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Development of mathematical model to predict the quantum energy of an electron in an orbit of hydrogen, lithium and sodium

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A R T I C L E I N F O

Article type:
Research article
Article history:
Received November 2019
Accepted February 2020
October 2020 Issue
Keywords:
Model development
Quantum energy prediction
Electron-orbit
Hydrogen
Lithium
Sodium

A B S T R A C T

The basic particle electron obeys various theories like electrodynamics, quantum mechanics and special relativity. Particle under different experimental conditions behaves differently, allowing us to observe different characteristics which are the basis for this work. In this paper, we have made an attempt to predict the quantum energy of an electron in an orbit using hydrogen, lithium and sodium atom as a base. As it is 'difficult' to find structure of electron experimentally, we make a mathematical attempt to predict the quantum energy number of an orbit when not in motion, we have studied atoms with same number of orbits, different atomic numbers and discovered that an increase in orbits has a major effect on the energy level of an atom also energy differs in different orbits. An attempt has been made to give a model that predicts the quantum energy of an electron in an orbit, the focus of these work is to develop a mathematical model that can predict quantum energy of electron in an orbit.

Capsule Summary: Mathematical model was developed to predict the energy of an e^- in an orbit of H, Li and Na atoms.

Cite This Article As: C. P. Ukpaka. Development of mathematical model to predict the quantum energy of an electron in an orbit of hydrogen, lithium and sodium. Chemistry International 6(4) (2020) 179-186.
https://doi.org/10.5281/zenodo.3667443

INTRODUCTION

A quantum mechanical system or particle that is bound and confined spatially can only take on certain discrete values of energy levels. This contrasts with classical particles, which can have any amount of energy. The term is commonly used for the energy levels of electrons in atoms, ions, or molecules, which are bound by the electric field of the nucleus, but can also refer to energy levels of nuclei or vibrational or rotational energy levels in molecules. The energy spectrum of a system is quantized. The atom consists of a central positively charged nucleus and an electron circulates around and as a whole atom is neutral. The nuclear charge is Ze^+, where e^- has negative charge and Z is an integer. Z is thus equal to the number of orbiting e^- and is known as the atomic number, each element has a different atomic number (Bransden and Joachain, 2004). Electrons move around the nucleus of an atom in circular motion. Electrons have a set number of orbitals, ring-like paths around the nucleus and travel in called stationary states. If the e^- stays in one orbital, the energy of the e^- remains constant. The first orbital is n=1, the second orbital n=2 and so on (n is called quantum numbers). An e^- is a negatively charged sub-atomic particle. It can be either free or bound to the nucleus of an atom. Electrons in atoms exist in spherical shells of various radii, representing energy level; the flow of current is a result of the movements of e^- from atom to atom individually and from negative to positive electric poles in general (David, 2004).

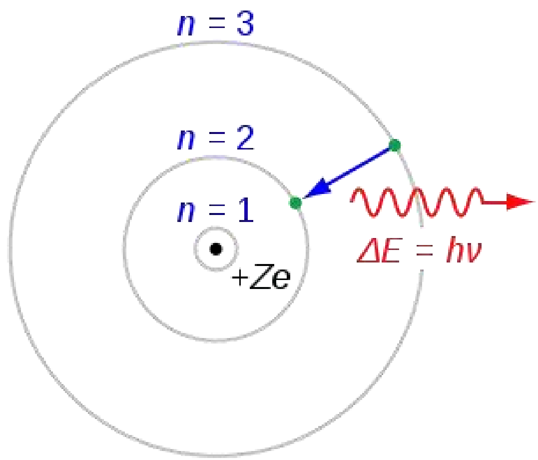

Fig. 1: Bohr model showing maximum electrons per shell (David, 2004).

