

Identification of elements and analysis of their properties using Bohr Model

Naini Diwan

Indian Institute of Science, Education and Research, Bhopal

Quantum mechanics, Atomic spectra

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Abstract

If an element is synthesised and is likely to find new slot in the modern periodic table, one needs to ensure it is not equivalent to any known member. This case study deals with the methods used to identify such elements, focusing on Scilab. It has several applications in the fields of heavy metal synthesis, material science, chemical engineering (chemical manufacturing), nuclear physics, etc. User needs to input experimental atomic mass of the element and principal quantum number of interest. On entering the tentative atomic number, the program provides standard values of physical quantities such as neutron/proton ratio, most probable separation between nucleus and first electron, various forms of energies possessed by the electron, its velocity, and the period of revolution. If all the theoretical data approximately matches the experimental properties of the element, then the atomic number guess is correct. Otherwise for the quantities that do not match, the user has to carefully observe dependency of those parameters on n and z, which is examined through graphs and change the guess of z or value of n accordingly. Thus, the study tells exactly where the newly discovered element fits in the periodic table. Additionally, by computing the energy of released/absorbed photon with the help of Scilab, we manifest how Bohr Model aligned with Ritz combination principle. Aim is to find the position of newly found elements by studying their properties along with urging the importance of correct presentation of Bohr Model.

1. Introduction

The Bohr model was first described by Niels Bohr and Ernest Rutherford in 1915. It is akin to the structure of the Solar System except that the cause of attraction is electrostatic force rather than gravity. It is drawn on Planck's quantum theory of radiation which states that energy is neither a complete wave nor it has an absolute particle nature, instead- it constitutes discrete packets known as quanta. The energy of the absorbed or emitted radiation is directly proportional to its frequency.

$$E = hv$$

Where h is the Plank's constant and v is frequency.

- According to this theory, electrons move in stationary levels that carry fixed energy, electrons cannot stay anywhere in between. Furthermore, an electron located away from the nucleus has more energy than the one that is closer.
- The energy levels are represented by circles for the sake of simplicity, although no restriction is placed on the eccentricity of the orbit, but length of the major axis is considered.
- These energy levels are represented by n (now known as 'principal quantum number'). The orbits are named as K, L, M, N... shells. On the nucleus side, there is n=1 (K shell or ground state). The following rule governs capacity of these orbits-

 $N = 2n^2$

Where N is the maximum number of electrons in nth Bohr orbit.

When an electron moves from lower to higher energy state, it gains the difference of energy between the levels. Likewise, on moving from higher to lower energy state (decay), it emits a photon.

2. Problem Statement

In the era of modern technology, science is developing rapidly but still there are areas in which discoveries are rare- The Periodic Table is one of them. A new element discovered has to get through several qualifications to secure its place in the periodic table. With the help of Scilab, we help the user determine exact position of the element in the periodic table by evaluating standard physical quantities and judging the stability of the nucleus with the help of neutron to proton ratio. As the user exclusively receives standard data analysis for whatever they input, the project is userfriendly.

It can be used in the field of spectroscopy because the program calculates energy of transition. Since each element has specific energy levels, it must have a distinctive emission spectrum (The same way we have unique fingerprints). We further explain this by taking the example of Balmer series.

In some instances, Bohr's Model is introduced in a more wrong than right way. So, one might wonder why, despite the passage of more than a century, it is still being taught. There even have been proposals that the model should not be taught anymore, as it is too simple to compete the lately accepted atomic structure. However, this is inappropriate as for a tree, the seed must be sown first. With Scilab, the correct picture of Bohr's model can be taught.

One might think that it would scarcely be possible, to bring Bohr's views about the atom into direct relation with the Ritz combination principle. However, a closer investigation through Scilab makes it clear that the relation between the spectra of the elements and the structure of their atoms based on the postulates can be obtained.

