

Chapter 2

ATOMIC THEORY

Basic Principles, Evidence and Examples

Among all physical constants there are two which will be universally admitted to be of predominant importance; the one is the velocity of light, which now appears in many of the fundamental equations of theoretical physics, and the other is the ultimate, or elementary, electrical charge, *Robert Millikan* (1868–1953)

1. INTRODUCTION

Around the 5th century BC, Greek philosopher Democritus invented the concept of the *atom* (from Greek meaning “indivisible”). The atom, *eternal, constant, invisible and indivisible*, represented the smallest unit and the building block of all matter. Democritus suggested that the varieties of matter and changes in the universe arise from different relations between these most basic constituents. He illustrated the concept of atom by arguing that every piece of matter could be cut to an end until the last constituent is reached. Today the word *atom* is used to identify the basic component of molecules that create all matter, but it is known that the atom itself is made of particles even more fundamental, some of which are elementary. The first theoretical and experimental models of the structure of matter came as late as the 19th century, which is the time marked as the beginning of modern science. At that time a more empirical approach, mainly in chemistry, opened a new era of scientific investigations.

The work of Democritus remained known through the ages in writings of other philosophers, mainly Aristotle. Modern Greece has honored Democritus as a philosopher and the originator of the concept of the atoms

through their currency; the 10-drachma coin, before Greek currency was replaced with the euro, depicted the face of Democritus on one side, and the schematic of a lithium atom on the other.

This chapter introduces the structure of atoms and describes atomic models that show the evidence for the existence of atoms and electrons.

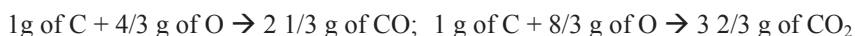
2. ATOMIC MODELS

2.1 The Cannonball Atomic Model

All matter on Earth is made from a combination of 90 naturally occurring different atoms. Early in the 19th century, scientists began to study the decomposition of materials and noted that some substances could not be broken down past a certain point (for instance, once separated into oxygen and hydrogen, water cannot be broken down any further). These primary substances are called *chemical elements*. By the end of the 19th century it was implicit that matter can exist in the form of a pure element, chemical compound of two or more elements or as a mixture of such compounds. Almost 80 elements were known at that time and a series of experiments provided confirmation that these elements were composed of atoms. This led to a discovery of the *law of definite proportions*: two elements, when combined to create a pure chemical compound, always combine in fixed ratios by weight. For example, if element *A* combines with element *B*, the unification creates a compound *AB*. Since the weight of *A* is constant and the weight of *B* is constant, the weight ratio of these two will always be the same. This also implies that two elements will only combine in the defined proportion; adding an extra quantity of one of the elements will not produce more of the compound.

Example 2.1: The law of definite proportion

Carbon (C) forms two compounds when reacting with oxygen (O): carbon monoxide (CO) and carbon dioxide (CO₂).



The two compounds are formed by the combination of a definite number of carbon atoms with a definite number of oxygen atoms. The ratio of these two elements is constant for each of the compounds (molecules): C:O = 3:4 for CO and C:O = 3:8 for CO₂.

The first atomic theory with empirical proofs for the law of definite

proportion was developed in 1803 by the English chemist John Dalton (1766–1844). Dalton conducted a number of experiments on gases and liquids and concluded that, in chemical reactions, the amount of the elements combining to form a compound is always in the same proportion. He showed that matter is composed of atoms and that atoms have their own distinct weight. Although some explanations in Dalton's original atomic theory are incorrect, his concept that chemical reactions can be explained by the union and separation of atoms (which have characteristic properties) represents the foundations of modern atomic physics. In his two-volume book, *New System of Chemical Philosophy*, Dalton suggested a way to explain the new experimental chemistry. His atomic model described how all elements were composed of indivisible particles which he called atoms (he depicted atoms like cannonballs, Fig.2-1) and that all atoms of a given element were exactly alike. This explained the law of definite proportions. Dalton further explained that different elements have different atoms and that compounds were formed by joining the atoms of two or more elements.

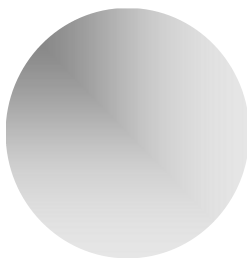


Figure 2-1. Cannonball atomic model (John Dalton, 1803)

In 1811, Amadeo Avogadro, conte di Quaregna e Ceretto (1776–1856), postulated that equal volumes of gases at the same temperature and pressure contain the same number of molecules. Sadly, his hypothesis was not proven until 2 years after his death at the first international conference on chemistry held in Germany in 1860 where his colleague, Stanislao Cannizzaro, showed the system of atomic and molecular weights based on Avogadro's postulates.

Example 2.2: Avogadro's law

As shown in Example 2.1, the ratio of carbon and oxygen in forming CO_2 is 3:8. Here is the explanation of this ratio: since a single atom of carbon has the same mass as 12 hydrogen atoms, and two oxygen atoms have the same mass as 32 hydrogen atoms, the ratio of the masses is $12:32 = 3:8$. This shows that the description of the reaction is independent of the units used since it is the ratio of the masses that determines the outcome of a chemical reaction. Thus, whenever you see wood burning in a fire, you should know that for every atom of carbon from the wood, two

oxygen atoms from the air are combined to form CO_2 ; the ratio of masses is always 12:32.

It follows that there must be as many carbon atoms in 12 g of carbon as there are oxygen atoms in 16 g of oxygen. This measure of the number of atoms is called a *mole*. The mole is used as a convenient measure of an amount of matter, similarly as “a dozen” is a convenient measure of 12 objects of any kind. Thus, the number of atoms (or molecules) in a mole of any substance is the same. This number is called Avogadro’s number (N_A) and its value was accurately measured in the 20th century as 6.02×10^{23} atoms or molecules per mole.

For example, the number of moles of hydrogen atoms in a sample that contains 3.02×10^{21} hydrogen atoms is

$$\text{Moles of H atoms} = \frac{3.02 \times 10^{21} \text{ atoms H}}{6.02 \times 10^{23} \text{ atoms/mole}} = 5.01 \times 10^{-3} \text{ moles H}$$

2.2 The Plum Pudding Atomic Model

Shortly before the end of the 19th century, a series of new experiments and discoveries opened the way for new developments in atomic and subatomic (nuclear) physics. In November 1895, Wilhelm Roentgen (1845–1923) discovered a new type of radiation called *X-rays*, and their ability to penetrate highly dense materials. Soon after the discovery of X-rays, Henri Becquerel (1852–1908) showed that certain materials emit similar rays independent of any external force. Such emission of radiation became known as *radioactivity* (described in all details in Chapter 5).

During this same time period, scientists were extensively studying a phenomenon called *cathode rays*. Cathode rays are produced between two plates (a cathode and an anode) in a glass tube filled with the very low-density gas when an electrical current is passed from the cathode to the high-voltage anode. Because the glowing discharge forms around the cathode and then extends toward the anode, it was thought that the rays were coming out of the cathode. The real nature of cathode rays was not understood until 1897 when Sir Joseph John Thomson (1856–1940) performed experiments that led to the discovery of the first subatomic particle, the *electron*. The most important aspect of his discovery is that the cathode rays are the *stream of particles*. Here is the explanation of his postulate: from the experiment he observed that cathode rays were always deflected by an electric field from the negatively charged plate inside the cathode ray tube, which led him to conclude that the rays carried a *negative electric charge*. He was able to determine the speed of these particles and obtain a value that was a fraction of the speed of light (one tenth the speed of

light, or roughly 30,000 km/s or 18,000 mi/s). He postulated that anything that carries a charge must be of material origin and composed of particles. In his experiment, Thomson was able to measure the charge-to-mass ratio, e/m , of the cathode rays; a property that was found to be constant regardless of the materials used. This ratio was also known for atoms from electrochemical analysis, and by comparing the values obtained for the electrons he could conclude that the electron was a very small particle, approximately 1,000 times smaller than the smallest atom (hydrogen). The electron was the first subatomic particle identified and the fastest small piece of matter known at that time.

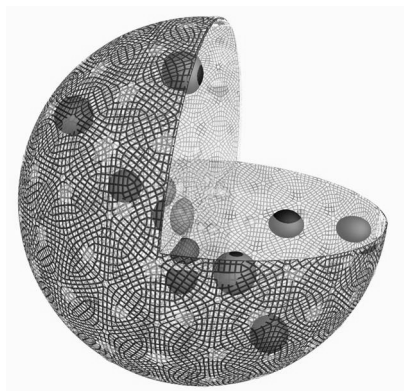


Figure 2-2. Plum pudding atomic model (J. J. Thomson, 1904)

In 1904, Thomson developed an atomic model to explain how the negative charge (electrons) and positive charge (speculated to exist since it was known that the atoms were electrically neutral) were distributed in an atom. He concluded that the atom was a sphere of positively charged material with electrons spread equally throughout like raisins in a plum pudding. Hence, his model is referred to as the *plum pudding model*, or *raisin bun atom* as depicted in Fig. 2-2. This model could explain

- The neutrality of atoms
 - The origin of electrons
 - The origin of the chemical properties of elements
- However, his model could not answer questions regarding
- Spectral lines (according to this model, radiation emitted should be monochromatic; however, experiments with hydrogen shows a series of lines falling into different parts of the electromagnetic spectrum)
 - Radioactivity (nature of emitted rays and their origin in the atom)
 - Scattering of charged particles by atoms

Thomson won the Nobel Prize in 1906 for his discovery of the electron. He worked in the famous Cavendish Laboratory in Cambridge and was one of the most influential scientists of his time. Seven of his students and collaborators won Nobel Prizes, among them his son who, interestingly, won the Nobel Prize for proving the electron is a wave (Chapter 4).

2.3 Millikan's Experiment

In 1909 Robert Millikan (1868–1953) developed an experiment at the University of Chicago to measure the charge of the electron. The experiment is known as the “Millikan oil-drop experiment”. Millikan determined the mass of the electron based on his experimentally measured value of the electron charge, 1.60×10^{-19} C, and Thomson's charge-to-mass ratio, 1.76×10^8 C/g. He found the electron mass to be 9.10×10^{-28} g (about 2000 times smaller than that of hydrogen, the lightest atom); the presently accepted value is 9.109382×10^{-28} g.

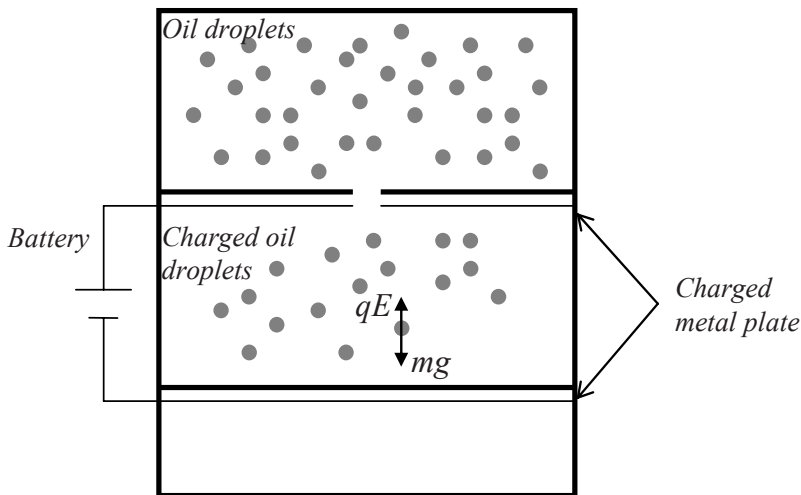


Figure 2-3. Schematics of Millikan's oil-drop experiment (1909)

How was the charge of an electron measured from the oil drops? Millikan's experimental apparatus consisted of a chamber with two metal plates connected to a voltage source where the oil droplets were allowed to fall between (Fig.2-3). In the absence of a voltage (electrical field, E , equal to zero) droplets were allowed to fall until they reached their terminal velocity (when the downward force of gravity, mg , is balanced with the upward force of air resistance). By measuring the terminal velocity he was able to determine the mass of the oil droplets. By introducing an electrical

field, the forces (gravitational and electrical) could be balanced and the drops would be suspended in mid-air. The resulting force is zero, because the gravitational force is equal to the electrical force:

$$mg = qE \quad (2-1)$$

where m is the mass of the oil drop, g is the acceleration of gravity and the total charge of the oil droplet, $q = N \cdot e$, is an integer times the charge of one electron (because the electron cannot be divided to produce a fractional charge). By changing the electric charge of oil droplets (irradiating them with X-rays known at that time to ionize the molecules), Millikan found that the charge was always a multiple of the same number. In 1913 he published the value of -1.5924×10^{-19} C. The accepted value today is $-1.60217653 \times 10^{-19}$ C (see also Appendix 2). Robert Millikan was awarded the Nobel Prize in 1923 for this work.

2.4 The Planetary Atomic Model

2.4.1 Disproof of Thomson's Plum Pudding Atomic Model

Thomson's atomic model described the atom as a relatively large, positively charged, amorphous mass of a spherical shape with negatively charged electrons homogeneously distributed throughout the volume of a sphere, the sizes of which were known to be on the order of an Ångström ($1 \text{ Å} = 10^{-8} \text{ cm} = 10^{-10} \text{ m}$). In 1911 Geiger and Marsden carried out a number of experiments under the direction of Ernest Rutherford (1871–1937) who received the Nobel Prize in chemistry in 1908 for investigating and classifying radioactivity. He actually did his most important work after he received the Nobel Prize and the 1911 experiment unlocked the hidden nature of the atom structure.

Rutherford placed a naturally radioactive source (such as radium) inside a lead block as shown in Fig. 2-4. The source produced α particles which were collimated into a beam and directed toward a thin gold foil. Rutherford hypothesized that if Thomson's model was correct then the stream of α particles would pass straight through the foil with only a few being slightly deflected as illustrated in Fig. 2-5. The "pass through" the atom volume was expected because the Thomson model postulated a rather uniform distribution of positive and negative charges throughout the atom. The *deflections* would occur when the positively charged α particles came very close to the individual electrons or the regions of positive charges. As expected, most of the α particles went through the gold foil with almost no deflection. However, some of them rebounded almost directly backward – a

phenomenon that was not expected (Fig. 2-6). The main challenge was to explain what caused such a large deflection angle and what caused other particles to go through the atom without noticeable scattering.

