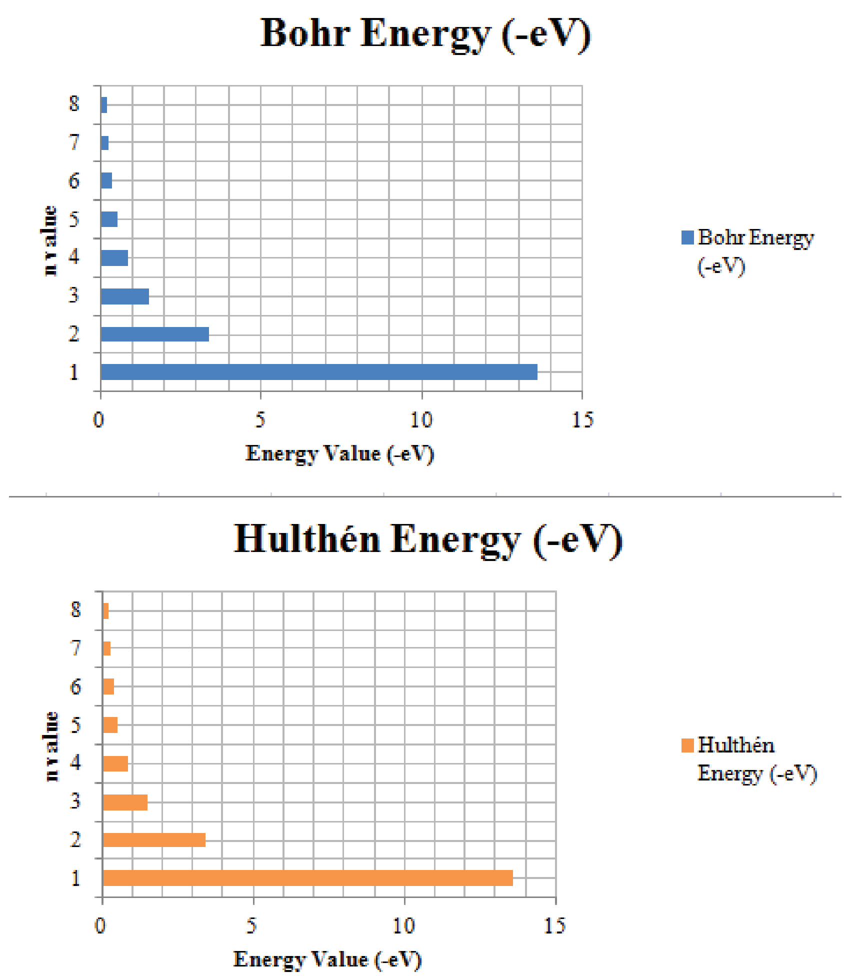

FIGURE 1. Graph of both Bohr and Hulthén's Energy Levels

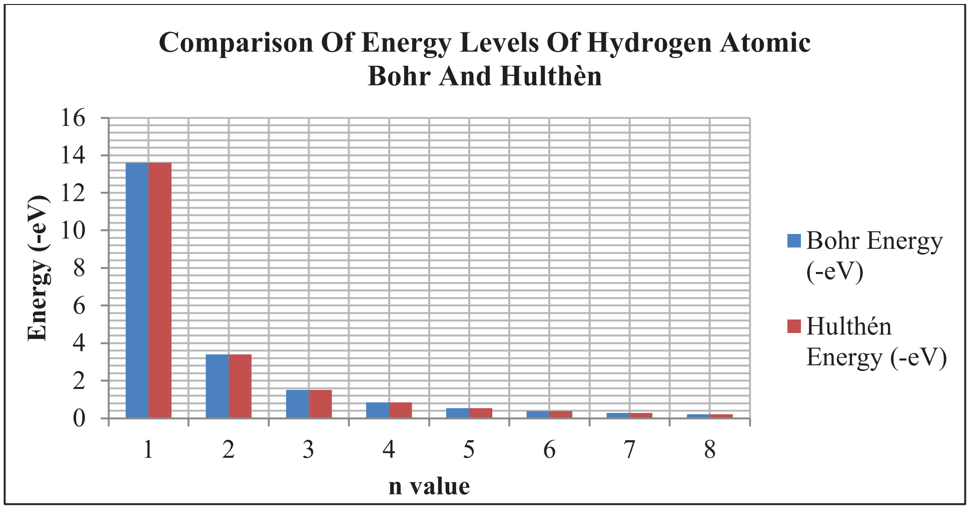

FIGURE 2. Energy Comparison of Bohr and Hulthén

The results illustrate that there is a method to estimate the energy level of the hydrogen atom apart from using the Bohr's method, and the method of using Hulthén potential in the Schrödinger equation also proves that energy is discrete in the quantum physics review. Through the Hulthén potential solution, a comparison of the estimated energy values of the Bohr & Hulthén hydrogen atomic level is lying on the same value with a ratio of 1: 1.

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