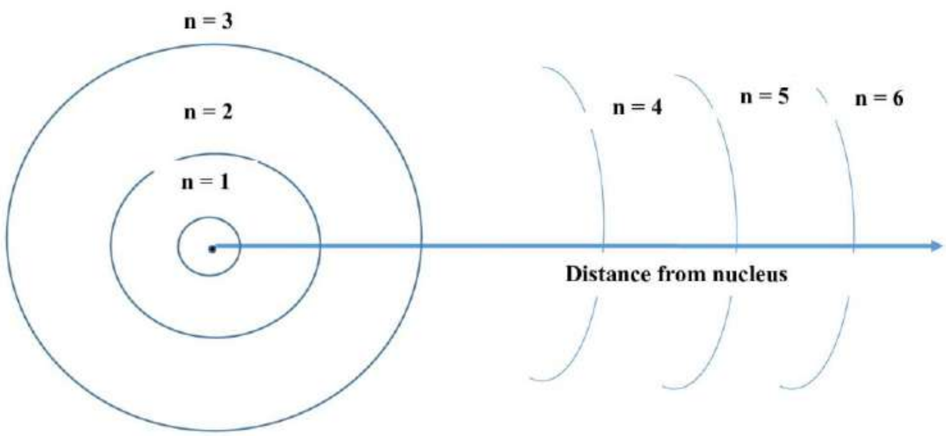

Fig. 2: Shows hydrogen orbits by Bohr model (Keith, 1964).

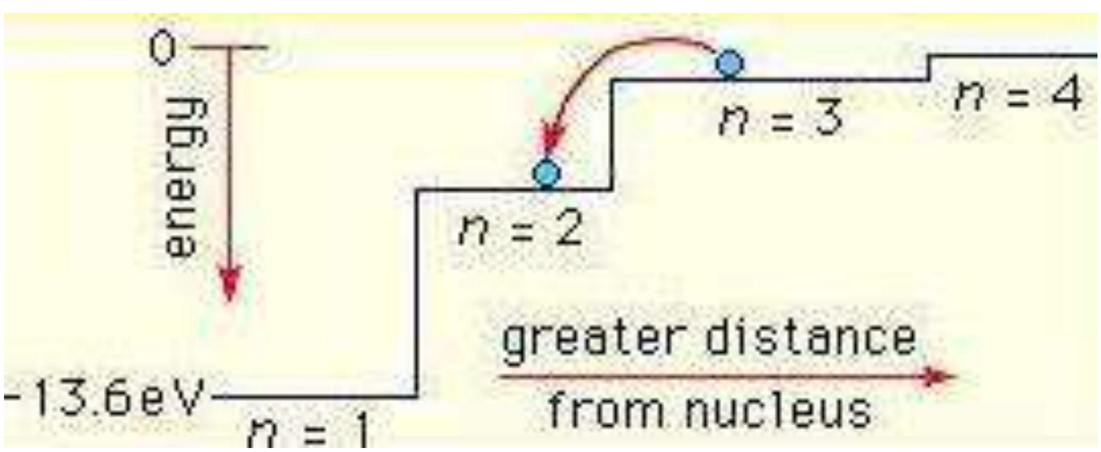

Fig. 3: Ballmer transition of electron (Max, 1901)

