Atomic Physics

Chapter 2

Bohr's Model of the Hydrogen
The Classical Atomic Model

The force of attraction on the electron due to the nucleus is

\[ \vec{F} = \frac{-e^2}{4\pi\varepsilon_0} \frac{\vec{r}}{r^3} \]

The electron's radial acceleration

\[ a_r = \frac{v^2}{r} \]

where \( v \) is the tangential velocity of the electron and Newton's second law now gives

\[ \frac{e^2}{4\pi\varepsilon_0} \frac{1}{r^2} = \frac{mv^2}{r} \]

and

\[ v = \frac{e}{\sqrt{4\pi\varepsilon mr}} \]
The total mechanical energy is

\[ E = \frac{1}{2}mv^2 - \frac{e^2}{4\pi\varepsilon_0 r} \]

with the equation about \( v \), we have

\[ E = \frac{e^2}{8\pi\varepsilon_0 r} - \frac{e^2}{4\pi\varepsilon_0 r} = -\frac{e^2}{8\pi\varepsilon_0 r} \]

The total energy is negative, indicating a bound system.

An accelerated electric charge continuously radiates energy in the form of electromagnetic radiation!
Bohr’s general assumptions

A. Certain “stationary states” exist in atoms, which differ from the classical stable states in that the orbiting electrons do not continuously radiate electromagnetic energy. The stationary states are states of definite total energy.

B. The emission or absorption of electromagnetic radiation can occur only in conjunction with a transition between two stationary states. The frequency of the emitted or absorbed radiation is proportional to the difference in energy of the two stationary states (1 and 2):

\[ E = E_1 - E_2 = h\nu \]

where \( h \) is Planck’s constant.
Bohr’s general assumptions

C. the angular momentum of the system in a stationary state being an integral multiple of $\hbar = \hbar/2\pi$

$$L = mvr = n\hbar$$

where $n$ is an integer called the principal quantum number.

The velocity can be solved

$$v = \frac{n\hbar}{mr}$$

with Newton’s second law

$$v^2 = \frac{e^2}{4\pi\varepsilon_0 m r} = \frac{n^2\hbar^2}{m^2 r^2}$$
Bohr model

Only certain values of radii are allowed

\[ r_n = \frac{4\pi\varepsilon_0 n^2 \hbar^2}{me^2} \equiv n^2 a_0 \]

where the Bohr radius \( a_0 \) is given by

\[ a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{me^2} = 0.53 \times 10^{-10} \text{ m} \]

The atomic radius is now quantized. The quantization of various physical values arises because of the principal quantum number \( n \).
Bohr model

Electron’s velocity in Bohr model

\[ v_n = \frac{n\hbar}{mr_n} = \frac{n\hbar}{mn^2a_0} = \frac{1}{n} \frac{\hbar}{ma_0} \]

or

\[ v_n = \frac{1}{n} \frac{e^2}{4\pi \varepsilon_0 \hbar} \]

and

\[ v_1 = \frac{\hbar}{ma_0} = 2.2 \times 10^6 \text{ m/s} \]

We define the dimensionless quantity ratio of \( v_1 \) to \( c \) as

\[ \alpha = \frac{v_1}{c} = \frac{\hbar}{ma_0 c} = \frac{e^2}{4\pi \varepsilon_0 \hbar c} \approx \frac{1}{137} \]

This ratio is called the fine structure constant. It appears often in atomic structure calculations.
Bohr model

The energies of the stationary states

\[ E_n = -\frac{e^2}{8\pi\varepsilon_0 r_n} = -\frac{e^2}{8\pi\varepsilon_0 a_0 n^2} \equiv -\frac{E_0}{n^2} \]

The lowest energy state (n=1) is \( E_1 = -E_0 \), where

\[ E_0 = \frac{e^2}{8\pi\varepsilon_0 a_0} = \frac{e^2}{8\pi\varepsilon_0} \frac{me^2}{4\pi\varepsilon_0 \hbar^2} = 13.6 \text{ eV} \]

This is the experimentally measured ionization energy of the hydrogen atom. Bohr’s assumption imply that the atom can exist only in “stationary state” with definite, quantized energies \( E_n \).
Bohr model

