Atomic and Molecular Physics

Presented by

Lec. Dr. Sarah Mahdi Obaid

Department of Medical Physics,

Al-Mustaqbal University,

Babil, Iraq

Email: sarah.mahdi@uomus.edu.iq

Second-year students

Lecture 4

Single electron atom (The Hydrogen atom)

4.1 Line spectra of Hydrogen atom

It is found that hydrogen always gives a set of line spectra in the save position, sodium another set, iron still another and so on the line structure of the spectrum extends into both the ultraviolet and infrared regions. It is impossible to explain such a line spectrum phenomenon without using quantum theory. For many years, unsuccessful attempts were made to correlate the observed frequencies with those of a fundamental and its overtones (denoting other lines here). Finally, in 1885, Balmer found a simple formula which gave the frequencies of a group lines emitted by atomic hydrogen. Since the spectrum of this element is relatively simple, and fairly typical of a number of others, we shall consider it in more detail.

Under the proper conditions of excitation, atomic hydrogen may be made to emit the sequence of lines illustrated in Fig. 4.1. This sequence is called *series*.

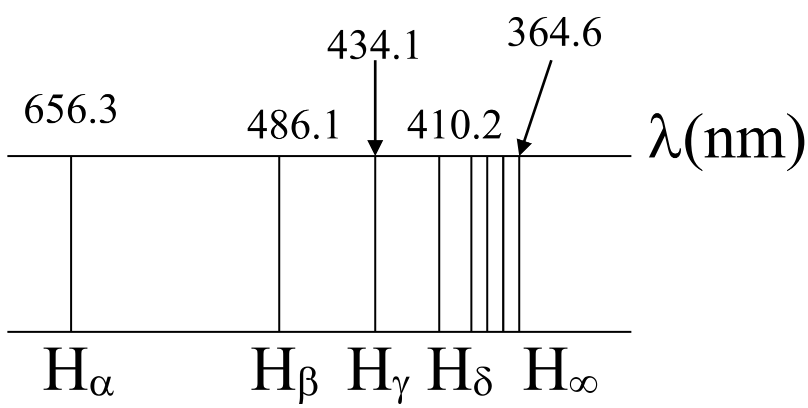

Fig. 4.1 The Balmer series of atomic hydrogen.

There is evidently a certain order in this spectrum, the lines becoming crowded more and more closely together as the limit of the series is approached. The line of longest wavelength or lowest

frequency, in the red, is known as H_α, the next, in the blue-green, as H_β, the third as H_γ, and so on.

Balmer found that the wavelength of these lines were given accurately by the simple formula

$$\frac{1}{\lambda} = R_\infty \left(\frac{1}{2^2} - \frac{1}{n^2} \right), \qquad n = 3, 4, 5, \cdots$$

where λ is the wavelength, *R_∞* is a constant called the *Rydberg constant*, and n may have the integral values 3, 4, 5, etc., if λ is in meters,

$$R_\infty = 1.097 \times 10^7 m^{-1}$$

Substituting R and n = 3 into the above formula, one obtains the wavelength of the Hα-line:

$$\lambda = 656.3nm$$

For n = 4, one obtains the wavelength of the H_β-line, etc. for n=∞, one obtains the limit of the series, at λ = 364.6nm –shortest wavelength in the series.

Other series spectra for hydrogen have since been discovered. These are known, after their discoveries, as Lymann, Paschen, Brackett and Pfund series. The formulas for these are

Lymann series: $$\frac{1}{\lambda} = R_\infty \left(\frac{1}{1^2} - \frac{1}{n^2} \right), \qquad n = 2,3,4,\cdots$$

Paschen series: $$\frac{1}{\lambda} = R_\infty \left(\frac{1}{3^2} - \frac{1}{n^2} \right), \qquad n = 4,5,6,\cdots$$

Brackett series: $$\frac{1}{\lambda} = R_\infty \left(\frac{1}{4^2} - \frac{1}{n^2} \right), \qquad n = 5,6,7,\cdots$$

Pfund series: $$\frac{1}{\lambda} = R_\infty \left(\frac{1}{5^2} - \frac{1}{n^2} \right), \qquad n = 6,7,8,\cdots$$

The Lymann series is in the ultraviolet, and the Paschen, Brackett, and Pfund series are in the infrared. All these formulas can be generalized into one formula which is called the general Balmer series.

$$\frac{1}{\lambda} = R_{\infty}\left(\frac{1}{k^2} - \frac{1}{n^2}\right), \qquad n = k+1, k+2, k+3, \cdots$$

All the spectra of atomic hydrogen can be described by this simple formula. As no one can explain this formula, it was ever called *Balmer formula puzzle*.

4.2 Bohr model for H-atom

Let's suppose an atom consists of nucleus with charge (Ze) and mass *M* and electron of charge (e) and mass *m* moving in circular orbit around the nucleus.