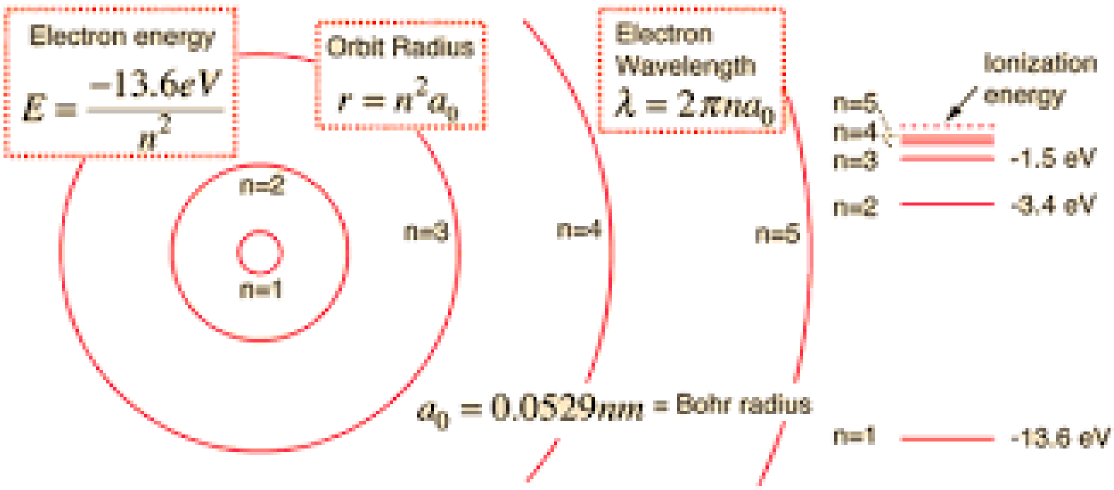

Fig. 4: Shows electron energy level diagram (Niels, 1913).

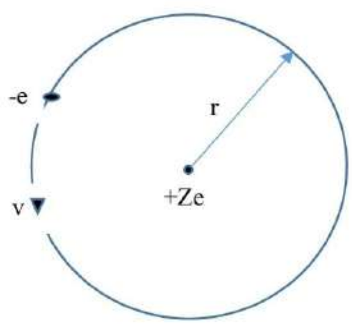

Fig. 5: The Bohr–Rutherford atom with one electron (Richard, 2003).

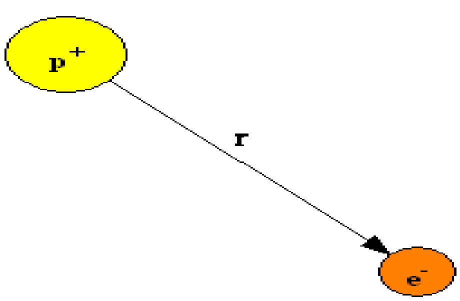

Fig. 6: Force of attraction in an electron

Ukpaka (2018) explain properly that an atom consists of a control positively charged nucleus around which circulates a number of electrons, sufficient to give electrical neutrality to the atom. The nuclear charge is +Ze, where –e is the charge on an electron and Z is an integer. Z is thus equal to the number of orbiting electrons and is known as the atomic number, each element having a different atomic number.

Characteristic of an electron

The electrons exist only in stable circular orbits of fixed energy, the angular momentum of an electron in an orbit being an integral multiple of $\frac{h}{2\pi}$ where h is Planck's constant (Godwin, 2012).

An electron will emit or absorb energy only when making a transition from one to another possible orbit. Figures 1-6 are presenting the e^- and atom properties.

In classical physics by Niels Bohr (1922) shows that the energy of an electron in a particular orbit is given below:

$$En = -\frac{Rhe}{n^2}$$

Where, R is Rydberg constant, h is Planck's constant, c is the speed of light and n is the number assigned to the orbit which is 1,2,3,4……… ∞ (John, 1965). In the above orbit illustration n is infinite; the distance of the orbit from the nucleus increases with increasing n, energy is emitted from the atom when the electron jumps from one orbit to another closer to the nucleus. Shown here is the first Ballmer transition, in which an electron jumps from orbit n = 3 to orbit n = 2, producing a photon of red light with an energy of 1.89 eV and a wavelength of 656 nanometers.

The closest shell to the nucleus is called the "1 shell" (also called "K shell"), followed by the "2 shell" (or "L shell"), then the "3 shell" (or "M shell"), and so on farther and farther from the nucleus. The shells correspond with the principal quantum numbers (n = 1, 2, 3, 4...) or are labeled alphabetically with letters used in the X-ray notation (K, L, M, ...).