3. Basic concepts related to the topic

- Physical quantities involved:
 - z atomic number
 - n principal quantum number
 - A– atomic mass in amu
 - h Plank's constant (6.626×10⁻³⁴ Joule-sec)
 - L-angular momentum of the electron
 - m mass of electron (9.109×10^{-31} kg)
 - v-velocity of electron

- r-radius of a stationary state
- e charge on an electron (1.602×10^{-19} C)
- k Coulomb's constant ($8.99 \times 10^9 Nm^2C^{-2}$)
- Postulates and assumptions of the model
 - The electron revolves in certain stable orbits, called Bohr Orbits around the nucleus without radiating any energy.
 - The stationary orbits are attained at distances for which the angular momentum is an integral multiple of the reduced Planck constant.
 Quantisation of angular momentum

$$mvr = \frac{nh}{2\pi}$$

- Electrons can only gain and lose energy by jumping from one allowed orbit to another, by absorbing or emitting electromagnetic radiation.
- The electron is held in a circular orbit by electrostatic attraction. The centripetal force is provided by the Coulomb force.

When it comes to the atomic scales, there are no structures which can be 100% perfect. Many excellent principles support this statement- including Heisenberg's Uncertainty Principle (the name gives the idea of what it is about). While the first postulate contemplates the general stability of an atom, second one principally has in view the existence of spectra with sharp lines. Rest of the postulates and assumptions are also necessary to present the complete picture of the model.

Stability of the nucleus

The A-z/z ratio or nuclear ratio for the nucleus of an atom is the ratio of its number of neutrons to its number of protons. For stable nuclei and naturally occurring nuclei, this ratio generally increases with increasing atomic number. Radioactive decay takes place to change the nuclear ratio in order to increase stability. Positron emission and electron capture increase the ratio, whereas beta decay decreases the ratio. > The radius of the stable Bohr orbits:

$$r = \frac{n^2 h^2}{4\pi^2 z m e^2}$$

> The velocity of electron in n^{th} energy level:

$$v = \frac{2\pi kze^2}{nh}$$

- Different forms of mechanical energy:
 - Total energy of the electron:

$$E = -\frac{4m\pi^2 k^2 z^2 e^4}{n^2 h^2}$$

It comes out to be negative. The greater the magnitude of energy, the more tightly the electron is bound to nucleus. Moreover, it is inversely proportional to n^2 , hence the separation between these stationary states decreases in a quadratic manner as you climb the energy level diagram.



Figure 1. (Made on MS Paint)

With a variation of energy on the vertical axis, an energy-level diagram is used to depict the Bohr orbits and the transition of an electron in them. Electrons in atoms and molecules can undergo transitions in these energy levels by emitting or absorbing electromagnetic radiation.

• Kinetic energy of the electron:

$$KE = \frac{4m\pi^2 k^2 z^2 e^4}{n^2 h^2}$$

It is always positive.

• Potential energy of electron:

$$U = -\frac{8m\pi^2 k^2 z^2 e^4}{n^2 h^2}$$

As the electron recedes the nucleus and the distance between them approaches infinity, the Coulombic force of attraction between them approaches zero. Conversely, as it approaches the nucleus, the motion accelerates

$$a_{centripetal} = rac{v^2}{r}$$

causing an increase in the (positive) kinetic energy of the system. Thus, by conservation of total energy, the increase of same amount in the potential energy of the object is taken to be negative.

Apart from these, we can also compute the energy of the photon radiated/ assimilated:

$$\Delta E = -13.6z^2 \left(\frac{1}{a^2} - \frac{1}{b^2}\right)$$

Here, transition occurs from shell a to shell b.

Period of electron's revolution around nucleus:

$$T = \frac{2\pi r}{v}$$

The time period in seconds is reciprocal of the frequency of revolution in Hertz.

4. Flowchart



5. Software/Hardware used

Operating System: Windows 11 Toolbox: None Hardware: Personal Computer with 12th Gen Intel Core Processor, 16GB RAM Software: Scilab Version: 2024.0.0 and Microsoft Office 2021

6. Procedure of execution

- I. On the computer, launch Scilab software.
- II. Open the Scilab file called "Scilab_FOSSEE_Project_Final.sce".
- III. Execute your code with the help of "Execute" menu along with "File with no echo" option, or press "Ctrl + Shift + E" on the keyboard.
- IV. Enter the value of atomic number, or 0 to exit.
- V. If atomic number is negative, correction message is displayed, and the user is directed back to step IV.
- VI. If the atomic number is in range (1,119) [open interval], the name of the element is displayed as the case already exists in the periodic table.
- VII. If z = 1 (the case is of H-atom which is known), n is to be entered, then all the physical quantities can be analysed.
- VIII. If z > 118, the console prompts a request for atomic mass and comments on the nuclear stability, and asks for n.
 - IX. Now the parameters can be investigated on providing suitable input.
 - X. For the analysis of other parameters/ different values, execute as many times as required, until all the experimental values approximately match with those provided by the Scilab program.