Emission of a quantum of light occurs when the atom is in an excited state (quantum number \( n_{u} \)) and decays to a lower energy state (quantum number \( n_{l} \))

\[
h\nu = E_{u} - E_{l}
\]

where, \( \nu \) is the frequency of the emitted light quantum (photon). Because

\[
\lambda \nu = c
\]

we have

\[
\frac{1}{\lambda} = \frac{\nu}{c} = \frac{E_{u} - E_{l}}{hc}
\]

\[
= -\frac{E_{0}}{hc} \left( \frac{1}{n_{u}^{2}} - \frac{1}{n_{l}^{2}} \right) = \frac{E_{0}}{hc} \left( \frac{1}{n_{l}^{2}} - \frac{1}{n_{u}^{2}} \right)
\]
Bohr model

where,

\[
\frac{E_0}{\hbar c} = \frac{me^4}{4\pi\varepsilon_0 h^3} \left(4\pi\varepsilon_0^2\right)^2 \equiv R_\infty
\]

is called the Rydberg constant (for an infinite nuclear mass) and

\[
\frac{1}{\lambda} = R_\infty \left(\frac{1}{n_l^2} - \frac{1}{n_u^2}\right)
\]

which was found by J. Rydberg.

Bohr’s model predicts the frequencies (and wavelengths) of all possible transitions in atomic hydrogen.
The spectrum of hydrogen

<table>
<thead>
<tr>
<th>Discoverer (year)</th>
<th>Wavelength</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lyman (1916)</td>
<td>Ultraviolet</td>
</tr>
<tr>
<td>Balmer (1885)</td>
<td>Visible, ultraviolet</td>
</tr>
<tr>
<td>Paschen (1908)</td>
<td>Infrared</td>
</tr>
<tr>
<td>Brackett (1922)</td>
<td>Infrared</td>
</tr>
<tr>
<td>Pfund (1924)</td>
<td>Infrared</td>
</tr>
</tbody>
</table>
Line spectra

Gas discharge tube containing hydrogen

Slits

Prism

Violet: 410.0 nm
Blue-violet: 434.0 nm
Blue green: 486.1 nm
Red: 658.2 nm

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Jinniu Hu
The absorption spectrum

When we pass white light (composed of all visible photon frequencies) through atomic hydrogen gas, we find that certain frequencies are absent. This pattern of dark lines is called an absorption spectrum.
The emission spectrum

The missing frequencies are precisely the ones observed in the corresponding emission spectrum.
Bohr’s correspondence principle: In the limits where classical and quantum theories should agree, the quantum theory must reduce to the classical result.

To illustrate this principle, let us examine the predictions of the radiation law.

Classically the frequency of the radiation emitted is equal to the orbital frequency $\nu_{\text{orb}}$ of the electron around the nucleus:

$$\nu_{\text{classical}} = \nu_{\text{orb}} = \frac{\omega}{2\pi} = \frac{1}{2\pi} \frac{\nu}{r}$$
The Correspondence Principle

With Newton's second law:

\[ \nu_{\text{classical}} = \frac{1}{2\pi} \sqrt{\frac{e^2}{4\pi\varepsilon_0 m r^3}} \]

Using Bohr model, the classical frequency in terms of fundamental constants and the principal quantum number \( n \)

\[ \nu_{\text{classical}} = \frac{m e^4}{4\varepsilon_0^2 h^3} \frac{1}{n^3} \]

In the Bohr model, the frequency of the transition from \( n+1 \) to \( n \) is

\[ \nu_{\text{Bohr}} = \frac{E_0}{h} \left[ \frac{1}{n^2} - \frac{1}{(n + 1)^2} \right] = \frac{E_0}{h} \left[ \frac{2n + 1}{n^2(n + 1)^2} \right] \]
The Correspondence Principle

It becomes for large $n$

$$\nu_{\text{Bohr}} \approx \frac{2nE_0}{\hbar n^4} = \frac{2E_0}{\hbar n^3}$$

When the $E_0$ is substituted, the result is

$$\nu_{\text{Bohr}} = \frac{me^4}{4\varepsilon_0^2\hbar^3} \frac{1}{n^3} = \nu_{\text{classical}}$$

so the frequencies of the radiated energy agree between classical theory and the Bohr model for large values of the quantum number $n$. Bohr’s correspondence principle is verified for large orbits, where classical and quantum physics should agree.
A straightforward analysis derived from classical mechanics shows that this two-body problem can be reduced to an equivalent one-body problem.
The Successes of Bohr Model

Reduced mass

\[ \mu_e = \frac{m_e M}{m_e + M} = \frac{m_e}{1 + \frac{m_e}{M}} \]

and \( M \) is the mass of the nucleus. In the case of the hydrogen atom, \( M \) is the proton mass, and the correction for the hydrogen atom is

\[ \mu_e = 0.999456 m_e \]

This difference can be measured experimentally. The Rydberg constant for infinite nuclear mass should be replaced by,

\[ R = \frac{\mu_e}{m_e} R_\infty = \frac{\mu_e e^4}{4\pi \epsilon_0} \frac{1}{4\pi \hbar^3 (4\pi \epsilon_0)^2} \]
The Successes of Bohr Model

The Rydberg constant for hydrogen is

\[ R_H = 1.096776 \times 10^7 \text{ m}^{-1} \]

The Bohr model may be applied to any single-electron atom (hydrogen-like) even if the nuclear charge is greater than 1 proton charge (+e), for example He\(^+\) and Li\(^{++}\).