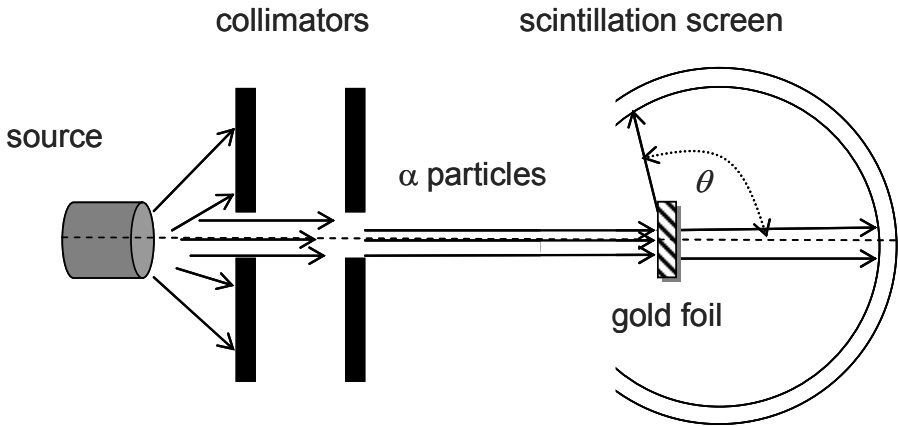


Figure 2-4. Schematics of Rutherford's experiment (1911)

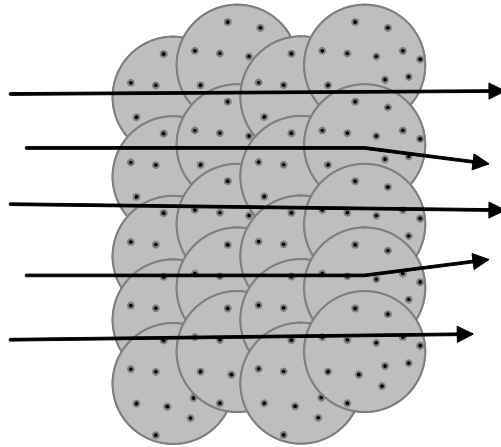


Figure 2-5. Expected scattering of α particles in Rutherford's experiment

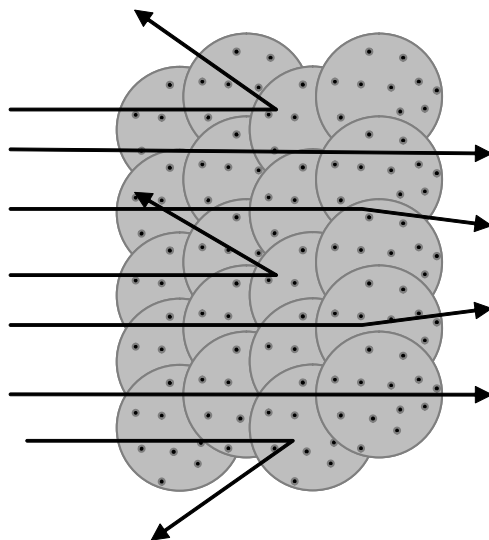


Figure 2-6. Actual scattering of α particles in Rutherford's experiment

Rutherford explained that most of the α particles pass through the gold foil with little or no divergence not because the atom is a uniform mixture of the positive and negative charges but because the atom is largely empty space and there is nothing to interact with the α particles. He explained the large scattering angle by suggesting that some of the particles occasionally collide with, or come very close to, the “massive” *positively charged nucleus* that is located at the center of an atom. It was known at the time that the gold nucleus had a positive charge of 79 units and a mass of about 197 units while the α particle had a positive charge of 2 units and a mass of 4 units. The repulsive force between the α particle and the gold nucleus is proportional to the product of their charges and inversely proportional to the square of the distance between them. In a direct collision, the massive gold nucleus would hardly be moved by the α particle. The diameter of the nucleus was shown to be $\sim 1/105$ the size of the atom itself, or $\sim 10^{-13}$ m. Clearly these ideas defined an atom very different from the Thomson's model.

Ernest Solvay (1838–1922), a Belgian industrial chemist, who made a fortune from the development of a new process to make washing soda (1863), was known for his generous financial support to science, especially

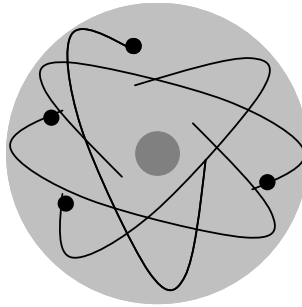


Figure 2-7. Planetary atomic model (Rutherford, 1911)

physics research. Among the projects he financially supported, was a series of international conferences, known as the Solvay conferences. The *First Solvay Conference on Physics* was held in Brussels in 1911 and it was attended by the most famous scientists of the time. Rutherford was one of them; he presented the discovery of the atomic nucleus and explained the structure of the atom. According to his explanation, the electrons revolve around the nucleus at relatively large distances. Since each electron carries one elementary charge of negative electricity, the number of electrons must equal the number of elementary charges of positive electricity carried by the nucleus for the atom to be electrically neutral. The visual model is similar to the solar planetary system and is illustrated in Fig. 2-7.

2.4.2 Idea of a Nucleus in the Center of an Atom

Rutherford's scattering experiment showed that a positive charge distributed throughout the volume of Thomson's atom could not deflect the α particles by more than a small fraction of a degree. A central assumption of Thomson's atomic model was that both the positive charge and the mass of the atom were distributed nearly uniformly over its volume. The electric field from this charge distribution is the field that must scatter the α particles, since the light-weight electrons would have a negligible impact. The expected deflection of an α particle from the gold nucleus according to Thomson's atomic model is shown in Fig. 2-8. The thickness of the gold foil used by Rutherford was about 400 atoms (or $\sim 5 \times 10^{-7}$ m). The gold atom has a positive charge of $79e$ (balanced by 79 electrons in its neutral state).

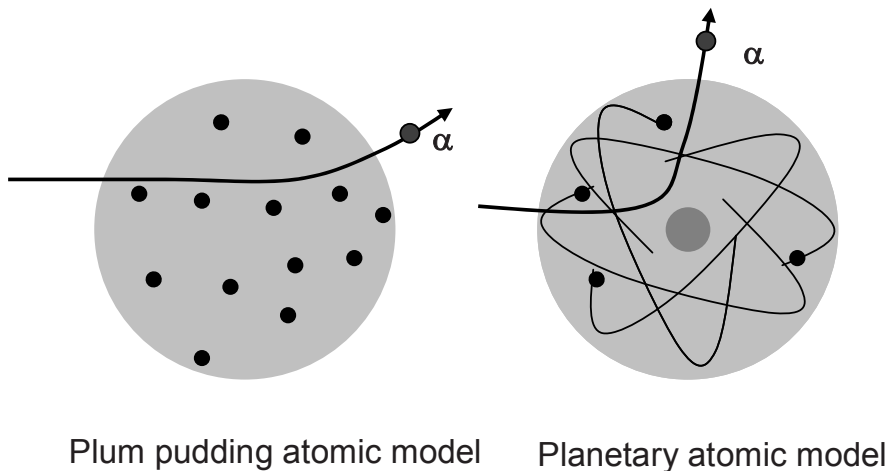


Figure 2-8. Trajectory of the α particle in the electric field of an atom in Rutherford's experiment according to the plum pudding and planetary atomic model

Neglecting the electrons, the maximum electric force the α particle would encounter is that at the surface of the positively charged sphere.

Johannes Kepler was the first to mathematically formulate Tycho Brahe's precise measurements of the motion of planets, showing that the orbit of the planets around the Sun is elliptical. Newton later proved that these elliptical orbits are a consequence of the attractive gravitational force (GmM/r^2). He also established that the motion of heavenly bodies in the field of a central attractive force with a $\sim 1/r^2$ dependence (such as the gravitational field of the Sun) is always a conical section, depending on the initial conditions: a *hyperbola* (body has sufficient kinetic energy to avoid capture by the gravitational field), an *ellipse* (the body is captured) and a *parabola* (a limiting case between these two). The scattering of particles in the electric field follows the same law that describes the motion of bodies in a gravitational field, except that the force can be both attractive and repulsive (the latter being the case for α particles and a positively charged nucleus). These two forces, electric and gravitational, are generated according to modern quantum physics by the exchange of a massless particle (or field quantum). In the case of the electric force the field quantum is a photon and in the case of the gravitational force the field quantum is called a graviton.

If the mass of an α particle is m with charge $q = 2e$, and the charge of the gold foil nucleus is $Q = Ze = 79e$, then the electric force acting on the α

particle (a Coulomb repulsion force due to the positively charged nucleus) is written as

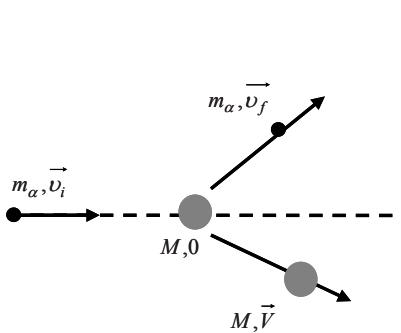
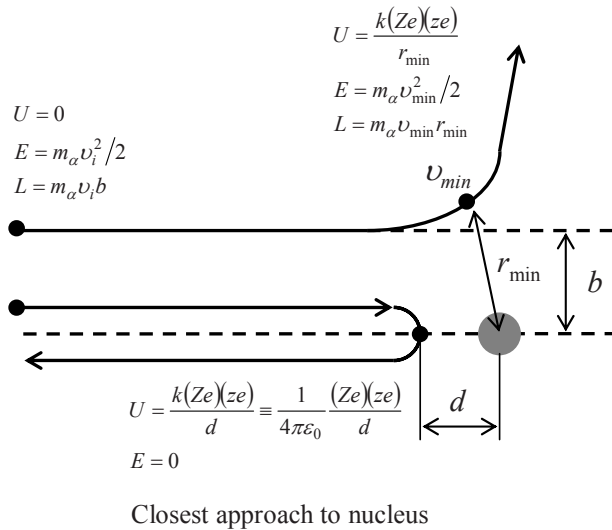
$$F = \frac{kQq}{r^2} = \frac{k(79e)(2e)}{r^2} \quad (2-2)$$

where k is the Coulomb force constant, $1/(4\pi\epsilon_0) = 8.9876 \times 10^9 \text{ N m}^2/\text{C}^2$. Assuming the atom to be represented by a sphere of radius 10^{-10} m , Eq. (2-2) gives the repulsive force that acts on the incoming α particle as $3.64 \times 10^{-6} \text{ N}$. The assumption that only the Coulomb force acts on the α particle was shown to be correct since the α particles never penetrated the gold nucleus and Rutherford's theoretical explanation agreed with the experimental measurements for all cases. Due to the nature of the Coulomb force acting on the α particle (inverse square law), the α particle follows a hyperbolic trajectory (Fig. 2-8) that is characterized by the *impact parameter*, b . The impact parameter represents the distance from the nucleus perpendicular to the line of approach of the incident α particle. The angle of deflection, θ , of any α particle is related to the impact parameter through the following relation (see Example 2.4)

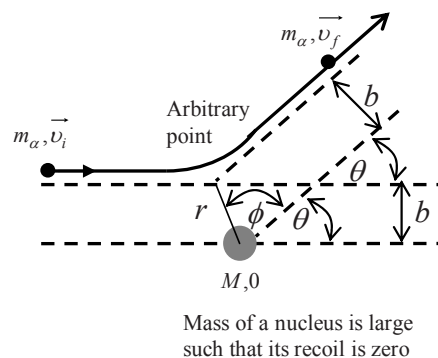
$$b = \frac{k(Ze)(ze)}{2E \tan(\theta/2)} = \frac{k(79e)(2e)}{2E \tan(\theta/2)} = \frac{(79e)(2e)}{8\pi\epsilon_0 E} \cot(\theta/2) \quad (2-3)$$

where E denotes the kinetic energy of the incident α particle ($=mv^2/2$). It follows from Eq. (2-3) that the impact parameter is smaller for larger scattering angles and larger energy of the incident particle. From the distribution of the α particle's scattering angles, Rutherford has concluded that the structure of an atom most likely mimics the solar planetary system. The size of the nucleus at the center of the atom was estimated based on the kinetic energy of the incident α particle and its potential energy at the point of the closest approach, d . The closest approach occurs in the case of a head-on collision in which the α particle comes to a rest before it bounces back at an angle of 180° (Fig. 2-9). At that point the kinetic energy is zero, and the potential energy equals the initial kinetic energy

$$E = \frac{k(79e)(2e)}{d} \quad (2-4)$$



Kinetics of Rutherford's experiment



Kinetics of Rutherford's scattering

Figure 2-9. Deflection of α particle (by angle θ) by the target nucleus (of radius R)

Knowing the kinetic energy of the incident α particle, its closest approach to any nucleus in the gold foil (on the order of 10^{-14} m) and the approximate size of the gold nucleus (on the order of 10^{-15} m) may be determined. The unit of 10^{-15} m is designated as a Fermi, fm. The small volume of the nucleus implies its high density and the need for a strong attractive force in the nucleus to overcome the Coulomb repulsive force. It was also understood that this attraction must be of a very short range.

Example 2.3 Size of the gold nucleus in Rutherford's experiment

In the Rutherford's experiment the kinetic energy of incident α particle was 7.7 MeV. Estimate the upper limit size of the gold nucleus and comment on the effect of

increased energy of the incident α particles in the experiment.

According to Fig. 2-8 the point of closest approach will determine the size of the nucleus. For the head-on collision it follows from Eq. (2-4) that

$$d < \frac{k(79e)(2e)}{7.7 \text{ MeV}} = \frac{(79)(2)ke^2}{7.7 \text{ MeV}} = \frac{(79)(2)(1.44 \text{ eV nm})}{7.7 \times 10^6 \text{ eV}} \approx 30 \text{ fm}$$

This implies that the gold nucleus has radius smaller than 30 fm (the actual measurement is about 8 fm). If the incident energy of the α particles in Rutherford's experiment is increased, some of the α particles would penetrate the nucleus, first in the head-on collisions and then for smaller angles as the energy is further increased. The limiting kinetic energy for the incident α particle above which the Rutherford experiment would not agree with theoretical explanation is

$$E \approx \frac{(79)(2)ke^2}{R} \cong 28.5 \text{ MeV where } R \text{ represents the radius of the gold nucleus.}$$

Example 2.4 Derivation of Eq. (2-3)

Considering the non-relativistic elastic scattering of an α particle from a stationary target in laboratory system derive Eq. (2-3). Kinetics of the scattering is shown in Fig. 2-9.

The law of conservation of linear momentum and kinetic energy applied to the scattering of α particle from target nucleus using notations from Fig. 2-9 and by neglecting for a moment the Coulomb force give

$$\begin{aligned} m_\alpha \vec{v}_i + 0 &= m_\alpha \vec{v}_f + M \vec{V} \\ \frac{m_\alpha v_i^2}{2} + 0 &= \frac{m_\alpha v_f^2}{2} + \frac{MV^2}{2} \end{aligned}$$

where $v_i = |\vec{v}_i|$, $v_f = |\vec{v}_f|$ and $V = |\vec{V}|$. Squaring the first equation and using the second equation we obtain the following:

$$\begin{aligned} m_\alpha^2 v_i^2 &= m_\alpha^2 v_f^2 + M^2 V^2 + 2m_\alpha M (\vec{v}_i \cdot \vec{V}) \quad \text{with} \quad m_\alpha^2 v_i^2 = m_\alpha^2 v_f^2 + m_\alpha MV^2 \\ m_\alpha MV^2 &= M^2 V^2 + 2m_\alpha M (\vec{v}_i \cdot \vec{V}) \quad \text{or} \quad V^2 \left(1 - \frac{M}{m_\alpha} \right) = 2(\vec{v}_i \cdot \vec{V}) \end{aligned}$$

We may discuss the last equation as follows:

- If the target is an electron in which case $M = m_e \ll m_\alpha$, there is no possibility for the large-angle scattering of the incoming α particle. The direction of scattering will be along or very close to the initial direction. [Because the thickness of the

gold foil was very small, the multiple small-angle scattering to produce a large-angle scattering was not possible.]

- If the target is heavy nucleus, $M=m_{Au} \gg m_{\alpha}$, the scattering angle may be large (because the left-hand side of the above equation becomes negative; the dot product of these two vectors is $|\vec{v}_i| |\vec{V}| \cos \theta$).