The electron moving around the nucleus under the influence of the Coulomb force keeps the electron in it's orbit therefore;

$$\frac{1}{4\pi\varepsilon_o}\frac{Ze^2}{r^2} = m\frac{\mathrm{v}^2}{r} \qquad \text{...(4.1)}$$

and by using the second postulate of Bohr

$$mvr = n\frac{h}{2\pi} \qquad n = 1,2,3,\cdots \qquad \textbf{(4.2)}$$

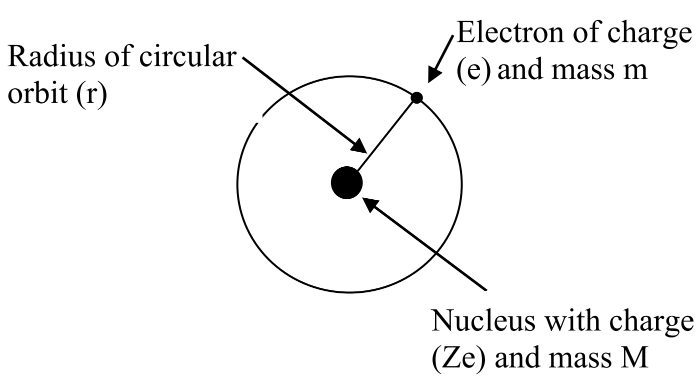

Fig. 4.1: Electron moving around the nucleus under the effect of Coulomb force

And by substituting the value of v from eq. (4.2) into eq. (4.1) we get;

$$Ze^2 = 4\pi\varepsilon_o m\mathrm{v}^2 r = 4\pi\varepsilon_o m\, r\left(\frac{n\hbar}{mr}\right)^2 = 4\pi\varepsilon_o \frac{n^2\hbar^2}{mr} \qquad \textbf{...(4.3)}$$

$$\therefore\ r_n = 4\pi\varepsilon_o \frac{n^2\hbar^2}{mZe^2} \qquad \textbf{...(4.4)}$$

where r_n is n^{th} Bohr radius

$$\mathrm{v_n} = \frac{n\hbar}{mr} = \frac{1}{4\pi\varepsilon_o}\frac{Ze^2}{n\hbar} \qquad \textbf{...(4.5)}$$

v_n is the velocity of the electron in the n^{th} orbit.

For hydrogen atom Z=1 and we take n=1 (ground state) and substitute into eq. (4.4) we will find first Bohr radius (a_o)

$$a_o = \frac{\hbar^2}{(e^2/4\pi\varepsilon_o)\ m} = 5.3\times10^{-11}\ \mathrm{m} = 0.53 \quad A^\circ$$

$$\mathrm{v} = \frac{e^2}{4\pi\varepsilon_o\hbar} = 2.2\times10^6 \quad \mathrm{m/s}$$

Therefore eq. 4.4 can be written in terms of first Bohr radius as

$$r = a_o n^2 \qquad\qquad n = 1,2,3\ \ldots$$

to calculate the total energy for the H-atom we use r_n and v_n from equations (4.4) and (4.5) respectively.

$$E_n = K.E + P.E = \frac{1}{2}m\mathrm{v}_n^2 + \frac{-e^2}{4\pi\varepsilon_o r_n} = -\frac{mZ^2e^4}{(4\pi\varepsilon_o)^2\,2\hbar^2}\frac{1}{n^2} \qquad \textbf{... (4.6)}$$

To calculate the electron energy in the ground state we put n=1 and Z=1 in eq. (4.6) we get;

$$E = -\frac{(9\times10^9)(9.11\times10^{-31})(1.6\times10^{-19})^4}{2(1.05\times10^{-34})} = -2.17\times10^{-18}J = -13.6 \quad eV$$

(-13.6 eV) is called the binding energy of the electron in the first orbit in H-atom.

The other energy levels can be calculated from the relation

$$E_n = -\frac{13.6 \ eV}{n^2} \qquad\qquad n = 1,2,3\ldots$$

It is easy to see that all the energy in atoms should be discrete not continuous. When the electron transits from n^{th} orbit to k^{th} orbit, the frequency and wavelength can be calculated as

$$\nu = \frac{E_n - E_k}{h} = \frac{me^4}{8\varepsilon_0^2 h^3}\left(\frac{1}{k^2} - \frac{1}{n^2}\right) \qquad\qquad n > k$$

$$\frac{1}{\lambda} = \frac{\nu}{c} = \frac{me^4}{8\varepsilon_0^2 h^3 c}\left(\frac{1}{k^2} - \frac{1}{n^2}\right) = R_\infty\left(\frac{1}{k^2} - \frac{1}{n^2}\right) \qquad\qquad ...(4.7)$$

Where $R_\infty = \frac{me^4}{8\varepsilon_0^2 h^3 c}$ is *Rydberg constant*. It is found that the value of R is matched with experimental data very well. Till then, the 30-years puzzle of line spectra of atoms was solved by Bohr since equation (4.7) is exactly the general Balmer formula.