The Rydberg equation becomes

\[ \frac{1}{\lambda} = Z^2 R \left( \frac{1}{n_i^2} - \frac{1}{n_u^2} \right) \]

Z is the nuclear charge. This equation is valid only for single-electron atoms. Charged atoms, such as He\(^+\), Li\(^+\), and Li\(^{++}\), are called ions.
The German physicists James Franck and Gustav Hertz decided to study electron bombardment of gaseous vapors to study the phenomenon of ionization.

We can explain the experimental results of Franck and Hertz within the context of Bohr's picture ofquantized atomic energy levels. In the most popular representation of atomic energy states, we say that the atom, when all the electrons are in their lowest possible energy states, is the **ground state**. We define this energy $E_0$ to be zero. The first quantized energy state above the ground state is called the **first excited state**, and it has energy $E_1$. The energy difference $E_1/E_0$ is called the **excitation energy** of the state $E_1$. We show the position of one

![Diagram of Franck-Hertz experiment](image)

**Figure 4.20** Schematic diagram of apparatus used in an undergraduate physics laboratory for the Franck-Hertz experiment. The hot filament produces electrons, which are accelerated through the mercury vapor toward the grid. A decelerating voltage between grid and collector prevents the electrons from registering in the electrometer unless the electron has a certain minimum energy.

**Figure 4.21** Data from an undergraduate student's Franck-Hertz experiment using apparatus similar to that shown in Figure 4.20. The energy difference between peaks is about 5 V, but the first peak is not at 5 V because of the work function differences of the metals used for the filament and grid.
John. Hu

Atomic Excitation by Electrons

Data from Franck-Hertz experiment

![Graph showing data from Franck-Hertz experiment]

The electron current registered in the electrometer continued to increase as $V$ increased. However, as the accelerating voltage increased above 5 V, there was a sudden drop in the current (see Figure 4.21, which was constructed using data taken by students performing this experiment). As the accelerating voltage continued to increase above 5 V, the current increased again, but suddenly dropped above 10 V. Franck and Hertz first interpreted this behavior as the onset of ionization of the Hg atom; that is, an atomic electron is given enough energy to remove it from the Hg, leaving the atom ionized. They later realized that the Hg atom was actually being excited to its first excited state.

We can explain the experimental results of Franck and Hertz within the context of Bohr’s picture of quantized atomic energy levels. In the most popular representation of atomic energy states, we say that the atom, when all the electrons are in their lowest possible energy states, is the ground state. We define this energy $E_0$ to be zero. The first quantized energy state above the ground state is called the first excited state, and it has energy $E_1$. The energy difference $E_1/E_0$ is called the excitation energy of the state $E_1$. We show the position of one collector.

**Figure 4.20**

Schematic diagram of apparatus used in an undergraduate physics laboratory for the Franck-Hertz experiment. The hot filament produces electrons, which are accelerated through the mercury vapor toward the grid. A decelerating voltage between grid and collector prevents the electrons from registering in the electrometer unless the electron has a certain minimum energy.

**Figure 4.21**

Data from an undergraduate student’s Franck-Hertz experiment using apparatus similar to that shown in Figure 4.20. The energy difference between peaks is about 5 V, but the first peak is not at 5 V because of the work function differences of the metals used for the filament and grid.
We can explain the experimental results of Franck and Hertz within the context of Bohr’s picture of quantized atomic energy levels.

In the most popular representation of atomic energy states, we say that the atom, when all the electrons are in their lowest possible energy states, is the ground state. The first quantized energy state above the ground state is called the first excited state.
The first excited state of Hg is at an excitation energy of 4.88 eV. As long as the accelerating electron’s kinetic energy is below 4.88 eV, no energy can be transferred to Hg because not enough energy is available to excite an electron to the next energy level in Hg.
When the accelerating voltage is increased to 7 or 8 V, even electrons that have already made an inelastic collision have enough remaining energy to reach the collector. However, when the accelerating voltage reaches 9.8 V, the electrons have enough energy to excite two Hg atoms in successive inelastic collisions, losing 4.88 eV in each
The limitations of Bohr Model

1. It could be successfully applied only to single-electron atoms (H, He+, Li++, and so on).

2. It was not able to account for the intensities or the fine structure of the spectral lines.

3. Bohr’s model could not explain the binding of atoms into molecules.
The extension of Bohr model

Sommerfeld succeeded partially in explaining the observed fine structure of spectral lines by introducing the following main modifications in Bohr’s theory:

1. Sommerfeld suggested that the path of an electron around the nucleus, in general, is an ellipse with the nucleus at one of the foci.