7. Result

As the Scilab file was executed, the console summoned input of atomic number(z) for the element of interest. 'z' corresponds to the direct address of an element in the periodic table. So, the user would be able to determine the exact position of the element he discovered, provided all their experimental data agrees with the output. Because of its flexibility, the allows any integral value of atomic number and principal quantum number. The Hydrogen Atom and Spectral Analysis

Bohr radius

It is an important quantity, equal to the most probable distance between nucleus and the electron at its ground state in hydrogen atom (52.9 pm).

Ionisation energy

It is defined as the energy required to remove an electron from ground state to

its free state. The first ionisation energy of hydrogen atom is 13.6 eV.

```
--> exec('C:\Users\Naini Diwan\OneDrive\FOSSEE_Scilab_Project\Scilab_FOSSEE_Project_Final.sce', -1;
------Welcome to the Scilab Code------
Enter the tentative atomic number (0 to quit): 1
"It is Hydrogen atom"
Principle quantum number of interest [any integer > 0]: 1
Which quantity is to be simulated ?
velocity, radius or total energy [Enter 0 to exit]: radius
Radius (in picometres) is: 52.9 pm
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? 0
velocity, radius or total energy [Enter 0 to exit]: total energy
Total energy in electronvolts is: -13.6 eV
This is Ionisation Energy of the element.
```

Simulation of Balmer series

Whenever in the atom, electron lands to L shell, it emits a radiation which

comes under Balmer series. In principle, first four of these wavelengths fall in

the visible range of spectra.

-

For the simulation of following physical quantitie:	s, numerical codes have been designated
Energy released or absorbed by the electron in the	
form of photon while undergoing transition	: 1
Period of revolution of electron in nth Bohr orbit	: 2
Kinetic energy of the electron	: 3
Potential energy of the electron	: 4
To exit	: 0
Enter a number: 1	
For calculation of the energy of transition	
Principal quantum number, from which transition hap	ppens [enter a natural number]: 3
Principal quantum number, to which transition happ	ens [enter a natural number]: 2
Positive energy change means that the electron abs	orbs energy, while negative energy change implies a release of energy
Energy of the photon is: -1.8888889 eV	
Enter a number for the quantity of interest (in ran	nge [0,4]): 1
For calculation of the energy of transition	
Principal quantum number, from which transition hap	ppens [enter a natural number]: 4
Principal quantum number, to which transition happ	ens [enter a natural number]: 2
Positive energy change means that the electron abso	orbs energy, while negative energy change implies a release of energy
Energy of the photon is: -2.55 eV	
Enter a number for the quantity of interest (in ran	nge [0,4]): 1
For calculation of the energy of transition	
Principal quantum number, from which transition hap	ppens [enter a natural number]: 5

```
Principal quantum number, to which transition happens [enter a natural number]: 2

Positive energy change means that the electron absorbs energy, while negative energy change implies a release of energy

Enter a number for the quantity of interest (in range [0,4]): 1

For calculation of the energy of transition

Principal quantum number, from which transition happens [enter a natural number]: 6

Principal quantum number, to which transition happens [enter a natural number]: 2

Positive energy change means that the electron absorbs energy, while negative energy change implies a release of energy

Energy of the photon is: -3.022222 eV
```

We tabulated the inference as shown below:

n (from which electron excites)	n (to which the electron lands)	Energy of photon emitted/ absorbed	Wavelength (in nm)	Colour observed
3	2	-1.88 eV	656	Red
4	2	<i>-2.55 eV</i>	486	Green
5	2	<i>-2.86 eV</i>	434	Blue
6	2	<i>-3.02 eV</i>	410	Violet



Figure 3. The Emission Spectra of Neon and Mercury respectively

• Ritz combination principle

It states that the frequency for each line in the spectrum of an element can be represented by the formula

$$v=T''-T'$$

where T' and T'' are spectral terms.