In deriving Eq. (2-3) we assume that the scattering of a non-relativistic α particle is from heavy nucleus that its recoil can be neglected (as indicated in Fig. 2-9). In the absence of any interaction the incoming particle approaching the target nucleus would travel in a straight line passing the nucleus at distance b (impact parameter). The incoming particle starting at the horizontal trajectory however slightly deflects from it due to the electrical repulsion making an angle of θ with the horizontal. This angle of deflection is related to the impact parameter. The impulse received by the α particle (due to Coulomb force, F) gives it a linear momentum. The change in that linear momentum in any direction over a given time interval is equal to the integrated force F in that direction over that time interval:

$$\Delta p = \int F dt \rightarrow \text{at arbitrary point along the particle trajectory}$$

Total time represents the time it takes for the α particle to travel through the atom. The arbitrary point as selected in Fig. 2-9 is the point of a closest approach. The line connecting that point to the target nucleus splits the angle $(\pi - \theta)$ in half. The component of the initial linear momentum is

$$\begin{aligned} -m_{\alpha} v_i \cos(\pi - \theta - \phi) &= -m_{\alpha} v_i \cos\left(\pi - \theta - \left(\frac{\pi}{2} - \frac{\theta}{2}\right)\right) \\ &= -m_{\alpha} v_i \cos\left(\frac{\pi}{2} - \frac{\theta}{2}\right) = -m_{\alpha} v_i \sin \frac{\theta}{2} \end{aligned}$$

By symmetry, the terminal velocity will be same as initial, and its component of a linear momentum in the same direction as shown in Fig. 2-9 is $+m_{\alpha} v_i \sin(\theta/2)$. Thus, it follows that the net change in the linear momentum of the α particle is $2m_{\alpha} v_i \sin(\theta/2)$. The component of the central force in the indicated direction in Fig. 2-9 is $F \cos(\phi)$. Therefore,

$$2m_{\alpha} v_i \sin(\theta/2) = \frac{k(Ze)(ze)}{r^2} \int_{-\infty}^{+\infty} \cos \phi dt$$

The angular momentum of the α particle with respect to the target nucleus location (Fig. 2-9) is $m_{\alpha} r$ at the arbitrary point on its trajectory where the location of the α particle is described by angle ϕ and its distance r from the nucleus. At that

point the α particle has a tangential velocity with respect to the location of the nucleus equal to $r d\phi / dt$ giving its angular momentum with respect to the nucleus of

$$L = m_{\alpha} r v_{\text{tangential}} = m_{\alpha} r^2 \frac{d\phi}{dt}$$

The angular momentum is conserved; thus we have

$$m_{\alpha} r^2 \frac{d\phi}{dt} = m_{\alpha} v_i b$$

The variable of integration is conveniently changed to ϕ instead of time. From the conservation of the angular momentum it follows that

$$\frac{d\phi}{dt} = \frac{v_i b}{r^2} \rightarrow dt = \frac{r^2}{v_i b} d\phi \quad \text{and} \quad \begin{cases} t = -\infty & \mapsto \phi = -(\pi - \theta)/2 \\ t = +\infty & \mapsto \phi = +(\pi - \theta)/2 \end{cases}$$

giving

$$2m_{\alpha} v_i \sin(\theta/2) = \frac{k(Ze)(ze)}{v_i b} \int_{-(\pi-\theta)/2}^{+(\pi-\theta)/2} \cos \phi d\phi$$

The integral is equal to $2 \cos(\theta/2)$; thus we obtain Eq. (2-3):

$$\begin{aligned} 2m_{\alpha} v_i \sin(\theta/2) &= 2 \frac{k(Ze)(ze)}{v_i b} \cos(\theta/2) \\ b &= \frac{k(Ze)(ze)}{v_i^2 m_{\alpha}} \cot(\theta/2) = \frac{k(Ze)(ze)}{2E} \cot(\theta/2) \\ &\equiv \frac{k(Ze)(ze)}{2E} \frac{1}{\tan(\theta/2)} \equiv \frac{(Ze)(ze)}{8\pi\epsilon_0 E} \cot(\theta/2) \end{aligned}$$

2.4.3 Rutherford's Scattering Formula

Rutherford's experiment eliminated Thomson's plum pudding atomic model on the basis of large-angle scattering. Relatively heavy α particles could not be turned around by much lighter electrons or by the combined mass of positive and negative charges if this mass were distributed uniformly over the whole volume (as demonstrated in Example 2.4). The

electrostatic repulsion would only be strong enough to deflect incoming α particles through such large angles if the positive charge is concentrated (as he proposed in a central nucleus). This scattering of charged particles by the nuclear electrostatic field is called *Rutherford scattering*. The probability of large-angle scattering is very small due to the extremely small size of the nucleus relative to the whole atom (radius of 10^{-15} m versus 10^{-10} m); indeed, according to Rutherford's experiment, only 1 out of ~ 8000 events resulted in large-angle scattering.

Based on his planetary model of the atom, Rutherford was able to define the angular distribution of the scattered α particles. A particle with an impact parameter less than b will be scattered at an angle larger than θ (Fig. 2-9 and 2-10). Therefore, all particles hitting the gold foil through the area πb^2 (where b is the radius) will scatter at an angle θ or larger (Fig. 2-10). Assuming that the incident beam is made of N α particles and has a cross-sectional area A , the number of particles scattered by θ or larger is $\pi b^2/A$. Thus, the number of particles scattered through an angle of θ or larger by one gold atom in the foil is

$$\frac{N_{scatt}}{\text{atom}} = N \left(\frac{\pi b^2}{A} \right) \quad (2-5)$$

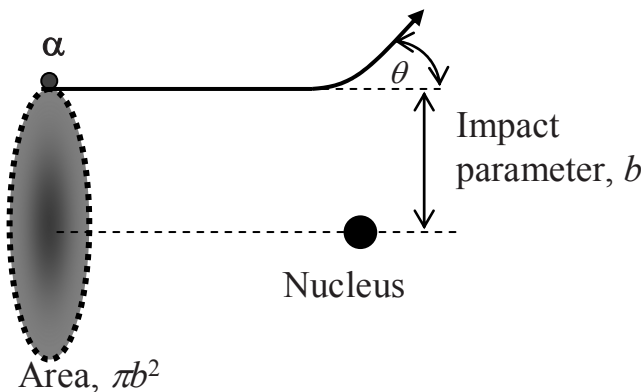


Figure 2-10. Correlation between the deflection angle of α particle and its impact parameter

The number of atoms encountered by the beam of particles in the gold is

$$N_{foil} = nAt \quad (2-6)$$

where t is the target (foil) thickness and n is the number of target atoms

per unit volume. Therefore, it follows from Eqs. (2-5) and (2-6) that the total number of α particles scattered through an angle θ or larger by the gold foil in Rutherford's experiment is

$$N_{tot-scatt} = \frac{N_{scatt}}{\text{atom}} \cdot N_{foil} = \frac{N\pi b^2}{A} \cdot nAt = N\pi b^2 nt \quad (2-7)$$

or

$$N_{tot-scatt} = N\pi nt \left(\frac{Zzke^2}{2E \tan(\theta/2)} \right)^2 \quad (2-8)$$

The number of particles that emerge between θ and $\theta + d\theta$ is obtained by differentiating Eq. (2-8)

$$N_{tot-scatt, \theta \rightarrow \theta+d\theta} = Nnt\pi \left[\frac{Zzke^2}{E} \right]^2 \frac{\cos(\theta/2)}{\sin^3(\theta/2)} d\theta \quad (2-9)$$

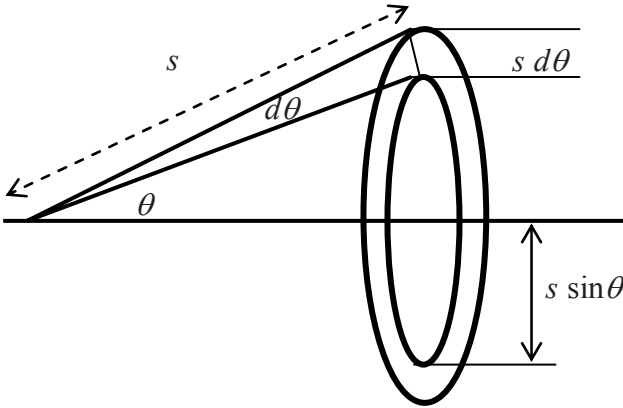


Figure 2-11. Detection of α particles after scattering through θ

At some distance s from the gold foil (where the detector is located) particles with a deflection angle between θ and $\theta + d\theta$ pass through the annulus as shown in Fig. 2-11 and are uniformly distributed over the surface area

$$A_{ring} = (2\pi \sin \theta)(s d\theta) = 4\pi s^2 \sin(\theta/2) \cos(\theta/2) \quad (2-10)$$

The number of particles per unit area that pass through the annulus at distance s and at angle θ is

$$n(\theta) \equiv \frac{N_{\text{tot-scatt}, \theta \rightarrow d\theta}}{A_{\text{ring}}} = \frac{Nnt}{4s^2} \left[\frac{Zze^2}{E} \right]^2 \frac{1}{\sin^4(\theta/2)} \quad (2-11)$$

This is called the *Rutherford scattering formula* or inverse square scattering formula. According to this formula, the number of particles scattered at a certain angle is proportional to the thickness of the foil and to the square of the nuclear charge of the foil and inversely proportional to the incident particle kinetic energy squared and to the fourth power of $\sin(\theta/2)$. This was confirmed in all of the experiments with gold foil. Rutherford derived Eq. (2-11) assuming that the only force acting between the nucleus and α particle is the Coulomb repulsive force, and since all of the experimental data agreed, this assumption was valid (see Example 2.3). However, some years later he repeated the experiment using the aluminum foil. The experimental results for small-angle scattering agreed with his formula, but large-angle scattering departed from it. Rutherford deduced that in the large-angle scattering that corresponded to a closer approach to the nucleus, the α particle was actually striking the nucleus. This meant that the size of the nucleus could be obtained by finding the maximum angle for which the Rutherford formula is valid and finding the incident particle's closest approach to the center of the nucleus.

2.4.4 Stability of the Planetary Atomic Model

The Rutherford planetary atomic model could not explain the following:

- How are the electrons (negatively charged bodies) held outside the nucleus (a positively charged body) despite the attractive electrostatic force? According to the planetary model electrons are revolving around the nucleus like planets around the Sun, though planets are electrically neutral and thus stay in their orbits. According to classical electromagnetic theory any charge placed in circular motion will radiate light (electromagnetic energy), which means that electrons orbiting around the nucleus would spiral inward and collapse into the nucleus due to the loss of kinetic energy. This would produce extremely unstable atoms.
- The radiated energy of photons from spiraling electrons would change in frequency during the deceleration process and produce a continuous spectrum; however, at that time, the spectra of some of the elements were known to show specific discrete lines.
- What does hold the positive charges in the nucleus together in spite of the repulsive electrostatic forces?

2.5 The Smallness of the Atom

Rutherford's gold foil experiment was the first indication and proof that the space occupied by an atom is huge compared to that occupied by its nucleus. In fact, the electrons orbiting the nucleus can be compared to a few flies in a cathedral. As a qualitative reference, a human is about two million times "taller" than the average *Escherichia coli* bacterium; Mount Everest is about 5,000 times taller than the average man; and a man is about ten billion times "taller" than the oxygen atom. If the atom were scaled up to a size of a golf ball, on that same scale a man would stretch from Earth to the Moon. Atoms are so small that direct visualization of their structure is impossible. Today's best optical or electron microscopes cannot reveal the interior of an atom.

The picture shown in Fig. 2-12 was taken with a scanning transmission electron microscope and shows a direct observation of cubes of magnesium oxide molecules, but details of the atoms cannot be seen.

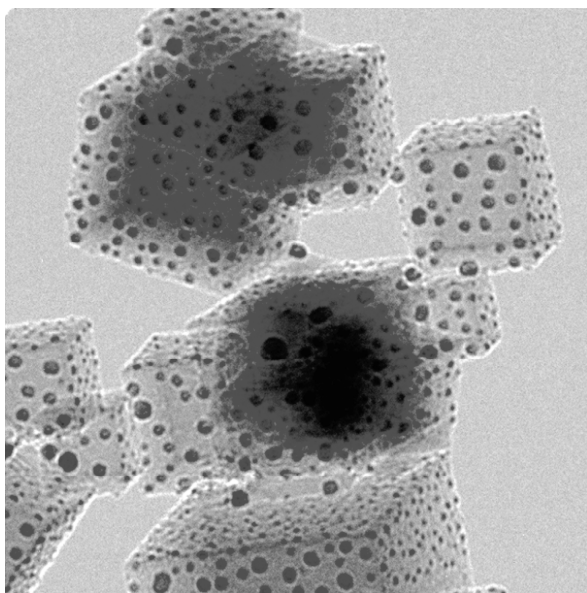


Figure 2-12. Magnesium oxide molecules as seen with scanning transmission electronic microscope produced at the Institute of Standards and Technology in the USA (Courtesy National Institute of Standards and Technology)

At the National Institute of Standards and Technology (NIST), however, the Nanoscale Physics Facility is used to manipulate and arrange atoms, one

by one, into desired patterns. The image shown in Fig. 2-13 represents an 8 nm square structure with cobalt atoms arranged on a copper surface. Such arrangements of atoms are used to investigate the physics of ultra-tiny objects. The shown structure was observed with a scanning tunneling microscope at a temperature of 2.3 K (about -455°F): the larger peaks (upper left and lower right) are pairs of cobalt atoms, while the two smaller peaks are single cobalt atoms. The swirls on the copper surface illustrate how the cobalt and copper electrons interact with each other.

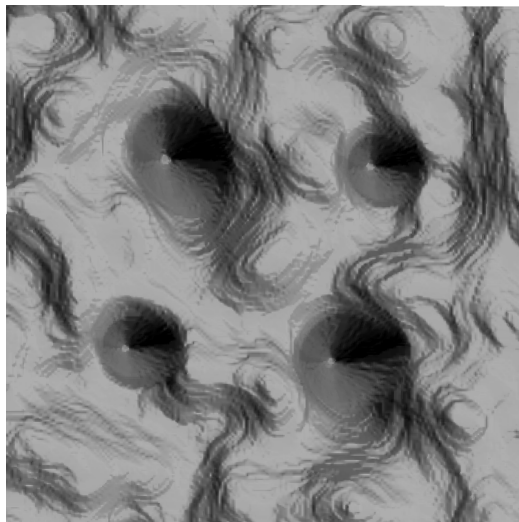


Figure 2-13. Nanoscale structure of cobalt and copper atoms produced at the Institute of Standards and Technology in the USA (Courtesy of J. Stroscio, R. Celotta, A. Fein, E. Hudson, and S. Blankenship, 2002)

2.6 The Quantum Atomic Model

2.6.1 Quantum Leap

In 1913, Niels Bohr (1885–1962) developed the atomic model that resolved Rutherford's atomic stability questions. His model was based on the work of Planck (energy quantization), Einstein (photon nature of light) and Rutherford (nucleus at the center of the atom).

In 1900, Max Planck (1858–1947) resolved the long-standing problem of black body radiation by showing that atoms emit light in bundles of radiation (called *photons* by Einstein in 1905 in his theory of the photoelectric effect). This led to formulation of Planck's *radiation law*: a light is emitted as well as absorbed in *discrete quanta* of energy. The magnitude of these discrete

energy quanta is proportional to the light's frequency (f , which represents the color of light):

$$E = hf = \frac{hc}{\lambda} \quad (2-12)$$

where h is Planck's constant ($h = 6.63 \times 10^{-34}$ J s), c is the speed of light and λ is the wavelength of the emitted or absorbed light.

Bohr applied this quantum theory of light to the structure of the electrons by restricting them to exist only along certain orbits (called the *allowed orbits*) and not allowing them to appear at arbitrary locations inside the atom. The angular momentum of the electrons is quantized and thus prohibits random trajectories around the nucleus. Consequently the electrons cannot emit or absorb electromagnetic radiation in arbitrary amounts since an arbitrary amount would lead to an energy that would force the electron to move to an orbit that does not exist. Electrons are thus allowed to move from one orbit to another. However, the electrons never actually cross the space between the orbits. They simply appear or disappear within the allowed states; a phenomenon referred to as a *quantum leap* or *quantum jump*.

For his theory of atoms that introduced the new discipline of quantum mechanics in physics, Bohr received a Noble Prize in 1922. He was also a founder of the Copenhagen school of quantum mechanics. One of his students once noticed a horseshoe nailed above his cabin door and asked him: "Surely, Professor Bohr, you don't believe in all that silliness about the horseshoe bringing good luck?" With a gentle smile Bohr replied, "No, no, of course not, but I understand that it works whether you believe it or not".

2.6.2 Absorption and Emission of Photons

In Bohr's atomic model, an electron jumps to a higher orbit when the atom absorbs a photon and back to a lower orbit when the atom emits a photon. In other words, a quantum leap to a higher orbit requires energy, while a quantum leap to a lower orbit emits that energy (Fig. 2-14).

Bohr's atomic model resolved the problem of atomic instability (Section 2.4.4) by changing the classical mechanics into quantum mechanics. This explains the existence of discontinuities in the absorption and emission of energy which is determined by the allowable electronic states in atoms. These allowed orbits are also called *stationary orbits* or *stationary states*. Since the orbits are discrete and quantized, so are their energies. The electrons in an atom can thus only have discrete energies. According to Bohr's theory, in an electrically neutral atom, an electron is in its stationary state and does not radiate energy as long as it is not disturbed. This

explained the stability of atoms but does not explain why electrons do not radiate energy while orbiting along their stationary trajectories. The theory also explained the reason for the discontinuities in the atomic spectra. When an electron jumps to a higher orbit a photon must be absorbed and its energy is equal to the energy difference of the two orbits. Conversely, a photon is emitted when an electron drops to a lower orbit and the photon energy is again equal to the energy difference of these two orbits (Fig. 2-14):

$$hf = E_n - E_m, \quad n > m \quad (2-13)$$

Both, the emission and absorption of energy by an atom, correspond to the electron transition representing a movement of an electron from one level to another. The electrons of an electrically neutral atom are normally all in the lowest possible energy levels. The addition of energy excites the electrons and the resulting atom is in an excited state (absorption of energy by an atom). Generally the electrons remain in this excited state for a short time and soon return to a more stable, lower energy level by releasing the extra energy (emission of energy by an atom).