Table 1: Computation of quantum energy number of Hydrogen (H) (Ukpaka, 2018)

S/N	N	Z	n_1^2	Z_1^2	1Ry (J)	$E_n = -2.18 \times 10^{-18} \left(\frac{Z^2}{n^2} J\right)$
1	1	1	1	1	-2.18×10^{-18}	-2.18×10^{-18}
2	2	1	4	1	-2.18×10^{-18}	-0.55×10^{-18}
3	3	1	9	1	-2.18×10^{-18}	-0.24×10^{-18}
4	4	1	16	1	-2.18×10^{-18}	-0.14×10^{-18}
5	5	1	25	1	-2.18×10^{-18}	-0.09×10^{-18}

Table 2: Computation of quantum energy number of Lithium (Li) (Ukpaka, 2018)

S/N	N	Z	n_1^2	Z_1^2	1Ry (J)	$E_n = -2.18 \times 10^{-18} \left(\frac{Z^2}{n^2} J\right)$
1	1	3	1	9	-2.18×10^{-18}	-19.62×10^{-18}
2	2	3	4	9	-2.18×10^{-18}	-4.91×10^{-18}
3	3	3	9	9	-2.18×10^{-18}	-2.18×10^{-18}
4	4	3	16	9	-2.18×10^{-18}	-1.23×10^{-18}
5	5	3	25	9	-2.18×10^{-18}	-0.78×10^{-18}

Table 3: Computation of quantum energy number of Sodium (Na) (Ukpaka, 2018)

S/N	N	Z	n_1^2	Z_1^2	1Ry (J)	$E_n = -2.18 \times 10^{-18} \left(\frac{Z^2}{n^2} J\right)$
1	1	11	1	121	-2.18×10^{-18}	-263.78×10^{-18}
2	2	11	4	121	-2.18×10^{-18}	-65.95×10^{-18}
3	3	11	9	121	-2.18×10^{-18}	-29.31×10^{-18}
4	4	11	16	121	-2.18×10^{-18}	-16.49×10^{-18}
5	5	11	25	121	-2.18×10^{-18}	-10.55×10^{-18}

Each shell can contain only a fixed number of electrons: The first shell can hold up to two electrons, the second shell can hold up to eight (2 + 6) electrons, the third shell can hold up to 18 (2 + 6 + 10) and so on. The general formula is that the *n*th shell can in principle hold up to $2(n^2)$ electrons. Since electrons are electrically attracted to the nucleus, an atom's electrons will generally occupy outer shells only if the more inner shells have already been completely filled by other electrons.

Quantum number

A quantum number is a value that is used when describing the energy levels available to atoms and molecules. Principle quantum number (n) it describes the energy level. Azimuthal or angular momentum quantum number (ℓ) it describes the subshell. Magnetic quantum number (Ms) it describes the spin of an orbit.

Quantum energy

The principal quantum number n represents the relative overall energy of each orbital. The energy level of each orbital increase as its distance from the nucleus increases. The sets of orbitals with the same n value are often referred to as an electron shell. The energy released is a result of jumping of electrons from infinity or an outer orbit to an orbit nearer the nucleus, this process decreases its total energy that is equal to the difference in its energy in two or more orbits. The Bohr – Rutherford atom with one electron illustrate appropriately the force of attraction between the electrons and the nucleus. In present investigation, mathematical model was developed to predict the quantum energy of an electron in an orbit for hydrogen, lithium and sodium atoms.

MATERIAL AND METHODS

The materials used to predict the energy in an orbit is basically three atoms namely: hydrogen, lithium and sodium.

Mathematical expression

The total energy of an electron is the sum of its Kinetic and Potential energies (Robert, 1964).