This was proven by transition energy values. The differences in energy between energy states correspond **to unique wavelengths in the electromagnetic spectrum**.



Figure 3. The Emission Spectra of Neon and Mercury respectively

Classification of elements

It was observed that the program assisted in classifying the elements of periodic table. When such a z was entered, whose element is already in existence, the program displayed its name.

```
--> exec('C:\Users\Naini Diwan\OneDrive\FOSSEE Scilab Project\Scilab FOSSEE Project Final.sce', -1)
  -----Welcome to the Scilab Code------
Enter the tentative atomic number (0 to quit): 2
The element that already exists with atomic number 2 is: Helium
Enter the tentative atomic number (0 to quit): 11
The element that already exists with atomic number 11 is: Sodium
Enter the tentative atomic number (0 to quit): 31
The element that already exists with atomic number 31 is: Gallium
Enter the tentative atomic number (0 to quit): 39
The element that already exists with atomic number 39 is: Yttrium
Enter the tentative atomic number (0 to quit): 50
The element that already exists with atomic number 50 is: Tin
Enter the tentative atomic number (0 to quit): 83
The element that already exists with atomic number 83 is: Bismuth
Enter the tentative atomic number (0 to quit): 118
The element that already exists with atomic number 118 is: Oganesson
```

Analysis of newly discovered element with z=119

When z entered by the user were such that no corresponding element is known, prompt requested its experimental atomic mass. Then the user could get theoretical values for various important quantities.

Stability of nucleus

With the help of neutron to proton ratio, the program judged that nucleus of this isotope is likely to reduce the number of protons inside it.

• Velocity of electron in nth orbit

User obtained the value of velocity of the electron in K shell

Enter the tentative atomic number (0 to quit): 119 Atomic mass of the element in amu: 204 Heavy metals are radioactive. Nucleus is expected to undergo electron capture or positron emission. Principle quantum number of interest [any integer > 0]: 1 Which quantity is to be simulated ? velocity, radius or total energy [Enter 0 to exit]: velocity Velocity of electron (in SI Units) is: 2.593D+10 m/s Enter 0 to exit Plotting its graph, which quantity is to be kept on x axis, n or z? n Enter 0 to exit Plotting on graph, which quantity is to be kept on x axis, n or z? z Enter 0 to exit

With the help of plots, they found that it varies in a rectangular hyperbolic manner with n, but linearly with z. This makes clear the fact that proportionality of velocity with n and z has a special form-



Hence if a discoverer does not find the velocity equivalent to given data, they do not have to change the input of n and z randomly, but as per the above.

Radius of orbit

```
velocity, radius or total energy [Enter 0 to exit]: radius
Radius (in picometres) is: 0.4445378 pm
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? n
Enter 0 to exit
Plotting on graph, which quantity is to be kept on x axis, n or z? z
Enter 0 to exit
Plotting on graph, which quantity is to be kept on x axis, n or z? 0
```

User obtained the most probable distance between nucleus and the electron in K shell of the 119th element. On similar analysis, they saw that radius modifies itself parabolically with n, but hyperbolically with z.





Total energy

The negative value of total energy of an electron denotes that it is bound to the nucleus, one of the greatest triumphs of the Bohr model. The ground state of an atom possesses the lowest energy. The electrons in an atom tend to be arranged in such a way that the energy of the atom is as low as possible. We observed that the system of nucleus and electron is stable as total energy reaches its maximum value (0, global maximum) when the electron and nucleus are infinitely far apart.

```
Which quantity is to be simulated ?
velocity, radius or total energy [Enter 0 to exit]: total energy
Total energy in electronvolts is: -192589.6 eV
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? n
Enter 0 to exit
Plotting on graph, which quantity is to be kept on x axis, n or z?: z
Enter 0 to exit
Plotting on graph, which quantity is to be kept on x axis, n or z?: 0
velocity, radius or total energy [Enter 0 to exit]: 0
```

By the two plots that follow,





Comparison of energy gaps

By evaluating the energy of photon absorbed when an electron goes from K shell to L shell as compared to the transition from L shell to infinite distance from nucleus, the user got a marvellous detail!

