1, 2011). Retrieved from: https://ru.osvita.ua/vnz/reports/management/14087/

SIMULATION OF S-ORBITALS OF HYDROGEN IN A CLOSED SYSTEM

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Hydrogen is a chemical element with atomic number 1, which belongs to the 1st group, the 1st period of the periodic table of chemical elements, and is the first and simplest representative of all chemical elements in general and the most common element of the universe. In a hydrogen atom, the electron's orbital has a spherical (spherical) shape, which we will need to model.

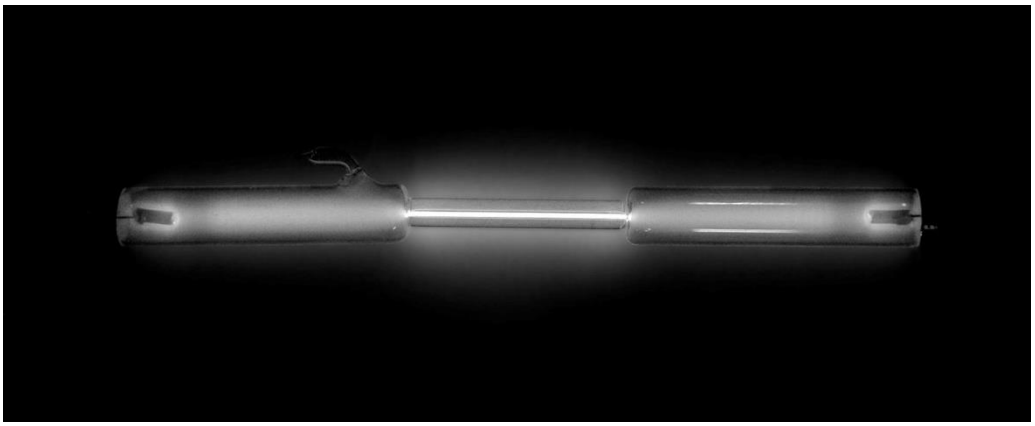


Figure 1. Spectral radiation of hydrogen in a gas discharge tube

In 1926, Erwin Schrödinger derived the famous wave equation that relates the energy of a system to its wave properties. Its application to the hydrogen atom is rather difficult, so first, we use the wave equation to solve the problem of "modelling the S-orbital of H in a closed system" (Lvovsky, 2019). Expressed in one-dimensional space, the Schrödinger wave equation has the form:

$$\frac{\partial^2\varphi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\varphi = 0$$

where

- φ = wave function or *eigenfunction*
- x = coordinate in space
- m = mass
- h = Planck's constant
- E = total energy or *eigenvalue*
- V = potential energy

To get the wave equation for quantum numbers, we have to convert it into the following three-dimensional format:

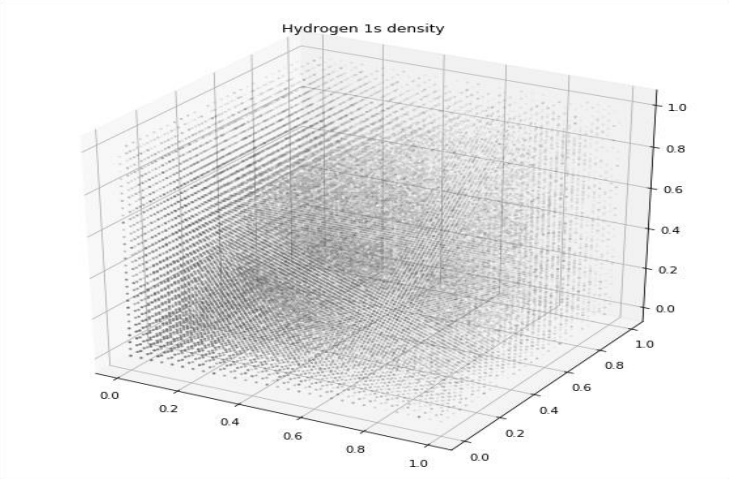
$$\varphi_{n,l,m}(r,\theta,\emptyset) = R_{n,l}(r).Y_{l,m}(\theta,\emptyset)$$

The separation of variables depends on the type of atom and is too complicated for this article. Instead, we just write the solution directly for plotting. Next, we will use the functions R and Y for the hydrogen atom without deriving them. Consider the 1s orbital first:

$$\varphi_{1,0,0} = (2e^{-r})\left(\frac{1}{2\sqrt{\pi}}\right) = \frac{e^{-r}}{\sqrt{\pi}}$$

The wave function of the 1s-orbital shows that the probability of an electron appearing exponentially decreases with distance from the nucleus. It also exhibits a spherical orbital shape.

It is a little difficult to look at it on the electron density graph above, but it is possible to see the sphere as a whole. Density decreases with distance from the center. As a rule, the starting point is the moment when the probability of the appearance of an electron is 99%. The same density plots can be obtained for other orbitals: s, p, d and f.



Simulation of the S-orbital of Hydrogen is written in a high-level programming

language – python.

References:

1. Coursera (2021). *Getting Started with Quantum Machine Learning*. Retrieved October 18, 2021, from https://www.coursera.org/projects/getting-started-quantum-machine-learning.

2. Lutz, M. (2020). *L86 Learning Python, Vol. II and JSC "First Exemplary Printing House*. Retrieved May 11, 2020, from https://www.yakaboo.ua/izuchaem-python-tom-2.html

3. Lutz M. (2020). *Learning Python, Vol. I and JSC "First Exemplary Printing House".* Retrieved December 11, 2020, from https://shultais.education/blog/best-python-books-for-beginners/learning-python-book.

4. Lvovsky A. (2019). *Excellent quantum mechanics: states, operators, Schrödinger equations, hydrogen atom.* Retrieved July 10, 2020, from https://nashol.biz/searchdoc/116936

GENERAL STATE OF THE ENVIRONMENT IN UKRAINE

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According to the UN Framework Convention on Climate Change, as a result of human activities, there was a considerable increase in the concentration of greenhouse gases in the atmosphere, which can lead to the additional surface warming and Earth's atmosphere as well as adversely affect natural ecosystems and humanity (United Nations Framework Convention on Climate Change, 1992).

The IPCC Working Group documents state that the greatest investment to climate change is related to "greenhouse gases", first of all, carbon dioxide and methane (Climate Change, 2007).

Most carbon dioxide emission from stationary sources of pollution in 2017 was