P.E = (Force of attraction) x (radius)

$$= -k\,\frac{Ze^2}{r} \quad (1)$$

$$\mathrm{K.E} = \frac{1}{2}mv^2 \quad (2)$$

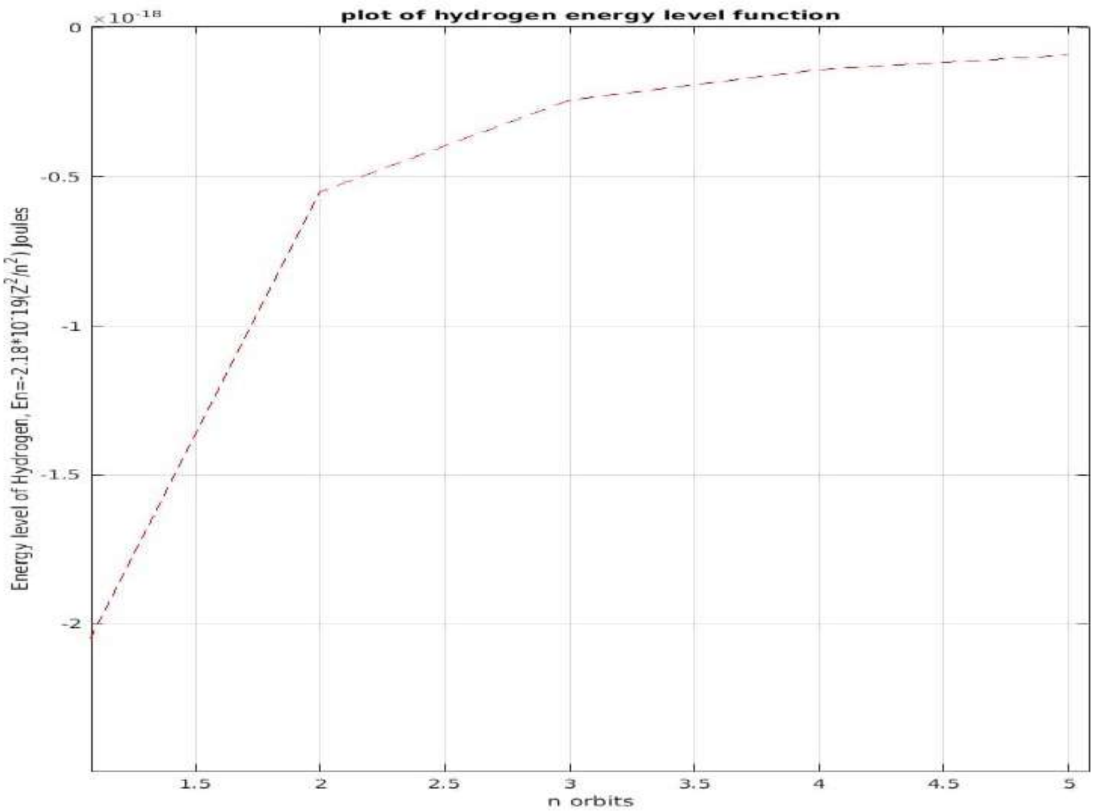

Fig. 7: Graph of energy of