The energy difference between ground state (n=1) and first excited state (n=2)

is LARGER than that between n=2 and $n \rightarrow \infty$.

For the simulation of following physical quantities, numerical codes have been designated Energy released or absorbed by the electron in the form of photon while undergoing transition Period of revolution of electron in nth Bohr orbit: 2 Kinetic energy of the electron Potential energy of the electron : 3 : 4 To exit : 0 Enter a number: 1 For calculation of the energy of transition Principal quantum number, from which transition happens [enter a natural number]: 1 Principal quantum number, to which transition happens [enter a natural number]: 2 Positive energy change means that the electron absorbs energy, while negative energy change implies a release of energy Energy of the photon is: 144442.2 eV Enter a number for the quantity of interest (in range [0,4]): 1 For calculation of the energy of transition Principal quantum number, from which transition happens [enter a natural number]: 2 Principal quantum number, to which transition happens [enter a natural number]: 9999999999999999 Positive energy change means that the electron absorbs energy, while negative energy change implies a release of energy Energy of the photon is: 48147.4 eV

 \blacktriangleright Analysis of newly discovered element with z=200

Stability of nucleus

As the atomic mass is 700 amu (all of which is almost contributed by protons and neutrons- nucleons), it is expected that the nucleus experiences a beta decay in order to reduce the number of neutrons in the isotope.

Velocity of electron

The electron revolves with a speed of 1.452×10^8 m/s in 300th shell of the atom. As it is inversely proportional to n, comparing this velocity with K shell in the previous case makes it evident that the latter has a velocity that is about hundred times of 300th shell.

Radius of n = 300 energy level

When the electron is in this shell, its most probable separation from the nucleus is: 23805 pm

Total energy

The energy of 300th shell or that of the electron staying in it is: -6.04 eV.

Energy of transition

The difference between first two energy states nearest to nucleus of this atom is: 408000 eV.

Time period

The period of revolution of the electron in 300^{th} energy state came out to be roughly the order of attoseconds. On the other hand, the interval of electron's transition from one energy eigen state to another is 10^{-8} sec, which is a significant difference.

"An attosecond is to one second as one second is to the age of the universe."

Kinetic energy

It was found that it has a positive value of 6.04 eV.

Potential energy

Negative potential energy is a relative concept as depends on the frame of reference. We found that this case bears a resemblance to the simple harmonic oscillator for which,

$$W = \int_{x_i}^{x_f} F_x \, dx = \int_{x_i}^{x_f} -kx \, dx = -\left(\frac{1}{2}kx_f^2 - \frac{1}{2}kx_i^2\right) = -\left[U_f - U_i\right] = -\Delta U.$$

```
--> exec('C:\Users\Naini Diwan\OneDrive\FOSSEE Scilab Project\Scilab FOSSEE Project Final.sce', -1)
 -----Welcome to the Scilab Code-----
Enter the tentative atomic number (0 to quit): 200
Atomic mass of the element in amu: 700
Heavy metals are radioactive.
Negative electron (beta) decay is expected from nucleus.
Principle quantum number of interest [any integer > 0]: 300
Which quantity is to be simulated ?
velocity, radius or total energy [Enter 0 to exit]: velocity
Velocity of electron (in SI Units) is: 1.452D+08 m/s
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? 0
velocity, radius or total energy [Enter 0 to exit]: radius
Radius (in picometres) is: 23805 pm
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? 0
velocity, radius or total energy [Enter 0 to exit]: total energy
Total energy in electronvolts is: -6.0444444 eV
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? 0
```

```
velocity, radius or total energy [Enter 0 to exit]: 0
For the simulation of following physical quantities, numerical codes have been designated
Energy released or absorbed by the electron in the
form of photon while undergoing transition
                                                  : 1
Period of revolution of electron in nth Bohr orbit: 2
Kinetic energy of the electron
Potential energy of the electron
                                              : 3
                                                  : 4
                                                  : 0
To exit
Enter a number: 1
For calculation of the energy of transition
Principal quantum number, from which transition happens [enter a natural number]: 1
Principal quantum number, to which transition happens [enter a natural number]: 2
Positive energy change means that the electron absorbs energy, while negative energy change implies a release of energy
Energy of the photon is: 408000 eV
Enter a number for the quantity of interest (in range [0,4]): 2
Time period of the revolution (in picoseconds) is:
0.0010298 ps
Enter a number for the quantity of interest (in range [0,4]): 3
Kinetic Energy (in electronvolts) is 6.0444444 eV
Enter a number for the quantity of interest (in range [0,4]): 4
Potential Energy (in electronvolts) is -12.088889 eV
Enter a number for the quantity of interest (in range [0,4]): 0
 "Winding up... Thank you"
```