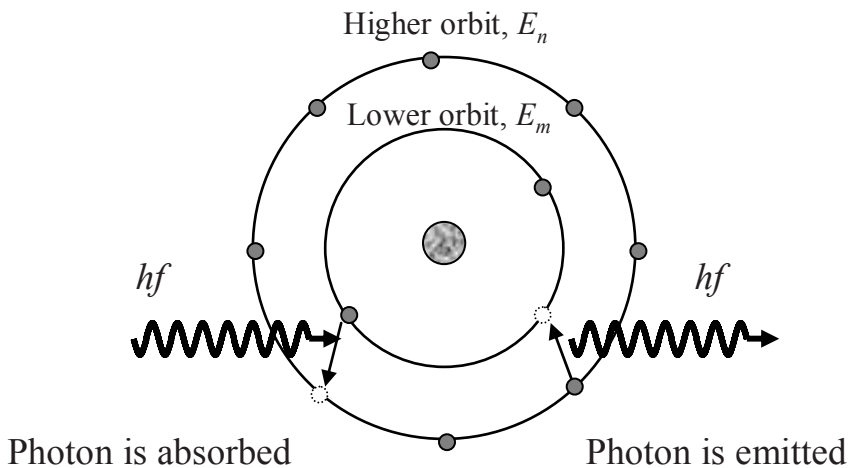


Figure 2-14. Schematic representation of a quantum leap of electrons according to the quantum atomic model (Niels Bohr, 1913)

2.6.3 The Bohr Model of the Hydrogen Atom

According to the Bohr atomic model, the hydrogen atom consists of an electron of mass m and charge $-e$, which orbits around a nucleus of charge

$+e$ (Fig. 2-15). For simplicity, it is assumed that the electron orbits the nucleus in a circular motion and that the nucleus is fixed in its position (since the hydrogen nucleus consists of one proton that is much heavier than the electron, this assumption does not affect the final result). Thus, the only force that is acting on the electron is the attractive Coulomb force from the positively charged nucleus:

$$F = \frac{ke^2}{r^2} \quad (2-14)$$

where k is the Coulomb force constant, $k=1/4\pi\epsilon_0=8.99\times10^9 \text{ N m}^2/\text{C}^2$ and $\epsilon_0=8.8542 \times 10^{-12} \text{ C}^2/\text{N m}^2$ is the permittivity of free space.

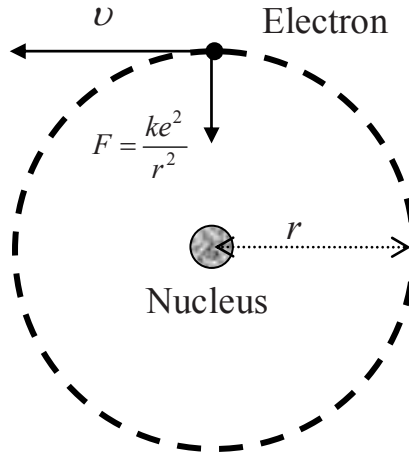


Figure 2-15. Circular motion of an electron in the Bohr model of the hydrogen atom

The Coulomb force of attraction is equal to the electron's centripetal force and according to Newton's second law of motion it can be written as

$$m \frac{v^2}{r} = \frac{ke^2}{r^2} \quad (2-15)$$

where v^2/r is the centripetal acceleration. Equation (2-15) can be rewritten as follows:

$$mv^2 = \frac{ke^2}{r} \quad (2-16)$$

and according to classical mechanics, this indicates possible values for electron velocity and its distance from the nucleus that range continuously from 0 to ∞ . The electron's kinetic energy is $E = mv^2/2$ and its potential energy in the field of the proton is $U = -ke^2/r$. By convention the potential energy is zero ($U = 0$) when the electron is far away from the nucleus ($r \rightarrow \infty$). For an electron in a circular orbit around a positively charged nucleus, kinetic and total energies are

$$E = -\frac{1}{2}U \quad (2-17)$$

$$E_{tot} = E + U = \frac{1}{2}U = -\frac{1}{2} \frac{ke^2}{r} \quad (2-18)$$

The negative value for the total energy indicates that the electron is bound to the nucleus and cannot escape to infinity. Since the distance from the nucleus ranges from 0 to ∞ , it follows from Eq. (2-18) that the electron's total energy can have values between $-\infty$ and 0.

This analysis is based on classical mechanics and does not show that the energy of the electron is quantized. Bohr's hypothesis was that the electron's angular momentum ($L = mvr$) was quantized in multiples of Planck's constant (this is because Planck's constant has a unit of angular momentum) and for circular orbits (see also Chapter 4, Section 3.9)

$$L = mvr = n \frac{h}{2\pi} = n\hbar \quad (n = 1, 2, 3, \dots) \quad (2-19)$$

where $\hbar = h/2\pi = 1.055 \times 10^{-34}$ J s (read as “ h bar”).

Combining Eqs. (2-16) and (2-19) it follows that

$$m \left[\frac{n\hbar}{mr} \right]^2 = \frac{ke^2}{r} \Rightarrow r_n = \frac{n^2 \hbar^2}{ke^2 m} = n^2 a_0 \quad (n = 1, 2, 3, \dots) \quad (2-20)$$

Eq. (2-20) gives quantized values for the radius of the electron's orbit. In addition, it defines the so-called *Bohr radius*, a_0 :

$$a_0 = \frac{\hbar^2}{ke^2 m} = 0.0529 \text{ nm} \quad (2-21)$$

The possible energy levels are obtained from the possible electron orbit radii as follows:

$$E_{tot} = E + U = \frac{1}{2}U = -\frac{1}{2} \frac{ke^2}{r} \text{ and } r_n = \frac{n^2 \hbar^2}{ke^2 m} = n^2 a_0 \text{ gives}$$

$$E_n = -\frac{ke^2}{2a_0} \frac{1}{n^2} \quad (n = 1, 2, 3, \dots) \quad (2-22)$$

The energy of the photons that are absorbed or emitted from the hydrogen atom during electronic transitions between orbits n and m ($n > m$, see Fig. 2-14) can be now determined:

$$E_\gamma = E_n - E_m = \frac{ke^2}{2a_0} \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad (2-23)$$

In the chapters that follow this equation is explored further and connected to the work of Rydberg.

2.7 Atomic Spectra

A spectrum is defined as the distribution of light (electromagnetic radiation) as a function of its frequency or its wavelength. Newton performed the first light color spectrum experiment in 1666 by shining white light through a glass prism. The experiment produced a rainbow of colors and showed that what we observe as white light is a mixture of many different colors. In 1814 a German physicist, Joseph von Fraunhofer, noticed a multitude of dark lines, indicating that certain colors are missing in the solar light spectrum. These dark lines were caused by the absorption of some of the solar light's components by the gases in the Sun's outer atmosphere. A series of experiments followed and by the middle of the 19th century it was understood that gases absorb light (specific frequencies of light) that are characteristic of the gas constituents.

If white light is shone through a gas that consists of only one kind of atom, the gas will absorb light of frequency (energy) that is characteristic to that atom. If the light is then subsequently transmitted through a glass prism, the resulting spectrum will lack the colors corresponding to the absorbed frequencies. This spectrum is called the *absorption spectrum* and the dark lines correspond to the absorbed frequencies (see the hydrogen *absorption* spectrum in Fig. 2-16). By 1859 Robert Bunsen discovered that sufficiently

heated gases also emit light and an *emission spectrum* is observed when the emitted light is transmitted through a glass prism (see the hydrogen *emission* spectrum in Fig. 2-16). The emission spectrum's bright lines correspond to the dark lines in the absorption spectrum. At the same time, his colleague, Gustav Kirchhoff, while analyzing the spectra of sunlight and heated sodium, realized that the dark lines in the solar spectrum represented the light frequencies that were absorbed by the sodium atoms in the solar gases.

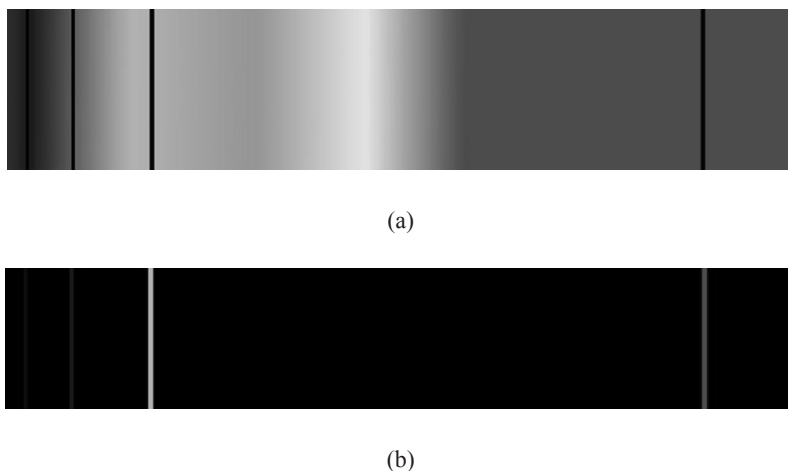


Figure 2-16. (a) Absorption and (b) emission spectra of the hydrogen atom

The emission and absorption spectra thus represent a “signature” of an atom. The Kirchhoff–Bunsen discovery was not fully understood until Bohr explained the transition of electrons between strictly defined orbits (energy levels), but it represents the beginning of the science of spectroscopy. By 1870 spectroscopy became a tool that was used to analyze the chemical compositions of the Sun and the stars.

2.7.1 The Balmer–Rydberg Formula

In 1885 a Swiss school teacher, Jakob Balmer (1825–1898), analyzed the hydrogen atomic spectral data and showed that the observed wavelengths correlate to the formula

$$\frac{1}{\lambda} = R \left[\frac{1}{4} - \frac{1}{n^2} \right] \quad (2-24)$$

where R is a constant with a dimension of inverse length, according to Balmer equal to 0.0110 nm^{-1} for the hydrogen spectrum, and n is an integer with values of 3, 4, 5 and 6 that correspond to the four observed hydrogen

spectral lines. Balmer correctly assumed that this dependence could not be a random coincidence and that other lines must exist (n can be greater than 6). The Balmer formula can be rewritten in the form

$$\frac{1}{\lambda} = R \left[\frac{1}{2^2} - \frac{1}{n^2} \right] \quad (n = 3, 4, 5, \dots) \quad (2-25)$$

Johannes Rydberg later extended Balmer's work to include all lines in the hydrogen atom emission spectrum:

$$\frac{1}{\lambda} = R \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad (n > m) \quad (2-26)$$

where n and m are both integers. Equation (2-26) is called the *Rydberg formula* and R is the *Rydberg constant*. At the time when this formula was developed, it only represented empirical data and no explanation was given as to why the spectral lines obey such regularities. In 1913, Neils Bohr developed an atomic model that explained this nature of absorption and emission spectra of atoms. Rewritten in terms of photon energy, the Rydberg formula becomes

$$E_\gamma = hc / \lambda \quad \text{and} \quad \frac{1}{\lambda} = R \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad (n > m) \quad \text{gives}$$

$$E_\gamma = Rhc \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad (n > m) \quad (2-27)$$

Recall from Section 2.6.3 (Eq. 2-23) that the energy of emitted or absorbed photons according to the Bohr atomic model is

$$E_\gamma = E_n - E_m = \frac{ke^2}{2a_0} \left[\frac{1}{m^2} - \frac{1}{n^2} \right]$$

From the last two relations it can be seen that Bohr's model predicts Rydberg formula and gives the value for the Rydberg constant

$$R = \frac{ke^2}{2a_0} \frac{1}{hc} = \frac{1.44 \text{ eV nm}}{2(0.0529 \text{ nm})(1240 \text{ eV nm})} = 0.0110 \text{ nm}^{-1} \quad (2-28)$$

which is in perfect agreement with the measured values. The term, hcR , is called the *Rydberg energy*, E_R :

$$E_R = hcR = \frac{ke^2}{2a_0} = \frac{m(ke^2)^2}{2\hbar^2} = 13.6 \text{ eV} \quad (2-29)$$

Thus, the allowed energies of the electron in a hydrogen atom can be expressed in terms of the Rydberg energy

$$E_n = -\frac{E_R}{n^2} \quad (2-30)$$

and the energies of the photons emitted or absorbed by the hydrogen atom are given by

$$E_\gamma = E_n - E_m = E_R \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad n > m \quad (2-31)$$

2.7.2 Properties of the Hydrogen Atom According to Bohr's Atomic Model

Bohr's model of the atom correctly predicts the following:

- Possible electron energies in a hydrogen atom are quantized and with values of $E_n = -E_R / n^2$ where $n = 1, 2, 3, \dots$
- The lowest possible energy level corresponds to the *ground state* for which $n = 1$ and $E_1 = -E_R = -13.6 \text{ eV}$.
- A minimum energy of $+13.6 \text{ eV}$ is needed to completely remove the electron from a hydrogen atom. This energy is called the binding energy of the hydrogen atom and it is in perfect agreement with the empirical value.
- The radius that corresponds to the ground state of a hydrogen atom is equal to the Bohr radius, $r_1 = a_0 = 0.0529 \text{ nm}$ which agrees well with measured values of the size of the hydrogen atom.
- The radius of the n^{th} circular electron orbit is $r_n = n^2 a_0$.
- The orbits with radii greater than the ground state radius are called the *excited states* of an atom. There are infinitely many levels and all are between the ground state and the zero energy levels. For the hydrogen atom, the energies of excited states are $E_2 = -E_R / 4 = -3.4 \text{ eV}$, $E_3 = -E_R / 9 = -1.5 \text{ eV}$ and so on. These energy levels are generally plotted as illustrated in Fig. 2-17 in a format commonly referred to as *energy-level diagrams*. The transition from the ground state ($n = 1$) to the

$n = 2$ energy level is called the *first excitation level*, and the energy required to raise the hydrogen atom to that level is $E_1 - E_2 = 10.2 \text{ eV}$.

The spectral lines of the hydrogen atom as shown in Fig. 2-18 are given names based on the names of the scientists who discovered them:

1. *Lyman series*: transition to the ground state $m = 1$
2. *Balmer series*: transition to the level $m = 2$
3. *Paschen series*: transition to the level $m = 3$
4. *Bracket series*: transition to the level $m = 4$.

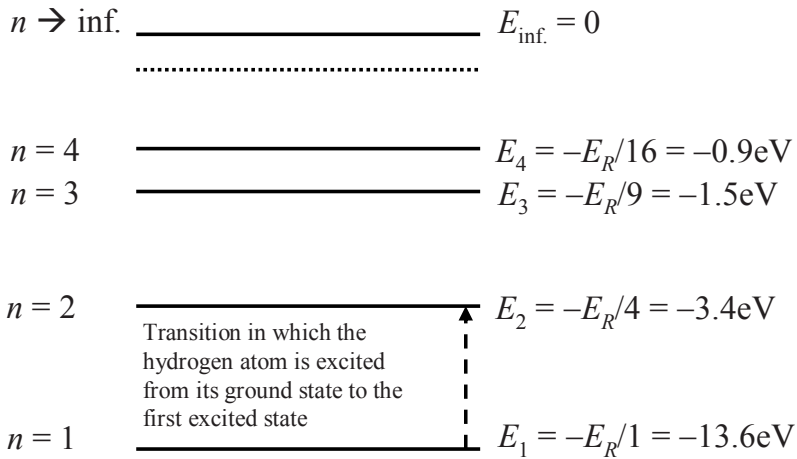


Figure 2-17. Energy-level diagram of the hydrogen atom

Example 2.5 Electron transitions in hydrogen atom

Calculate the wavelength and energy of the light emitted when the electron in a hydrogen atom falls from the first excited state to the ground level.