hydrogen atom against number of orbits

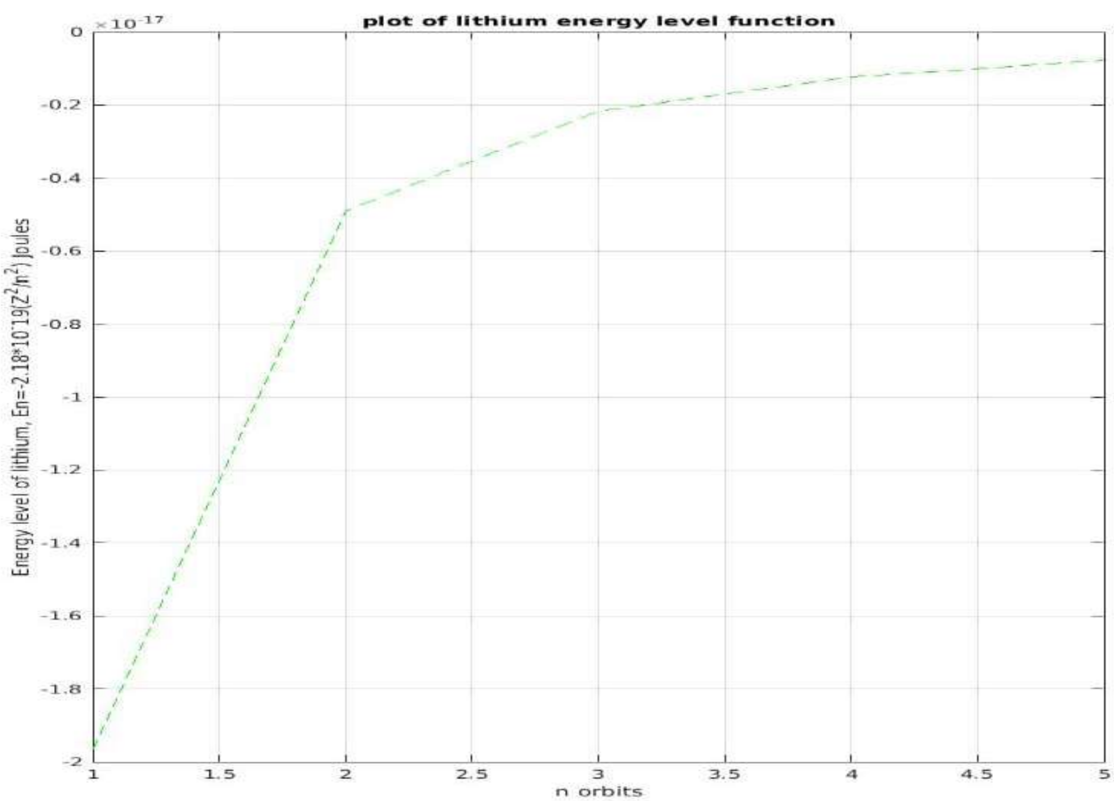

Fig. 8: Graph of energy of lithium atom against number of orbits

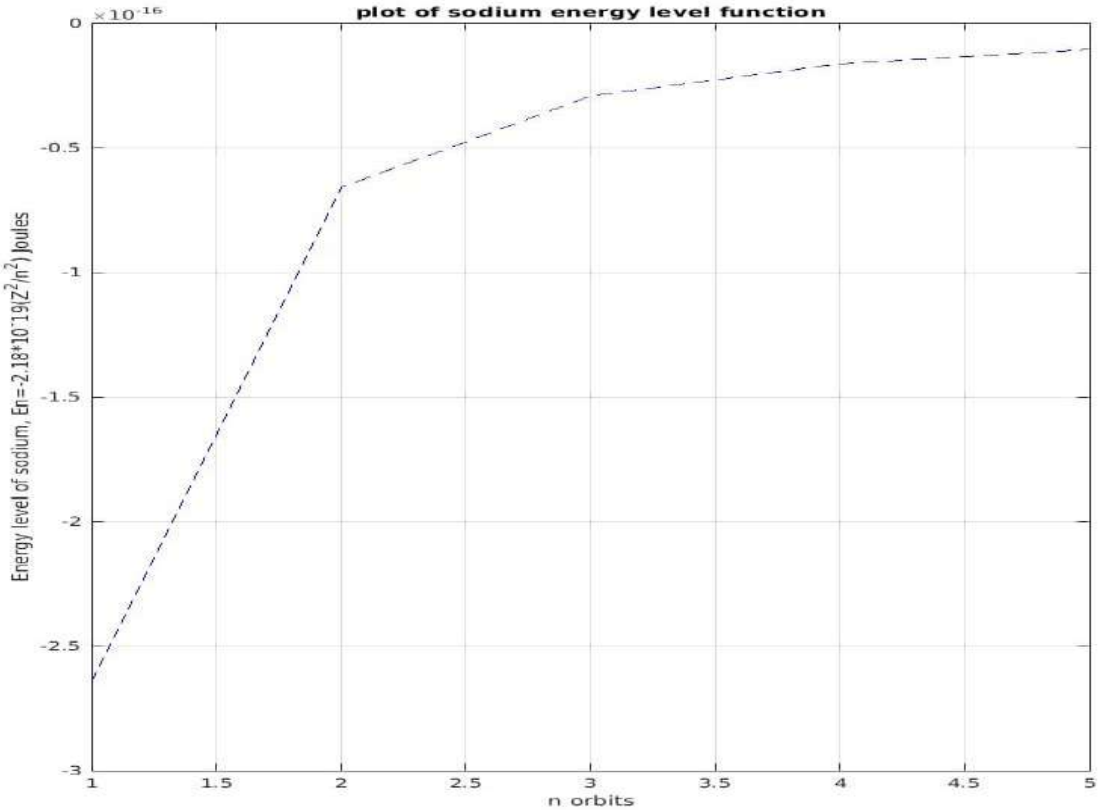