> Analysis of newly discovered element with atomic number 201

Stability of nucleus

Since the neutron number was almost equal to the proton number, nucleus was found to be stable. We derived an important conclusion here that the stability is not affected by the orbit number in which electron is present.

Velocity of electron

The electron revolves with a speed of 2.19 x 10^9 m/s in 20^{th} shell of this atom, which is about ten times faster than the previous case in which electron was in the 300^{th} shell of the atom with z = 200.

Radius of 20th stationary state

When the electron is in this shell, its most probable separation from the nucleus is found to be: 105.27 pm

Total energy

The total energy of 20th shell of this atom is: -1373.63 eV.

The values of radius, velocity and total energy which the program evaluated matched user's experimental data, so they did not need to see the graphs.

--> exec('C:\Users\Naini Diwan\OneDrive\FOSSEE_Scilab_Project\Scilab_FOSSEE_Project_Final.sce', -1)

```
Enter the tentative atomic number (0 to quit): 201
Atomic mass of the element in amu: 477
Heavy metals are radioactive.
Stable isotope.
Principle quantum number of interest [any integer > 0]: 20
Which quantity is to be simulated ?
velocity, radius or total energy [Enter 0 to exit]: velocity
Velocity of electron (in SI Units) is: 2.190D+09 m/s
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? 0
velocity, radius or total energy [Enter 0 to exit]: radius
Radius (in picometres) is: 105.27363 pm
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? 0
velocity, radius or total energy [Enter 0 to exit]: total energy
Total energy in electronvolts is: -1373.634 eV
Enter 0 to exit
Plotting its graph, which quantity is to be kept on x axis, n or z? 0
```

Energy of transition

The difference between 200th and 409th eigen states' energy of this atom is about 10.45 eV, which is very scant as compared to that between its 1st and 2nd orbit.

Time period

The period of revolution of the electron in 20^{th} shell is 3.0×10^{-19} sec.

Frequency
$$=\frac{1}{T}$$

Thus, its frequency of revolution is 3.33×10^{18} Hz.

Kinetic energy

It was found that indeed, kinetic energy is always positive, having a value of 1373.63 eV. This resembles to the absolute value of the total energy of the same electron

Potential energy

The value of potential energy of the electron is about -2747.268 eV.

velocity, radius or total energy [Enter 0 to exit]: 0 For the simulation of following physical quantities, numerical codes have been designated Energy released or absorbed by the electron in the form of photon while undergoing transition : 1 Period of revolution of electron in nth Bohr orbit: 2 Kinetic energy of the electron : 3 Potential energy of the electron : 4 To exit : 0 Enter a number: 1 For calculation of the energy of transition Principal quantum number, from which transition happens [enter a natural number]: 200 Principal quantum number, to which transition happens [enter a natural number]: 409 Positive energy change means that the electron absorbs energy, while negative energy change implies a release of energy Energy of the photon is: 10.451725 eV Enter a number for the quantity of interest (in range [0,4]): 2 Time period of the revolution (in picoseconds) is: 0.0000003 ps Enter a number for the quantity of interest (in range [0,4]): 3 Kinetic Energy (in electronvolts) is 1373.634 eV Enter a number for the quantity of interest (in range [0,4]): 4 Potential Energy (in electronvolts) is -2747.268 eV Enter a number for the quantity of interest (in range [0,4]): 5 Please enter an appropriate number Enter a number for the quantity of interest (in range [0,4]): 0 "Winding up... Thank you"

8. References

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N. Bohr

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Rejection of Rutherford's Planetary Model of the Atom, Bohr's Postulates and the Tunnel Effect

LG Sapogin, S Konstantinov

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