According to the Balmer formula

$$\frac{1}{\lambda} = R \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad (n > m);$$

therefore, the wavelength of the emitted light is

$$\frac{1}{\lambda} = R \left[\frac{1}{1^2} - \frac{1}{2^2} \right] = \frac{3}{4} R \Rightarrow \lambda = \frac{4}{3R} = \frac{4}{(3)(0.0110 \text{ nm}^{-1})} = 121 \text{ nm}$$

and the required energy for this transition is

$$E_\gamma = E_R \left[\frac{1}{1^2} - \frac{1}{2^2} \right] = \frac{3}{4} E_R = \frac{3}{4} (13.6 \text{ eV}) = 10.2 \text{ eV}$$

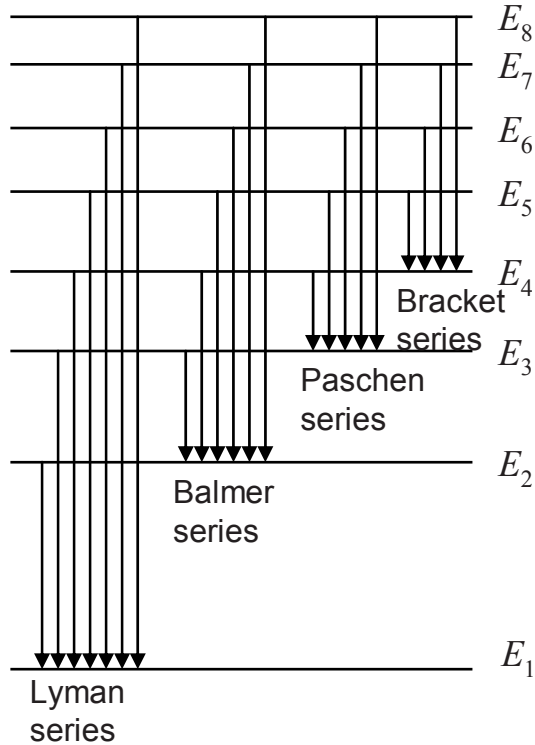


Figure 2-18. Spectral lines in hydrogen atom

Example 2.6 Orbiting velocity of the electron in hydrogen atom

Calculate the highest velocity, the smallest orbit radius and the time it takes for an electron to complete one revolution in a hydrogen atom.

The electron has its highest velocity and smallest orbit radius while in the ground state. The ground state radius in the hydrogen atom corresponds to the Bohr radius, $r_1 = a_0 = 0.0529 \text{ nm}$. The highest velocity is thus

$$m v_1 r_1 = n \hbar \quad r_1 = a_0 \quad n = 1 \quad \Rightarrow$$

$$v_1 = \frac{\hbar}{m a_0} = \frac{1.05 \times 10^{-34} \text{ kg m}^2/\text{s}}{(9.31 \times 10^{-31} \text{ kg})(0.0529 \times 10^{-9} \text{ m})} = 2.1 \times 10^6 \text{ m/s}$$

The time it takes for a ground state electron to complete one revolution around

the nucleus is

$$t = \frac{2\pi a_0}{\nu_1} = 1.52 \times 10^{-16} \text{ s}$$

2.7.3 Ionization and Excitation

Ionization or excitation of the atoms occurs when a photon or a charged particle (electron, α , proton) collides with an orbital electron, thereby transferring energy to and changing the energy level of the electron. Ionization refers to the case in which the transferred energy causes the ejection of an electron, while in the case of excitation the electron simply moves to a higher energy orbital. This is an important concept in health physics as it represents the mechanism through which energy is transferred from radiation to tissue.

Table 2-1. First ionization potential (IP) for the first few atoms

Atom	IP (eV)
Hydrogen	13.6
Helium	24.6
Lithium	5.4
Beryllium	9.3
Boron	8.3
Carbon	11.3
Nitrogen	14.5
Oxygen	13.6
Fluorine	17.4
Neon	21.6
Sodium	5.14

The ionization energy (also called the ionization potential, *IP*) of an atom is the amount of energy required to remove the least tightly bound electron from the atom. To remove a second electron requires remarkably more energy and the removal of each subsequent electron becomes increasingly more difficult. For most elements, the first ionization potential is on the order of several eV (Table 2-1). The first ionization potential of the hydrogen atom is described in Section 2.7.2. When a photon with energy greater than the ionization energy collides with a bound electron of an atom, the photon vanishes and the electron is ejected from the atom with a kinetic energy, E_{pe} , equal to the difference between the photon’s initial energy and the ionization potential:

$$E_{pe} = hf - IP \tag{2-32}$$

This mechanism is called the *photoelectric effect* and is described in Chapter 6.

Example 2.7 Excitation of the hydrogen atom

Sketch the excitation of the hydrogen atom for the corresponding absorption and emission of light of energy 10.2 eV.

The absorption of a photon with energy 10.2 eV will move the electron from its ground state to orbit $n = 2$. Conversely, the jump back to ground state will emit a photon of energy 10.2 eV (Fig. 2-19).

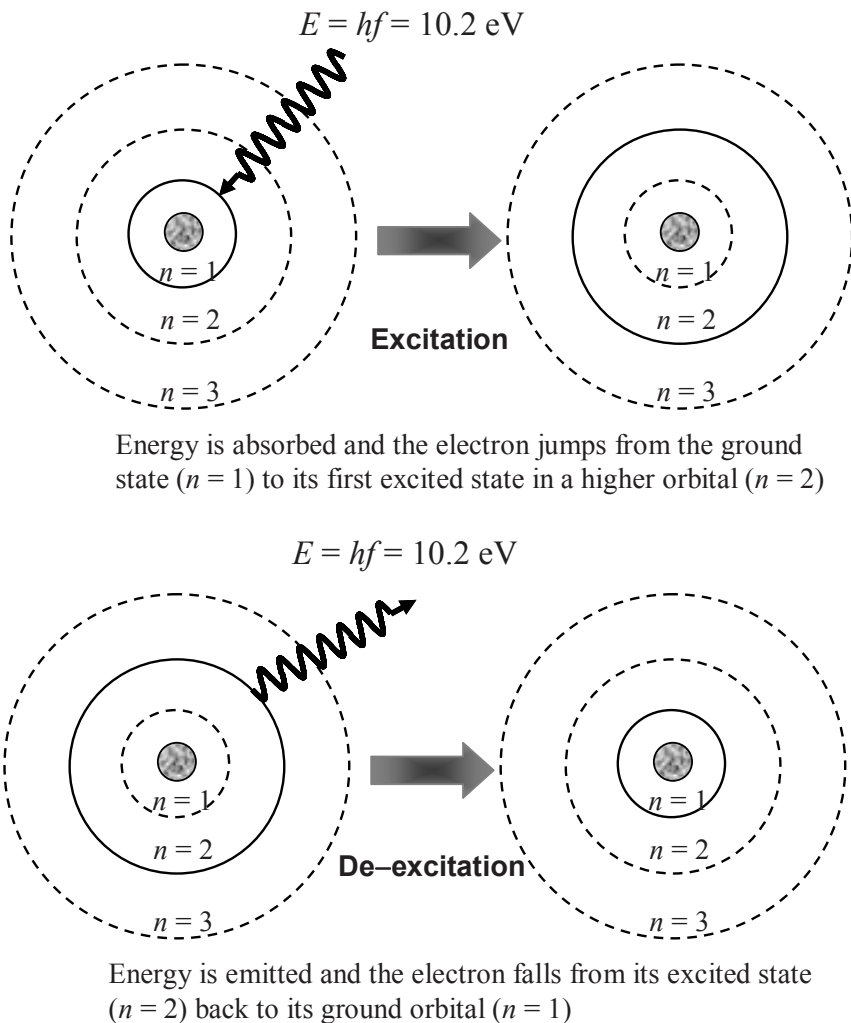


Figure 2-19. Excitation and de-excitation of the hydrogen atom

Example 2.8 Ionization potential (*IP*)

For a photon of wavelength 10^{-7} m striking the outer orbital electron of a sodium atom, calculate the kinetic energy of the photoelectron (ejected electron). What is the maximum photon wavelength (minimum energy) required to ionize the sodium atom? The *IP* for sodium is given in Table 2-1.

The energy of the photon of wavelength 10^{-7} m is calculated by

$$E_{\gamma} = \frac{hc}{\lambda} = \frac{1240 \text{ eV nm}}{100 \text{ nm}} = 12.4 \text{ eV}$$

The kinetic energy of the photoelectron is $E_{\text{pe}} = hf - IP = 12.4 \text{ eV} - 5.14 \text{ eV} = 7.26 \text{ eV}$. The maximum photon wavelength (minimum energy) required for the ionization of a sodium atom is then

$$\lambda_{\text{min}} = \frac{hc}{IP} = \frac{1240 \text{ eV nm}}{5.14 \text{ eV}} = 241 \text{ nm}$$

The electron is ejected because the wavelength of the photon is less than the required maximum wavelength (i.e., the photon energy exceeds the ionization potential).

2.7.4 Hydrogen-Like Ions

The Bohr's atomic model was valid for the hydrogen atom. Any attempt to generalize it for atoms having multiple electrons was unsuccessful until quantum mechanics development took place in 1925. Bohr's model can, however, be applied to all atoms that are like hydrogen, that is the atoms that have lost all but one of their electrons. In such atoms (ions) the remaining electron revolves around the nucleus of charge $+Ze$ in the same way as the electron in a hydrogen atom. All of the formulas developed for the hydrogen atom in the previous sections are thus applicable to these ions, with the exception that the e^2 term is replaced by Ze^2 . Therefore,

- The radius of an electron moving around a nucleus of charge Ze is inversely proportional to Z :

$$r_n = \frac{n^2 \hbar^2}{kZe^2 m} = \frac{n^2}{Z} a_0 \quad (n = 1, 2, 3, \dots) \quad (2-33)$$

- The potential energy of the electron in a hydrogen-like ion is

$$U = -\frac{kZe^2}{r} \quad (2-34)$$

- The total energy of the electron in a hydrogen-like ion is

$$E_{tot} = E + U = \frac{1}{2}U = -\frac{1}{2} \frac{kZe^2}{r} \quad (2-35)$$

- The allowed energies for the electron in a hydrogen-like ion are Z^2 times the corresponding energies in hydrogen atom:

$$E_n = -\frac{kZe^2}{2a_0} \frac{1}{n^2} = -Z^2 \frac{E_R}{n^2} \quad (n = 1, 2, 3, \dots) \quad (2-36)$$

- The energies of the photons emitted and absorbed by the electron in hydrogen-like ions are

$$E_\gamma = E_n - E_m = Z^2 E_R \left[\frac{1}{m^2} - \frac{1}{n^2} \right] \quad n > m \quad (2-37)$$

Example 2.9 Helium ion and reduced mass correction

Calculate the ratio of the allowed energies in the helium ion to that in the hydrogen atom taking into account the effect of nuclear motion.

The assumption that the electron orbits around a fixed nucleus is not entirely correct. In reality, they both revolve around the common center of mass. Since the nucleus is much heavier than the electron, the center of mass is close to the nucleus, which is therefore almost stationary. In the equations for allowed energies as well as for the Rydberg energy, the electron mass, m , must be corrected for the motion of the nucleus (mass = M). This is done by replacing the electron mass with the so-called *reduced mass*, μ , which is defined as

$$\mu = \frac{m}{1 + m/M} \quad (2-38)$$

The reduced mass is always less than the actual mass of the electron. In a hydrogen atom, the nucleus consists of a single proton and $m/M \sim 1/1800$. The helium ion (He^+) nucleus is four times heavier than that of the hydrogen atom (H) and thus m/M is four times smaller:

$$E_n^{\text{He}^+} = 2^2 \frac{E_R}{n^2} = -4 \frac{\mu^{\text{He}^+} (ke^2)^2}{2\hbar^2 n^2} \quad E_n^{\text{H}} = -\frac{\mu^{\text{H}} (ke^2)^2}{2\hbar^2 n^2}$$

$$\frac{E_n^{\text{He}^+}}{E_n^{\text{H}}} = \frac{4\mu^{\text{He}^+}}{\mu^{\text{H}}} = \frac{4 \times \frac{1}{1+1/(4 \times 1800)}}{\frac{1}{1+1/(1800)}} = 4.0017$$

When nuclear motion is accounted for, the ratio of allowed energy levels in the helium ion to that of hydrogen increases from exactly 4 to 4.0017. This small difference is observed in the measurements of atomic and ionic spectra.

2.7.5 Empirical Evidence of Bohr's Theory

Although Bohr's theory was shown to be almost completely valid for the hydrogen atom, great success was also achieved when it was used to describe hydrogen-like ions (as discussed in Section 2.7.4). Bohr's theory also proved to be valid for calculating the allowed energy levels of the innermost electron in multi-electron atoms. The latter application approximates the charge of the outer electrons to be uniformly distributed in a sphere surrounding the innermost electron. It follows that, due to the spherical symmetry of the electric field, the innermost electron experiences no net force from the outer electrons. The only force acting on the innermost electron is the electrostatic force from the positively charged nucleus (Ze). The allowed energies for the innermost electron in multi-electron atoms are given by Eq. (2-36):

$$E_n = -\frac{kZe^2}{2a_0} \frac{1}{n^2} = -Z^2 \frac{E_R}{n^2} \quad (n=1,2,3,\dots)$$

For example, the energy required to remove the innermost electron from its ground state orbit ($n = 1$) in an iron atom ($Z = 26$) is

$$E_1 = -Z^2 E_R = -(26)^2 (13.6 \text{ eV}) \approx 9,194 \text{ eV}$$

For heavier atoms the energy needed to remove the innermost electrons is on the order of thousands of eV and thus photons emitted or absorbed in such transition are in the range of X-rays (see Chapter 3). Henry Moseley

(1887–1915), a British physicist (killed at the age of 27 in World War I), was measuring the wavelengths of X-rays emitted by various atoms when he discovered that the dependence on atomic number exactly followed Bohr's theory. His explanation of characteristic X-rays was that if an innermost electron ($n = 1$) is ejected, the vacancy created is filled by an outer electron.

The transition of the outer electron to the inner shell will produce the emission of a characteristic photon with energy that is equal to the difference in allowed energies of the levels involved in the electron jump. For example, in the transition of an electron from level $n = 2$ to level $n = 1$, traditionally called K_α , the energy of the emitted photon is given by Eq. (2-37):

$$E_\gamma = E_2 - E_1 = Z^2 E_R \left(1 - \frac{1}{4}\right) = \frac{3}{4} Z^2 E_R$$

Moseley measured the frequencies of emitted photons for about 20 different elements and found that frequency changes with the square of the atomic number Z . He then plotted the square root of the frequencies as a function of known values of Z and verified that it is a linear function. This helped in the identification of the atomic numbers of several elements that were not known at the time (one of which was technetium, $Z = 43$, which does not occur naturally and was produced artificially in 1937).

The plot shown in Fig. 2-20 indicates that the line does not start from the origin as the relation would suggest. After detailed examination of the plot, Moseley concluded that the line crosses the Z -axis at a point close to $Z = 1$, implying that $\sqrt{f} \propto (Z - 1)$ or $E_\gamma \propto (Z - 1)^2$. The prediction that characteristic X-rays are emitted with frequencies proportional to Z^2 was based on the assumption that inner electrons experience a force due to the positive charge of nucleus ($+Ze$) but are not affected by the charges of the other (outer) electrons in the atom.