2. Sommerfeld took into account the relativistic variation of the mass of the electron with velocity. Hence this model of the atom is called the relativistic atom model.
Elliptical orbits for hydrogen

Two quantization conditions are

\[ \int p_\phi \, d\phi = n_\phi h \]
\[ \int p_r \, dr = n_r h \]

where \( n_\phi \) and \( n_r \) are the two quantum numbers introduced by Sommerfeld and

\[ n_r + n_\phi = n \]
The extension of Bohr model

The energies for hydrogen with elliptical orbits

\[ E_n = - \frac{mZ^2 e^4}{8 \varepsilon_0^2 h^2 n^2} = - \frac{mZ^2 e^4}{8 \varepsilon_0^2 h^2} \left[ \frac{1}{n_r + n_\phi} \right]^2 \]

which is identical with the expression for the energy of the electron in a circular orbit of quantum number \( n \). Thus, the introduction of elliptical orbits does not result in the production of new energy terms. Thus the introduction of elliptical orbits gives no new energy levels and hence no new transition.
The extension of Bohr model

Sommerfeld, including the relativistic correction in the treatment of elliptical orbits, showed that equation of the path of the electron was not simply that for an ellipse but was of the form

\[
\frac{1}{r} = \frac{1 + \varepsilon \cos \psi \phi}{a(1 - \varepsilon^2)}
\]

where,

\[
\psi^2 = 1 - \left[ \frac{Ze^2}{4\pi \varepsilon_0 pc} \right]^2
\]

and \(\varepsilon\) is the eccentricity (离心率) and the path of the electron is, therefore, a rosette (玫瑰花结).
The extension of Bohr model

It can be shown that the total energy with a principal quantum number $n$ in the relativistic theory is

$$E_n, n_\phi = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2n^2} - \frac{mZ^2e^4\alpha^2}{8\varepsilon_0^2h^2} \left[ \frac{n}{n_\phi} - \frac{3}{4} \right] \frac{1}{n^4}$$

The second term is Sommerfeld’s relativity correction arising from the rosette motion of the electron orbit with principal quantum number $n$ and azimuthal quantum number $n_\phi$.

$H_\alpha$ line is due to the transition from $n = 3$ state to $n = 2$ state of hydrogen atom.
Alkali Atom

The alkali atoms have a weakly bound outer electron, the so-called valence electron, and all other \((Z-1)\) electrons are in closed shells.

![Diagram showing energy levels and transitions for alkali-metal atoms]
Penetrating effect

Non-Penetrating orbits

When the outer electron has a non-penetrating orbit, as in the figure. If it's accepted that the mean symmetry of the cloud formed by \((Z-1)e\) electrons is similar, the electron experiences the electrostatic potential of the nuclear charge of \(Ze\) and of the spherical distribution of charge \((Z-1)e\). The discussion presented for the hydrogen atom remains valid.

Penetrating orbits

On the other hand, if the orbit of the outer electron penetrates inside the core of the atom, the problem is much more complex. Simple solution by Somerfield, is this,
Effective nuclear charge

The effective nuclear charge (often symbolized as $Z_{\text{eff}}$) is the net positive charge experienced by an electron in a polyelectronic atom.
Heart curve

\[
r = \sqrt{\sin(0.5(x - 1.5\pi))} + 1, \{x, -0.5\pi, 1.5\pi\}
\]

\[
\left(x^2 + \frac{9}{4}y^2 + z^2 - 1\right)^3 - x^2z^3 - \frac{9}{80}y^2z^3
\]

\[
(x^2 + y^2 - 1)^3 - x^2y^3 = 0
\]

\[
x = \sin(t)\cos(t)\log(|t|)
\]

\[
y = |t|^{0.5}\sqrt{\cos(t)}
\]

\[
x = 16\sin^3(t)
\]

\[
y = 13\cos(t) - 5\cos(2t) - 2\cos(3t) - \cos(4t)
\]
Homework

The Physics of Atoms and Quanta

8.1, 8.2, 8.3, 8.6, 8.8, 8.18