Fig. 9: Graph of energy of Sodium atom against number of orbits

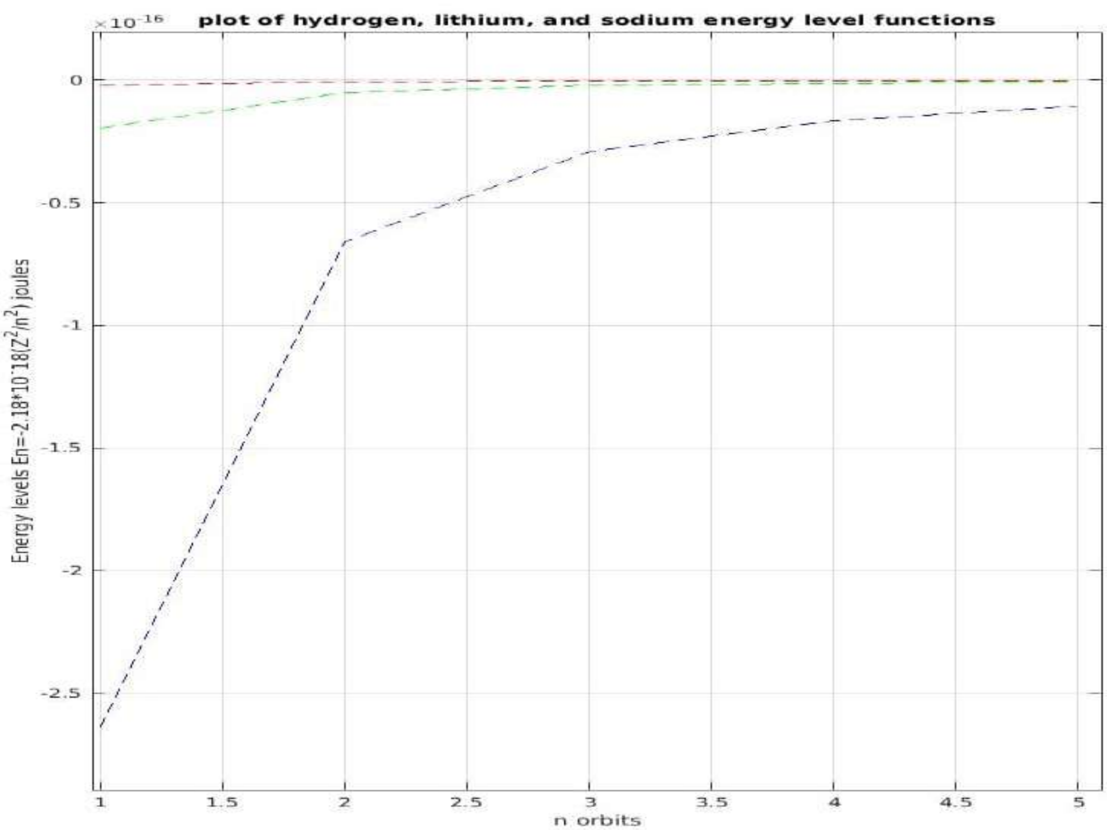

Fig. 10: Graph of energy level of hydrogen, lithium, and hydrogen atom against number of orbits