In reality, however, the inner electrons do experience a force from the outer electrons in the form of a screening of the nuclear attraction force; in other words, the attractive force of the nucleus is somewhat diminished due to the presence of the outer electrons. This so-called *screening factor*, a , is usually close to unity and the energy of emitted (or absorbed) K_α X-rays is

$$E_\gamma = \frac{3}{4} (Z - a)^2 E_R \quad a \cong 1 \quad (2-39)$$

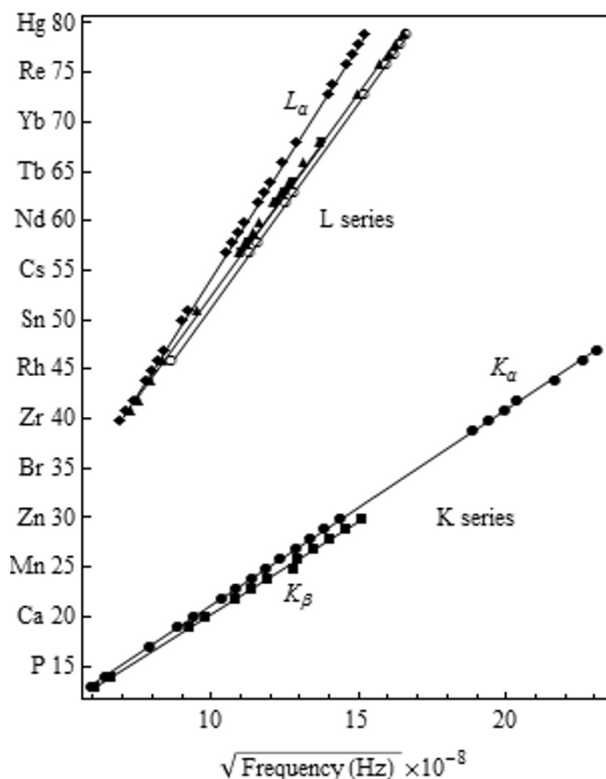


Figure 2-20. Plot of K_{α} X-ray characteristic lines known at the time of Moseley's experiments

Example 2.10 Characteristic K_{α} line

Estimate the wavelength of the characteristic K_{α} X-ray from niobium, which has the atomic number $Z = 41$. Assume that the screening factor is approximately equal to 1.

$$E_{\gamma} = \frac{3}{4}(Z - a)^2 E_R = \frac{3}{4}(41 - 1)^2 (13.6 \text{ eV}) = 16,320 \text{ eV} \rightarrow \lambda = \frac{hc}{E_{\gamma}} = 0.076 \text{ nm}$$

Example 2.11 Cascade of atomic vacancies

Calculate the wavelength and determine the spectral region for a krypton atom ($Z = 36$) when an electron from $n = 2$ fills a vacancy in the $n = 1$ level. What happened to the $n = 2$ level when the electron fell to the $n = 1$ level?

Allowed energies for these two levels, taking into account the screening effect, are according to Eq.(2-37):

$$E_1 = -(36 - 1)^2 (13.6 \text{ eV}) = -16,660 \text{ eV}; E_2 = -(36 - 1)^2 \left(\frac{13.6 \text{ eV}}{4} \right) = -4,165 \text{ eV}$$

The energy of the emitted photon in this transition is 12,495 eV and the corresponding wavelength is 0.099 nm, which belongs to the X-ray region of the spectrum. After the $n = 2$ electron falls to the $n = 1$ level, an $n = 3$ or an $n = 4$ electron fills this orbital and emits another photon.

2.8 Atoms of Higher Z

2.8.1 Quantum Numbers

The light spectra of atoms with more than one electron are much more complex than that of the hydrogen atom (many more lines). The calculations of the spectra for these atoms with the Bohr atomic model are complicated by the screening effect of the other electrons (see Section 2.7.5). Examination of the hydrogen spectral lines with high-resolution spectroscopes shows these lines to have very fine structures, and the observed spectral lines are each actually made up of several lines that are very close together. This observation implied the existence of sublevels of energy within the principal energy level, which makes Bohr's theory inadequate even for the hydrogen atomic spectrum.

Bohr recognized that the electrons are most likely organized into orbital groups in which some are close and tightly bound to the nucleus, and others less tightly bound at larger orbits. He proposed a classification scheme that groups the electrons of multi-electron atoms into "shells" and each shell corresponds to a so-called quantum number n . These shells are given names that correspond to the values of the principal quantum numbers:

- $n = 1$ (K shell) can hold no more than 2 electrons
- $n = 2$ (L shell) can hold no more than 8 electrons
- $n = 3$ (M shell) can hold no more than 18 electrons, etc.

Moseley's work (described in Section 2.7.5) contributed to the understanding that the electrons in an atom existed in groups visualized as electron shells, and according to quantum mechanics, the electrons are distributed around the nucleus in *probability regions* also called the *atomic orbitals*. In order to completely describe an atom in three dimensions, Schrödinger introduced three quantum numbers in addition to the principal quantum number, n . There are thus a total of four quantum numbers that specify the behavior of electrons in an atom, namely

- principal quantum number, $n = 1, 2, 3, \dots$
- azimuthal quantum number, $l = 0$ to $n - 1$
- magnetic quantum number, $m = -l$ to 0 to $+l$
- spin quantum number, $s = -1/2$ or $+1/2$.

The *principal quantum number* describes the shells in which the electrons orbit. The maximum number of electrons in a shell n is $2n^2$.

The sub-energy levels (s , p , d , etc.) are the reason for the very fine structure of the spectral lines and result from the electron's rotation around the nucleus along elliptical (not circular) orbits. The *azimuthal quantum number* describes the actual shape of the orbits. For example, $l = 0$ refers to a spherically shaped orbit, $l = 1$ refers to two obloid spheroids tangent to one another and $l = 2$ indicates a shape that is quadra-lobed (similar to a four leaf clover). For a given principal quantum number, n , the maximum number of electrons in an $l = 0$ orbital is 2, for an $l = 1$ orbital it is 6 and an $l = 2$ orbital can accommodate a maximum of 10 electrons.

$l =$	0	1	2	3	4	5
$n = 1$	1s					
$n = 2$	2s	2p		Not Allowed		
$n = 3$	3s	3p	3d			
$n = 4$	4s	4p	4d	4f		
$n = 5$	5s	5p	5d	5f	5g	
$n = 6$	6s	6p	6d	6f	6g	6h
$n = 7$	7s	7p	7d	7f	7g	7h

Figure 2-21. Allowed combinations of quantum numbers

The *magnetic quantum number* is also referred to as the *orbital quantum number* and it physically represents the orbital's direction in space. For example when $l = 0$, m can only be zero. This single value for the magnetic quantum number suggests a single spatial direction for the orbital. A sphere is uni-directional and it extends equally in all directions, thus the reason for a single m value. If $l = 1$ then m can be assigned the values -1 , 0 or $+1$. The three values for m suggest that the double-lobed orbital has three distinctly different directions in three-dimensional space into which it can extend. In the absence of any perturbing force (such could be an external magnetic field) the orbitals with the same n and l are equal in energy and are called *degenerate*. In the presence of a perturbing force caused by the magnetic field the orbitals would differ in energy, and thus this quantum number is called the *magnetic quantum number*.

The *spin quantum number* describes the spin of the electrons. The electrons spin around an imaginary axis (as Earth spins about the imaginary axis connecting the north and south poles) in a clockwise or counter-clockwise direction; for this reason there are two values, $-1/2$ or $+1/2$.

The allowed combination of quantum numbers is given in Fig. 2-21.

Example 2.12 Quantum numbers of the hydrogen atom

Write the quantum numbers of the ground and first-excited levels of the electron in a hydrogen atom. Comment on the values of angular momentum of the ground state atom using Bohr's atomic model. Use an energy-level diagram to indicate the quantum levels.

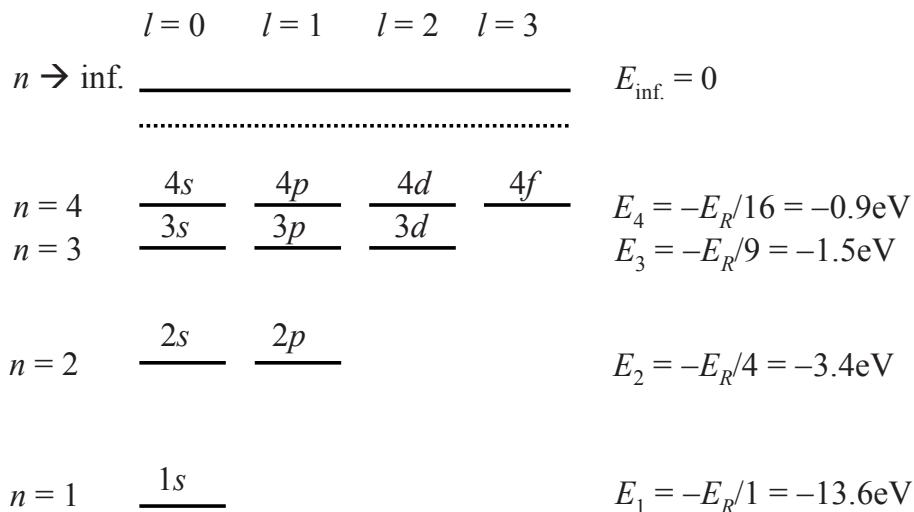


Figure 2-22. Energy-level diagram for the hydrogen atom including the quantum numbers

From Fig. 2-21 it follows that for the ground level, $n = 1$. The only possible value for the azimuthal quantum number is then zero ($l = 0$), indicating that the ground state of a hydrogen atom has zero angular momentum. (In general the angular momentum is zero if the motion of the particle is directly toward or away from the origin, or if it is located at the origin.) This in turns gives only one value for the magnetic quantum number, $m = 0$. According to Bohr's atomic model, the ground state of a hydrogen atom has an angular momentum equal to $L = 1 \times \hbar$. However, the Schrödinger equation (see Chapter 4) predicts that $L = 0$. For the first excited level, $n = 2$, which gives two values for the azimuthal quantum number, namely $l = 0$ and $l = 1$. When $l = 0$, the only possible value for m is zero. However, when $l = 1$, m assumes three values, $m = 1, 0$ or -1 and this results in three possible orientations for the angular momentum. The energy-level diagram is shown in Fig. 2-22:

Ground state: $n = 1, l = 0, m = 0$

First excited level: $n = 2, l = 0$ or $l = 1, m = 0$ or $m = 1, 0$ or -1 .

2.8.2 The Pauli Exclusion Principle

Quantum numbers describe the possible states that electrons can occupy in an atom. Additional rules are required to define how the electrons occupy these available states and thus explain the structure of multi-electron atoms and the periodic system of elements. An atom in its ground state has the minimum possible energy and electrons are distributed among the available and allowed states according to the principle formulated by the Austrian physicist Wolfgang Pauli (1900–1958). This principle, called the *Pauli exclusion principle*, states that no two electrons in any atom can share the same set of four quantum numbers. As an analogy, consider the fact that a single seat in the bus can be occupied by only one passenger and not by all the passengers. The electron states for the first three elements are used to describe the Pauli exclusion principle:

Hydrogen, the first and simplest atom, has a nuclear charge of $+1$ ($Z = 1$), and thus only one electron. The principal quantum number must be 1. Therefore, $n = 1, l = 0, m = 0, s = +\frac{1}{2}$ or $-\frac{1}{2}$. Since there is only one electron, the spin orientation can be either of the two values.

Helium, the second element, has two orbital electrons and positive nuclear charge of $+2$ ($Z = 2$). The first electron in a helium atom may have the same set of quantum numbers as the electron in a hydrogen atom, but the second electron must differ. Since there are two possible values for spin orientation, these two electrons will have different spin quantum numbers (Fig. 2-23). Thus, for the first electron $n = 1, l = 0, m = 0, s = +\frac{1}{2}$ and for the second $n = 1, l = 0, m = 0, s = -\frac{1}{2}$. The second electron in a helium atom exhausts all possibilities for $n = 1$. The anti-parallel orientation of the spins in the $1s$ state results in a zero magnetic moment, which is observed for the helium atom in its ground state, thus providing proof of the exclusion principle. If the spins of these two electrons were parallel (forbidden states), this would produce a non-zero magnetic moment, which has never been observed. In an excited helium atom as shown in Fig. 2-24, one electron can be in the $1s$ state and the other in $2s$. In this case, according to Pauli exclusion principle, the spins of the two electrons can be parallel, which would give a non-zero magnetic moment, or anti-parallel, in which case the magnetic moment is zero. Both cases have been observed in reality and thus contribute evidence of the exclusion principle.

Lithium, which has three orbital electrons and atomic number $Z = 3$. The first two electrons occupy the $1s$ level with anti-parallel spins. The $1s$ level is

thus filled and cannot accommodate any more electrons (all seats are taken!). Thus, the third electron, according to the exclusion principle, must occupy the next higher energy level and thus have a principal quantum number equal to 2. The lowest level in this state is the $2s$ level (Fig.2-25). This orbital may be circular or elliptical, i.e., the azimuthal quantum number may be either 0 or 1: (a) if $l = 0 \Rightarrow m = 0$ and (b) if $l = 1 \Rightarrow m = -1, 0$ or $+1$. Each of these states may contain two electrons, with each electron having a spin of $+\frac{1}{2}$ or $-\frac{1}{2}$.

The Pauli exclusion principle also applies to any electron-like particle, *i.e.* a particle with a half-integer spin. For example, neutrons, like the electrons, have a half-integer spin and the arrangement of neutrons inside the nucleus is similar to that of the electrons in their orbits around the nucleus (see Chapter 4).

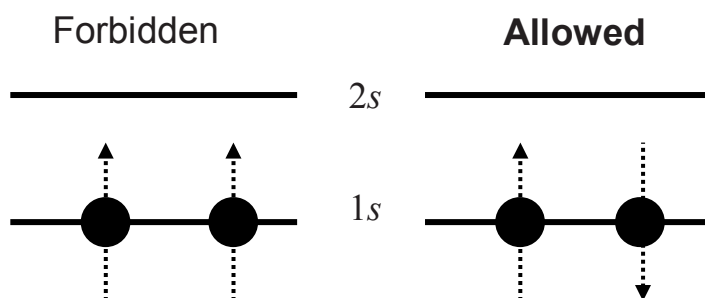


Figure 2-23. The ground state of a helium atom according to the Pauli exclusion principle

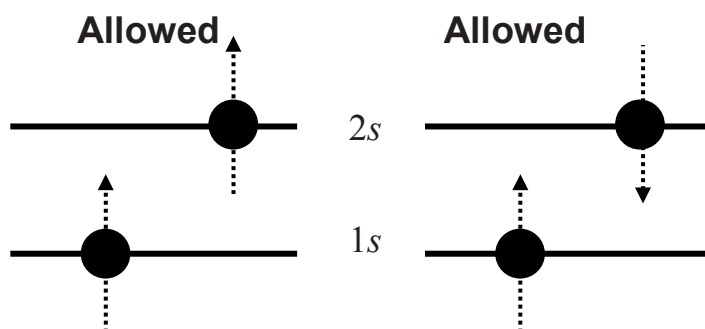


Figure 2-24. The lowest excited states of a helium atom

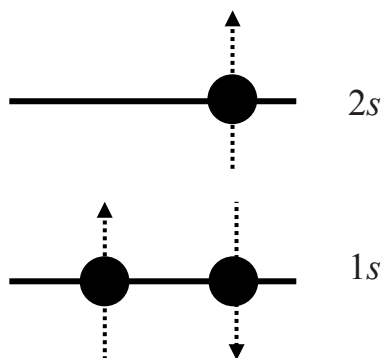


Figure 2-25. The ground state of a lithium atom

2.8.3 The Aufbau Principle

The quantum numbers and the Pauli exclusion principle define the maximum number of the electrons that can be found in each of the electron orbits in an atom and also explain how the electrons are arranged. The *aufbau principle* (German meaning “to build up” thus also known as the building-up principle) explains the order in which the electrons occupy the orbitals. According to this principle the lowest energy orbitals in an atom are filled before those in the higher energy levels. Each orbital can accommodate at most two electrons (confirmed by spectroscopic and chemical analysis). According to additional rule, called the Hund’s rule, if two or more energetically equivalent orbitals are available (such as orbitals p , d , f) the electrons spread out before they start to pair. The reason for this is that because the electrons repel each other and because each orbital is directed toward a different section in space, the electrons can depart from each other. The Hund’s rule also says that the unpaired electrons in degenerate orbitals have the same spin alignment.

All these rules explain the regularities in the chemical properties of the elements and the periodic table of elements as described in Section 2.9.

2.8.4 Screening Effect

Previous sections described how the multi-electron (polyelectron) atoms are built; when one proton attracts one electron, the hydrogen atom is created; each successive electron if added requires additional proton in the nucleus to assure the neutrality of the atom. The energy of attraction of one electron in one-electron atom (or ion) is proportional to Z^2/n^2 . Thus, in an atom with one electron, that electron experiences the full charge of the

positive nucleus and the effective nuclear charge can be calculated from Coulomb's law. In an atom with more than one electron, the outer electrons are simultaneously attracted to the positive nucleus but also repelled by other electrons. Because of this repulsion, each electron feels a nuclear charge that is smaller than the actual charge. The effective nuclear charge, Z_{eff} , on an electron is given with $(Z - a)$, as defined by Eq. (2-39). Parameter a as described in Section 2.7.5 represents the average number of electrons between the nucleus and the electron in question. It can be estimated using the Slater's rule or simply by deducing the number of electrons excluding the valence electrons from the total number of protons.