When Bohr's theory met problems in explaining a little bit more complex atoms (He) or molecules (H_2), Bohr realized that his theory is full of contradictions as he used both quantum and classical theories. The problem was solved completely after De Broglie proposed that electron also had the wave-particle duality. Since then, the proper theory describing the motion of the micro-particles, quantum mechanics, have been gradually established by many scientists.

MCQ Lecture 4

Multiple Choice Questions

1. **Which formula did Balmer propose to explain the wavelengths of the hydrogen spectrum?**
   A. Bohr's Formula
   B. Rydberg Formula
   C. Balmer Formula
   D. Planck's Formula

2. **What is the wavelength of the Hα line in the Balmer series?**
   A. 364.6 nm
   B. 656.3 nm
   C. 486.1 nm
   D. 434.1 nm

3. **Which series of the hydrogen spectrum is in the ultraviolet region?**
   A. Paschen Series
   B. Lyman Series
   C. Brackett Series
   D. Pfund Series

4. **What constant is used in the Balmer formula for hydrogen?**
   A. Planck's Constant
   B. Speed of Light
   C. Rydberg Constant
   D. Avogadro's Constant

5. **Which quantum number determines the orbit of an electron in the Bohr model?**
   A. Principal Quantum Number
   B. Orbital Angular Momentum Quantum Number
   C. Magnetic Quantum Number
   D. Spin Quantum Number

6. **In Bohr's model, what is the energy of the electron in the ground state of hydrogen?**
   A. 6.13 eV
   B. -13.6 eV
   C. 0 eV
   D. -6.13 eV

7. **What is the Bohr radius for the hydrogen atom?**
   A. 1.5×10^{-10} m
   B. 5.3×10^{-11} m
   C. 9.2×10^{-11} m
   D. 2.1×10^{-10} m

8. **What does the Rydberg formula describe?**
   A. The energy of electrons in hydrogen
   B. The wavelengths of spectral lines in hydrogen

C. The transition of electrons between shells
D. The spin of an electron

9. **Which of the following series is NOT part of the hydrogen spectral lines?**
   A. Lyman Series
   B. Paschen Series
   C. Fleming Series
   D. Brackett Series

10. **Which transition of the electron in hydrogen gives rise to the Hα line?**
   A. n=2 to n=1
   B. n=3 to n=2
   C. n=4 to n=3
   D. n=5 to n=4

11. **What is the formula used to calculate the wavelength in the Balmer series?**
   A. $\lambda = (1/n^2) \times R_\infty$
   B. $\lambda = R_\infty \times (1/n^2 - 1/m^2)$
   C. $\lambda = h/n$
   D. $\lambda = R_\infty \times (1/n^2)$

12. **What does the term "Bohr radius" refer to?**
   A. The radius of the electron's orbit in the hydrogen atom
   B. The energy level of the electron in the hydrogen atom
   C. The charge of the nucleus in hydrogen
   D. The wavelength of the emitted light in the hydrogen spectrum

13. **In Bohr's model, what happens when an electron moves from a higher energy orbit to a lower one?**
   A. The electron absorbs energy
   B. The electron emits energy
   C. The electron changes its mass
   D. The electron's velocity increases

14. **What is the value of the Rydberg constant in SI units?**
   A. 1.097×10^7 m^{-1}
   B. 2.18×10^{-18} J
   C. 3.28×10^8 m/s
   D. 6.626×10^{-34} J $\cdot$ s

15. **In the Bohr model, the electron's angular momentum is quantized in integer multiples of which constant?**
   A. Planck's constant (h)
   B. Rydberg constant (R)
   C. Electron mass (m)
   D. Coulomb constant (k)

16. **What series of spectral lines is emitted when an electron moves from a higher orbit to n=2?**
   A. Lyman Series
   B. Balmer Series
   C. Paschen Series
   D. Pfund Series

17. **What is the shortest wavelength in the Balmer series of hydrogen?**
   A. 364.6 nm
   B. 656.3 nm
   C. 434.1 nm

D. 486.1 nm

18. **In the hydrogen atom, what does the principal quantum number (n) represent?**

    A. The electron's angular momentum
    B. The energy level of the electron
    C. The direction of the electron's spin
    D. The shape of the electron's orbit

19. **Which of the following equations relates to Bohr's energy calculation for the hydrogen atom?**

    A. $E = -13.6/n^2$ eV
    B. $E = 13.6/n^2$ eV
    C. $E = -13.6m/n^2$
    D. $E = 13.6m/n^2$

20. **What physical principle did Bohr's model incorporate to explain the stability of electron orbits in hydrogen?**

    A. Wave-particle duality
    B. Heisenberg uncertainty principle
    C. Coulomb's law
    D. Quantization of angular momentum