Putting equation (2) into (1) we have

$\frac{1}{2}m \times K \frac{Ze^2}{mr}$

$$\frac{1}{2}K \frac{Ze^2}{r} \tag{3}$$

Thus the total energy is given by the sum of the two results:

Total Energy $= K\frac{Ze^2}{r} + \frac{1}{2}K\frac{Ze^2}{r}$

$$\frac{Ze^2}{4\pi\varepsilon_o r^2} \tag{4}$$

In equation (4): Z = an integer known as atomic number, e = the charge, r = the distance, while $4\pi\varepsilon_o$ = a constant of –2.18.

$$\text{En} = \frac{Ze^2}{4\pi\varepsilon_o r^2} \tag{5}$$

Let $r = n$, which is the number of orbits in shell of an atom

$$E_n = \frac{Ze^2}{4\pi\varepsilon_o n^2} \tag{6}$$

$$E_n = A\frac{Z}{n^2} \tag{7}$$

Replacing A (constant) in equation (7) with Rydberg's constant) we have the expression below as

$$E_n = \frac{MC^4 Z^2}{8\,\varepsilon_0^2 h^2 n^2} = \frac{MC^4}{8\varepsilon_0^2 h^2} \times -\left(\frac{Z^2}{n^2}\right) \tag{8}$$

$$1Ry \equiv hcR\infty = \frac{m_e e^4}{8\varepsilon_0^2 h^2}$$

$$= 13.605\ eV(1eV = 1.60 \text{ x } 10^{-19}J)$$

$$\approx 2.179 \text{ x } 10^{-18}J$$

$$En = -\frac{Z^2}{n^2}\ 1Ry \tag{9}$$

$$En = -2.18 \text{ x } 10^{-18}\left(\frac{Z^2}{n^2}\right) J$$

Equation (9) is the mathematical expression developed to predict the total energy of electron in an orbit, which was applied to the atoms under consideration are Hydrogen, Lithium and Sodium (Ali et al., 2017).

RESULTS AND DISCUSSION

Figure (7) demonstrates the relationship between the energy level of hydrogen atom and the number of orbit. The result presented in figure (7) shows an increase in the energy level of hydrogen atom with increase in orbit. The energy level increase via the negative values, these increase of hydrogen atom negatively shows the state of the atom (stationary state) not in motion. The energy increase proportionally with increase in orbits until it attains it maximum energy at the last orbits where it stabilizes (equilibrium state). The graph also shows that, at the maximum energy (last orbits) energy increases more than previous orbits meaning electrons are trying to attain a higher energy level if any, which is impossible at the last orbits.

Figure 8 also demonstrates the relationship between the energy level of lithium atom and the number of orbit. The result presented in figure 8 shows an increase in the energy level of lithium with increase in orbit, the negative values in the graph of energy level in lithium atom shows that the atom is in it stationary state and therefore no extra external energy is acted upon the atom. The curve in the graph at it maximum state indicate that the atom has attain equilibrium (last orbit) and cannot jump into any other orbit.

Figure 9 shows the relationship between the energy level of sodium atom and the number of orbit. The result presented in figure 8 shows an increase in the energy level of sodium atom with increase in orbit. Figure 10 demonstrates at a glance the relationship between energy level of hydrogen, lithium and sodium atom against number of orbits, it shows that the energy level of an atoms is determined by the orbits. The atomic number of an atom does not necessary predict it energy level. Electron jumps from one orbit to another when it has attained it maximum energy level at an orbits. Different orbit has different energy level.

CONCLUSIONS

To develop mathematical model that can predict the quantum energy of an electron in an orbit, a clear understanding of orbits, quantum energy, and movement of electrons is necessary. Electron moves from a lower to a higher orbit, so its energy increases at stationary state, to maintain a higher energy level in any atom an extra amount of energy is required and for it to retain such higher energy it most remain in the higher energy state. Electrons naturally at a higher state cannot fall back to lower state unless there is a lower energy state, which does not at that moment contain an electron.

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