For a given electron, important screening (shielding) is only presented by electrons in the same or smaller shells; electrons in the larger shells do not importantly affect the Z_{eff} . The electrons in s orbit have the highest probability to be closest to the nucleus. The p or d or f or other higher orbits have regions in which electrons will never be found; therefore electrons in these orbits are never close to the nucleus as electrons in s orbit. Because of that the s orbits are called the penetrating orbits and these electrons have greater screening effect than electrons in higher orbits. For example, the electronic configuration of the carbon atom $1s^2 2s^2 2p^2$ indicates that the two electrons in $1s$ orbit shield better electrons in $2p$ than those in $2s$ orbit. The Z_{eff} is higher for the s electrons than it is for the p electrons (see Section 2.9.5).

2.9 The Periodic Table and Properties of the Elements

By the mid-19th century, several chemists had discovered that when the elements are arranged by atomic mass they demonstrate periodic behavior. In 1869, while writing a book on chemistry, Russian scientist Dmitri Mendeleev (1834–1907) realized this periodicity of the elements and he arranged them into a table that is today called the periodic table of elements. The table, as first published, was a simple observation of regularities in nature; the principles that defined this periodicity were not understood. Mendeleev's table contained gaps due to the fact that some of the elements were yet unknown. In addition, when he arranged the elements in the table he noticed that the weights of several elements were wrong.

In the modern periodic table, the elements are grouped in order of increasing atomic number and arranged in rows (Fig. 2-26). Elements with similar physical and chemical properties appear in the same columns. A new row starts whenever the last (outer) electron shell in each energy level (principal quantum number) is completely filled. Properties of an element are discussed in terms of their chemical or physical characteristics. Chemical properties are often observed through a chemical reaction, while physical properties are observed by examining a pure element.

The chemical properties of an element are determined by the distribution of electrons around the nucleus, particularly the outer, or valence, electrons. Since a chemical reaction does not affect the atomic nucleus, the atomic number remains unchanged. For example, Li, Na, K, Rb and Cs behave chemically similarly because each of these elements has only one electron in its outer orbit. The elements of the last column (He, Ne, Ar, Kr, Xe and Rn) have filled inner shells and all except helium have eight electrons in their outermost shells. Because their electron shells are completely filled, these elements cannot interact chemically and are therefore referred to as the inert, or noble, gases.

		Group																																													
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																												
Period	1	1 H																	2 He																												
	2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne																												
	3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar																												
	4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr																												
	5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe																												
	6	55 Cs	56 Ba	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn																												
	7	87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo																												
		<table><tr><td>57 La</td><td>58 Ce</td><td>59 Pr</td><td>60 Nd</td><td>61 Pm</td><td>62 Sm</td><td>63 Eu</td><td>64 Gd</td><td>65 Tb</td><td>66 Dy</td><td>67 Ho</td><td>68 Er</td><td>69 Tm</td><td>70 Yb</td></tr><tr><td>89 Ac</td><td>90 Th</td><td>91 Pa</td><td>92 U</td><td>93 Np</td><td>94 Pu</td><td>95 Am</td><td>96 Cm</td><td>97 Bk</td><td>98 Cf</td><td>99 Es</td><td>100 Fm</td><td>101 Md</td><td>102 No</td></tr></table>																		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No
57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb																																		
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No																																		

Figure 2-26. The periodic table of elements

Each horizontal row in the periodic table of elements is called a period. The first period contains only two elements, hydrogen and helium. The second and third periods each contain eight elements, while the fourth and fifth periods contain 18 elements each. The sixth period contains 32 elements that are usually arranged such that elements from $Z = 58$ to 71 are detached from main table and placed below it. The seventh and last period is also divided into two rows, one of which, from $Z = 90$ to 103, is placed below the second set of elements from the sixth period. The vertical columns are called groups and are numbered from left to right. The first column, Group 1, contains elements that have a closed shell plus a single s electron in the next higher shell. The elements in Group 2 have a closed shell plus two s electrons in the next shell. Groups 3–18 are characterized by the elements

that have filled, or almost filled, *p* levels. Group 18 is also called Group 0 and contains the noble gases. The columns in the interior of the periodic table contain the transition elements in which the electrons are present in the *d* energy level. These elements begin in the fourth period because the first *d* level (*3d*) is in the fourth shell. The sixth and the seventh shells contain *4f* and *5f* levels and are called lanthanides, or rare earth elements, and actinides, respectively.

The elements are also grouped according to their physical properties; for instance, they are grouped into metals, non-metals, and metalloids. Elements with very similar chemical properties are referred to as families; examples include the halogens, the inert gases, and the alkali metals. The following sections only focus on those atomic properties that are closely related to the principles of nuclear engineering.

2.9.1 Ground States of Atoms

The most common way to illustrate the electronic structure of the atoms in their ground states is to use the energy-level diagrams (like these shown in Fig. 2-23 and 2-25) or notations as shown in Table 2-2.

Table 2-2. Electron configuration of the first 18 elements

First shell	Second shell	Third shell
Hydrogen, H-1: $1s^1$	Lithium, Li-3: $1s^2 2s^1$	Sodium, Na-11: $1s^2 2s^2 2p^6 3s^1$
Helium, He-2: $1s^2$	Beryllium, Be-4: $1s^2 2s^2$	Magnesium, Mg-12: $1s^2 2s^2 2p^6 3s^2$
	Boron, B-5: $1s^2 2s^2 2p^1$	Aluminum, Al-13: $1s^2 2s^2 2p^6 3s^2 3p^1$
	Carbon, C-6: $1s^2 2s^2 2p^2$	Silicon, Si-14: $1s^2 2s^2 2p^6 3s^2 3p^2$
	Nitrogen, N-7: $1s^2 2s^2 2p^3$	Phosphor, P-15: $1s^2 2s^2 2p^6 3s^2 3p^3$
	Oxygen, O-8: $1s^2 2s^2 2p^4$	Sulfur, S-16: $1s^2 2s^2 2p^6 3s^2 3p^4$
	Fluorine, F-9: $1s^2 2s^2 2p^5$	Chlorine, Cl-17: $1s^2 2s^2 2p^6 3s^2 3p^5$
	Neon, Ne-10: $1s^2 2s^2 2p^6$	Argon, Ar-18: $1s^2 2s^2 2p^6 3s^2 3p^6$

How to determine the ground state of an atom? Simply as the data in Table 2-2 indicates, the number of electrons of that atom (*Z*) is to be assigned to the lowest energy levels taking into account the Pauli exclusion principle and the aufbau principle. The ground states of the first few elements are explained in Section 2.8.2 in the discussion of the quantum numbers and the electron spin orientation. Recall analyzing Table 2-2, for the first two elements, hydrogen and helium, H-1 and He-2, the *1s* level is used to create the ground state. Starting from lithium, Li-3 through neon, Ne-10, *1s* level is filled with the maximum allowed number of electrons, and the new shells are open, first the *2s* level and then the *2p* level. For sodium, Na-11, through argon, Ar-18, the levels, *1s*, *2s* and *2p*, are already occupied; thus the electrons are filling the next shells, i.e., the energy levels *3s* and then *3p*. The atoms from Ar-18 to potassium, K-19, have electrons filling the

orbits with the lower angular momentum and thus lower energies (these are the penetrating orbits as described in Sections 2.8.4 and 2.9.5), which would be $4s$ and not $3d$. Therefore, K-19 has the following electronic configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$.

Example 2.13 Electronic configuration

For Na and Li, write the electronic configurations in short notation based on the previous completed electron shell.

From Table 2-2 it follows that

Lithium, Li-3: $1s^2 2s^1 = [\text{He}] 2s^1$

Sodium, Na-11: $1s^2 2s^2 2p^6 3s^1 = [\text{Ne}] 3s^1$

Example 2.14 Electron energy shell diagram

Draw the energy diagram for the first six shells to illustrate the orders in which the electron energy levels (shells) are occupied taking into account all discussions presented in this and in the previous sections.

Shell	Energy levels	Max*	Z**
6	<div><div><div>6s</div></div><div><div>6p</div></div><div><div>5d</div></div><div><div>4f</div></div></div>	2+6+10 +14	86
5	<div><div><div>5s</div></div><div><div>5p</div></div><div><div>4d</div></div></div>	2+6+10	54
4	<div><div><div>4s</div></div><div><div>4p</div></div><div><div>3d</div></div></div>	2+6+10	36
3	<div><div><div>3s</div></div><div><div>3p</div></div></div>	2+6	18
2	<div><div><div>2s</div></div><div><div>2p</div></div></div>	2+6	10
1	<div><div><div>1s</div></div></div>	2	2

*Indicates the maximum number of electrons that can be found at that level

** Indicates the atomic number of the atom with the closed shells

2.9.2 Excited States of Atoms

For an atom to be in its excited state, one or more of its electrons is supposed to be moved from the ground (lowest energy) state to higher energy levels. Electron can be moved to any of the available levels and in many-electron atoms more than one electron can be moved to higher levels

at the same time. Let us assume that the atom has its last and only one electron in its ground state located in the shell $3s$. From Table 2-2 it is clear that the levels $1s$, $2s$ and $2p$ are filled with the electrons indicating thus that the smallest energy needed to excite this atom would be to move the last electron to a higher level orbit. Since this last electron occupies shell $3s$ according to the schematics from Example 2.14, with the addition of energy, it can be moved to $3p$, or $4s$, or $4p$ and so on. The excitation energies of the most outer electrons (valence electrons) are usually in the order of few eV; these excitations are usually called the optical excitations (because the energy of few eV corresponds to a visible spectrum of light). The higher incoming energy of the photon is required to excite the atom by moving some of the inner electrons to higher energy levels. The highest energy needed is to remove the $1s$ electrons and is nearly equal to $-Z^2 E_R$ (Section 2.7.4). The $1s$ electron when excited can move only to those shells that Pauli exclusion principle allows; in other words these electrons cannot occupy already filled shells. Therefore, $1s$ electrons are moved to the valence shells or the higher levels that require much smaller energy. The difference (in energy required to remove $1s$ electron in the order of keV or higher to valence shell of energy in the order of few eV) is therefore emitted in the form of X-rays and this type of atom excitation is called the X-ray excitations. When $1s$ electron is removed, the formed vacancy is filled by any of the electrons from the higher energy levels. The difference in energy is again emitted in the form of X-rays. This is described by the Mosley experiment in Section 2.7.5.

2.9.3 Atomic Radius

The size of an atom, expressed as the atomic radius, represents the distance between the nucleus and the valence, or outermost, electrons. The boundary between the nucleus and the electrons is not easy to determine and the atomic radius is therefore approximated. For example, the distance between the two chlorine atoms of Cl_2 is known to be nearly 2\AA . In order to obtain the atomic radius, the distance between the two nuclei is assumed to be the sum of the radii of two chlorine atoms. Therefore the atomic radius of chlorine is $\sim 1\text{\AA}$ (or 100 pm, see Fig. 2-27).

The atomic radius changes across the periodic table of elements and is dependent on the atomic number and the electron distribution. Since electrons repel each other due to like charges, the overall size of the atom increases with an increase in the number of electrons in each of the groups (see Fig. 2-27). For example, the radius of a hydrogen atom is smaller than the radius of the lithium atom. The outer electron of lithium is in the $n = 2$ level, so its radius must be larger than the radius of hydrogen which has its

outermost electron in the $n = 1$ level. However, in spite of the increase in the number of electrons, the atomic radius decreases when going from left to right across the periodic table. This is a result of an increase in the number of protons for these elements, which all have their valence electrons in the same quantum energy level. Since the electrons are attracted to the protons, the increased charge of the nucleus (more protons) binds the electrons more tightly and brings them closer to the nucleus, causing the overall atomic radius to decrease. For example, the first two elements in the second period of the periodic table are lithium and beryllium.

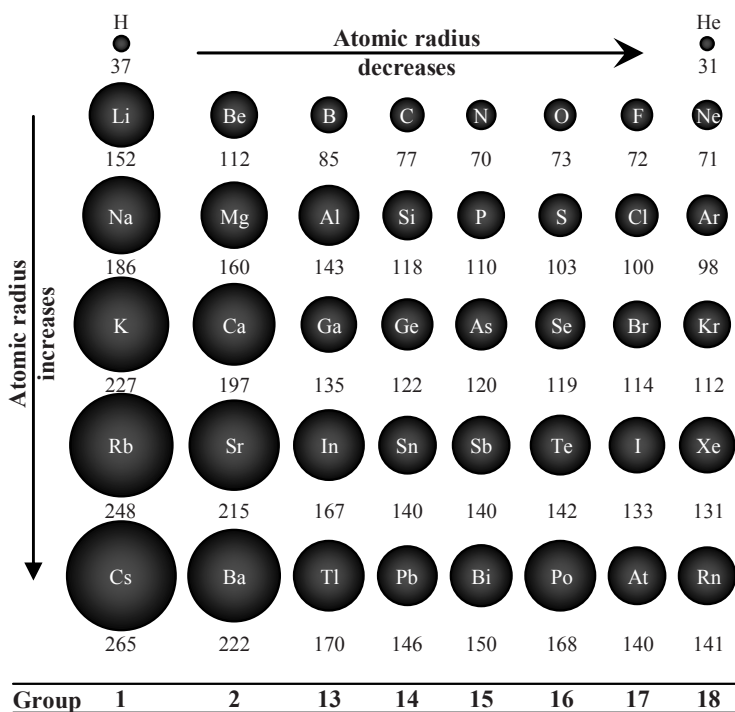


Figure 2-27. Trends of atomic radii (listed in picometers) in the periodic table

The radius of a beryllium atom is 112 pm, which is smaller than that of lithium (152 pm). In beryllium, $Z = 4$, the fourth electron joins the third in the $2s$ level, assuming their spins are anti-parallel. The charge is thus larger and this causes the electrons to be bound more tightly to the nucleus; as a result the beryllium radius is less than the lithium radius. The effect of the increased charge should, however, be seen in the context of the quantum energy levels. For example, cesium has a large number of protons but it is one of the largest atoms. The valence electrons are furthest from the nucleus and the inner electrons shield them from the positive charge of the nucleus;

thus the valence electrons experience a reduced effective nuclear charge and not the total charge of the nucleus. The effect of the increase in the nuclear charge thus only plays a role in the periods from left to right, e.g., from sodium to argon in the third period, since the additional valence electrons (in the same quantum energy level) are exposed to a greater effective nuclear charge along the period.

2.9.4 Ionization Energy

Another important property that shows a trend in the periodic table is the ionization energy (the energy required to remove an electron from an atom). An atom has as many ionization energies as there are electrons. By definition, the *first ionization energy* is the energy required to remove the most outer electron from a neutral atom (Table 2-1):



The second ionization energy is the energy required to remove the next outer electron from the singly charged ion:



Each successive removal of an electron requires more energy because, as more electrons are removed, the remaining electrons experience a greater effective attraction.

The first ionization potential increases across a period (Fig. 2-28), which is a direct result of the decrease in atomic radius (Fig. 2-27). As the atomic radius becomes smaller the electrons feel a greater attraction from the nucleus. As the force of attraction increases, more energy is required to remove the electrons. The larger nuclear charge in helium ($Z = 2$) that is responsible for the smaller radius (31 pm) results in a higher ionization potential (24.6 eV) compared to that of hydrogen (radius 37 pm and ionization potential 13.6 eV). Lithium, however, has one more electron than helium and this electron is at a higher quantum energy level. The lithium radius is thus greater and the ionization potential is less. The outermost electron in lithium is located in the $2s$ level, which is outside the $1s$ level occupied by the first two electrons. The $2s$ electron is screened by the other two and experiences a charge on the order of one. Thus, the ionization energy of this electron can be estimated to be nearly that of the $2s$ hydrogen state (which is 3.4 eV). The observed lithium ionization potential, however, is 5.4 eV (see Table 2-1). The value is larger because the outer electron is not perfectly shielded by inner electrons and the effective charge is greater

than the assumed value of one. Because lithium has such small ionization energy it is a chemically active element. Next to lithium is beryllium. Due to the larger charge, the radius is smaller (Fig. 2-27) and the ionization potential is thus larger. Next is boron; the first four electrons occupy the $1s$ and $2s$ levels and the fifth electron is in $2p$ level. The increased charge causes the electrons in the new energy level to be more tightly bound, but the new energy level is further away from the nucleus and the valence electron is thus bound with a slightly weaker force. Consequently, the radius is reduced; the ionization potential is also reduced. Although there is an anomaly in the overall trend of ionization potential values across the period, the differences are small (the ionization potentials of beryllium and boron are 9.3 eV and 8.3 eV, respectively). In the next elements leading up to neon, the electrons occupy the $2p$ level (maximum of six electrons). The increasing charge decreases the atomic radius (Fig. 2-27) and ionization potential increases as indicated in Fig. 2-28. The next period starts with sodium. Since the valence electrons of neon fill the $2p$ level, the sodium valence electron can only occupy the higher $3s$ level. This accounts for the larger atomic radius and smaller ionization potential.

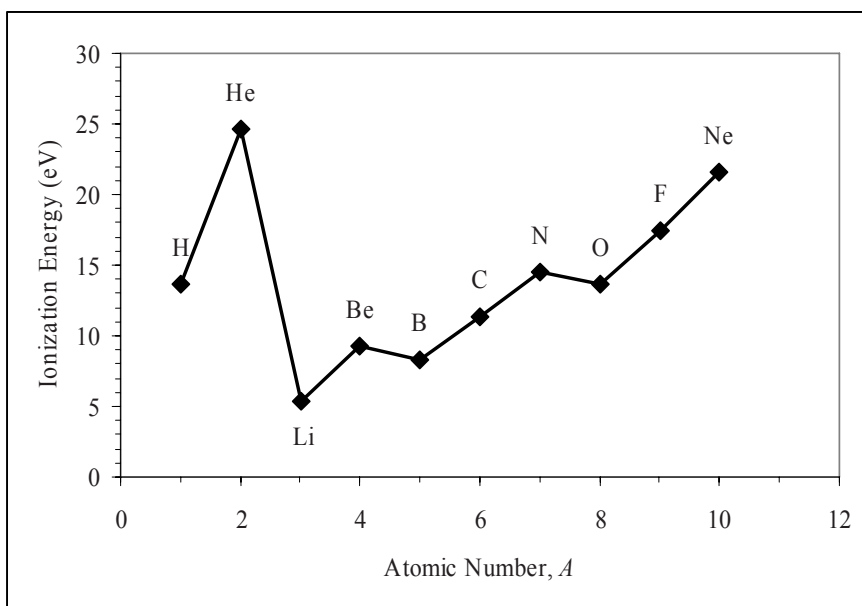


Figure 2-28. Ionization potential of the first ten elements

The small drop in ionization potential of oxygen compared to nitrogen is due to the arrangement of electrons. In nitrogen, two electrons occupy the $1s$ level and two others occupy the $2s$ level. The remaining three electrons

occupy the $2p$ level. These three electrons occupy three available and distinct orbitals ($2p$ level accommodates three orientations of the electron's orbital, see Section 2.8.1). This keeps them well separated and reduces the repulsion between them. This in turn makes nitrogen relatively stable with relatively large ionization energy. In oxygen, the fourth electron occupies the $2p$ level and must share one of the orbitals (with opposite spin). These two electrons thus overlap in the orbital they share which increases the repulsion between them and decreases the ionization potential relative to nitrogen.

Examples of the periodic behavior of the elements are evident from the similarities between helium and neon (both very stable, with large ionization potential and small radii), or lithium and sodium (both with very low ionization potential and very large radii).

Example 2.15 First ionization potential

Explain which element from the list has the larger first ionization energy and why: Mg, Na or Al.

Magnesium (Mg), when compared to sodium (Na), has a larger first ionization potential because the first ionization energy tends to increase across a row of the periodic table from left to right (period 3, see Fig. 2-27). Mg also has a larger ionization potential than aluminum (Al) even though Al is to the right of Mg in the periodic table. The electron configurations for Mg and Al are (see Table 2-2)

Mg (12 electrons): $1s^2 2s^2 2p^6 3s^2$

Al (13 electrons): $1s^2 2s^2 2p^6 3s^2 3p^1$

The outermost electron of Al (in the $3p$ level) is further away from the nucleus than the outermost Mg electrons which are in the $3s$ level. Less energy is thus required to remove the outermost Al electron.

2.9.5 Independent Particle Approximation for Electrons

The multi-electron atom is a complicated and complex structure that cannot be exactly modeled. The basic and most common approximation is called the independent particle approximation, known as the IPA. The approximation is derived from the classical theory of the many-body problem such as the solar system in which all forces in between the planets are neglected in comparison to the force from the Sun. This same approach is applied to the atom, assuming the most important force is the force of the nucleus. This is however very poor approximation as the effect of the electrons on each other cannot be neglected. The IPA therefore analyzes each electron independently but the force is the sum of the forces from the nucleus and the force from the average distribution of $Z-1$ electrons. One electron in a multi-electron atom will therefore possess the so-called IPA potential energy, $U(\vec{r})$. It is assumed that the charge distribution affecting

each electron is spherically symmetric, thus defining the IPA potential energy to be dependent only on distance from the nucleus, $U(r)$. According to the Gauss's law, any electron outside the charge that is spherically distributed experiences exactly the same force if it is assumed that that same charge, Q , is concentrated at the center of the sphere ($r = 0$)

$$F = k \frac{Qe}{r^2} \quad (2-40)$$

For the electron which is away from the rest of the electrons in an atom, $Z-1$, the total charge Q will be the charge of the nucleus (Ze) reduced by the charge of the rest of the electrons (located inside the radius r). In this extreme case, the charge Q becomes $Ze - (Z-1)e = e$. Thus this one electron experiences the same force as the electron in hydrogen atom, and Eq. (2-40) becomes

$$F = k \frac{e^2}{r^2} \quad (2-41)$$

For the electron located inside a spherical charge the electron will experience no force coming from that charge. This implies the following: the electron close to the nucleus is inside of the charge created by all other electrons; thus it will experience the attractive force from the nucleus (of charge Ze) and will not experience any force from other electrons

$$F = k \frac{Ze^2}{r^2} \quad (2-42)$$

If a force acting on a particle is a function of position only, the potential energy of that particle can be defined as an integral of the force. Thus it follows that when an electron is outside the charge created by all other electrons (at r outside all other electrons) its potential energy is defined by

$$U(r) = \int k \frac{e^2}{r^2} dr = -k \frac{e^2}{r} \quad (2-43)$$

For the electron inside the charge created by all other electrons

$$U(r) = \int k \frac{Ze^2}{r^2} dr = -Zk \frac{e^2}{r} \quad (2-44)$$

The last two equations could be written as follows

$$U(r) = -Z_{\text{eff}} k \frac{e^2}{r} \begin{cases} Z_{\text{eff}} = Z & \text{if } r \text{ (electron) is inside all other electrons} \\ Z_{\text{eff}} = 1 & \text{if } r \text{ (electron) is outside all other electrons} \end{cases} \quad (2-45)$$

Because this potential energy depends only on distance it implies the spherical symmetry of the potential field, and therefore the energy is the same for both spin orientation. For the lowest energy level (like in hydrogen), $n = 1$ and $l = 0$ (Section 2.8.1), the $1s$ shell is twofold degenerate (due to two possible spin orientations) and is the closest to the nucleus. In other words, in many-electron atoms in $1s$ shell the potential energy is large and its numeric value is close to hydrogen-like potential energy; thus $Z_{\text{eff}} \sim Z$, giving

$$E_{1s} = -Z^2 E_R \quad (2-46)$$

and the most probable radius is a_0/Z .

The next energy level is described with $n = 2$. As explained in Section 2.8.4 the shells $2s$ and $2p$ are located in the region where electrons experience the screening from the $1s$ shell seeing only Z_{eff} that is always smaller than Z . The $2s$ electrons penetrate closer to the nucleus, have lower energy than $2p$ electrons and experience almost full effect from Z . The energy levels with higher n than 1 are located at increasing distance from the nucleus and these electrons experience the screening effect thus seeing only Z_{eff} . This effective charge is becoming smaller as the orbit quantum number is becoming higher. The most probable radius for such orbits is $\sim n^2 a_0 / Z_{\text{eff}}$.

2.10 Atomic Parameters

Atomic mass is given in either the absolute unit of *grams* or in a relative unit called the *atomic mass unit* (u or amu):

- 1 mole of any substance contains 6.02×10^{23} molecules (Avogadro's number), N_a
- The weight in grams of 1 mole of a substance is numerically equal to its molecular weight
- The unified atomic mass unit is exactly one-twelfth of the mass of a C atom (C-12), i.e., the atomic mass of carbon-12 is equal to 12 amu

$$1 \text{ amu} = \frac{m_{\text{C-12}}}{12} = 1.661 \times 10^{-24} \text{ kg} = 931.5 \text{ MeV} / c^2 \quad (2-47)$$

Example 2.16 Number of atoms

How many ^{12}C atoms are there in 12 g of carbon? What is the mass of one atom of carbon in kg?

Number of atoms in 12 g of carbon is

$$\frac{12 \text{ g}}{(1.661 \times 10^{-24} \text{ g/amu})(12 \text{ amu/atom})} = 6.02 \times 10^{23} \text{ atoms}$$

Because the molar mass of carbon-12 is 12 g, the mass of one atom of carbon 12 can be found by dividing the molar mass by Avogadro's number:

$$\frac{12 \text{ g/mol}}{6.02 \times 10^{23} \text{ atoms/mol}} = 1.993 \times 10^{-23} \text{ g/atom} = 1.993 \times 10^{-26} \text{ kg/atom}$$

The chemical properties of atoms are determined by the distribution of electrons (Section 2.9), and the number of electrons is called the *atomic number* and is usually denoted by Z . The number of protons in an atomic nucleus is also equal to Z , which is a requirement for electrical neutrality. When a neutral atom loses some of its electrons the atom becomes positively charged and is called a *positive ion*. For example, Ca^{2+} is a calcium atom that has lost two of its electrons. An atom can, however, gain electrons and thus become a *negative ion*. For example, Cl^- is a chlorine atom that gained one electron. The *atomic mass number*, A , is an integer that is almost equal to the atomic mass in amu. It is equal to the number of nucleons in the nucleus; that is, it is equal to the sum of the number of protons (Z) and the number of neutrons (N). Atoms (the elements of the periodic table) are denoted as follows:



Atoms with the same atomic number Z (for example, ^{35}Ar , ^{38}Ar , ^{40}Ar) are called the *isotopes* of that element (argon). A naturally occurring sample of any element consists of one or more isotopes of that element and each isotope has a different weight. The relative amount of each isotope represents the isotope distribution for that element, and the *atomic weight* is obtained as the average of the isotope weights, weighted according to the isotope distribution.

Example 2.17 Atomic weight

Chromium (atomic weight 51.996) has four naturally occurring isotopes. Three of these are ^{50}Cr with isotopic weight 49.9461 and abundance 4.31%, ^{52}Cr with isotopic weight 51.9405 and abundance 83.76% and ^{54}Cr with isotopic weight 53.9389 and abundance 2.38%. Determine the isotopic weight of the fourth isotope.

$$M^{\text{Cr}} = \frac{4.31}{100} M^{50} + \frac{83.76}{100} M^{52} + \frac{2.38}{100} M^{54} + \frac{[100 - (4.31 + 83.76 + 2.38)]}{100} M^x = 51.996$$

$M^{53} = 52.9237$ with an abundance of 9.55 %.

Example 2.18 Mass of an atom

Calculate the mass in grams of a ^{52}Cr atom. The atomic mass is 51.94051 amu. A mole contains N_a number of same particles (atoms or molecules); thus

$$M(^{52}\text{Cr}) = \frac{52 \text{ (g/mol)}}{6.02 \times 10^{23} \text{ (atoms/mol)}} = 8.638 \times 10^{-23} \text{ g/atom}$$

However, knowing the atomic mass as given in the problem, the more precise mass of the atom is obtained as follows

$$M(^{52}\text{Cr}) = \frac{51.9405 \text{ (g/mol)}}{6.02 \times 10^{23} \text{ (atoms/mol)}} = 8.628 \times 10^{-23} \text{ g/atom}$$

Example 2.19 Atom number density

Calculate the molecular weight of water and then determine the atom density of hydrogen in water.

The molecular weight of water is

$$2A_{\text{H}} + A_{\text{O}} = 2 \times 1 + 16 = 18 \quad \text{giving the molecular density of water}$$

$$N(\text{H}_2\text{O}) = \frac{\rho N_a}{A} = \frac{(1 \text{ g/cm}^3)(6.02 \times 10^{23} \text{ molecules/mol})}{18 \text{ g/mol}} \\ = 3.35 \times 10^{22} \text{ molecules/cm}^3$$

The molecular weight of hydrogen is

$$N(\text{H}) = 2 \times N(\text{H}_2\text{O}) = 2 \times (3.35 \times 10^{22} \text{ atoms/cm}^3) \\ = 6.69 \times 10^{22} \text{ atoms/cm}^3$$

APPLICATIONS

Fluorescent Lamp

An atom gains or loses energy by adding or removing energy from the electrons influencing them to move from one orbital to another. Atom is in its neutral state if all electrons are in their lowest possible energy levels. Atoms gain energy by absorbing from photons or by colliding with another particle. As described earlier, when an atom gains energy one or more electrons will move to a higher (more energetic) orbital. Once excited the atoms hold that energy for a very short time, typically in the order of 10^{-12} s. After that time, the electron or electrons will go back to their original energy states, during which process the excess of energy is released in the form of a photon (Section 2.7.3). This emission of photon can be in any part of the light spectrum. The fluorescence lamps operate on that principle. The fluorescence occurs when atom absorbs usually a photon in the ultraviolet range and emits the photon (with the longer wavelength) in the visible part of a spectrum. The transition probability is explained at the end of Chapter 3, Section on APPLICATIONS.

Laser

Laser (light amplification by stimulated emission of radiation) is a device used to produce (amplify) the coherent light (emitted light is in a form of almost perfect sinusoidal waves) as a narrow, low-divergence photon beam, with a narrow wavelength spectrum (called the monochromatic light). The basic principle of the laser device is the transition of the electrons between the orbits in an excited atom and the emission of the photon of a desired frequency. A photon of correct wavelength will stimulate the transition of an electron in an excited atom to return to a lower energy level, thus emitting the photon of the same wavelength as the stimulating (incoming) photon. These two photons will then stimulate two more emissions producing four photons of the same wavelength and the process when continues will produce an amplified stimulated emission of radiation.

From 1960 when laser was invented, it has found numerous applications in science, medicine, engineering, industry, military, information technology and entertainment.

X-rays

The principle of the X-ray excitation is described in Section 2.9.2; the discovery of X-rays is described in Chapter 5; the interaction and effects are summarized in Chapter 6. The X-rays have wide applications in many disciplines: in medicine (medical imaging and cancer treatment), industry (industrial radiography for inspecting particularly the welding sections),

homeland security (for example, at the airports for detecting the metal objects), astronomy (X-ray astronomy studying the X-ray emission from celestial bodies in the universe) and biology (X-ray microscopy for imaging the small objects).

PROBLEMS

2.1 Write the electron configuration for potassium, lanthanum, copper and bromine.

2.2 Name the elements whose electron configuration is

(a) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$

(b) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^9$

(c) $1s^2 2s^2 2p^6 3s^2 3p^6$

2.3 How many electrons are in an atom specified by $1s^2 2s^2 2p^6 3s^2 3p^4$?

2.4 (a) The attractive electrostatic force of the positively charged atomic nucleus forces the negatively charged electron of the hydrogen atom to a circular motion. Write the equation that describes this statement.

(b) Knowing that only orbital radii are allowed for which angular momentum is an integer multiple of $h/(2\pi)$ and using the equation from (a) develop the relation for the allowed radii.

2.5. (a) Express the relation for the frequency of revolution of the electron in hydrogen atom for $n = 1$.

(b) For this case show that $\nu/c = (ke^2)(2\pi)/hc = 1/137$, which is called the fine structure constant, α .

2.6 Starting from the Bohr's equation for the energy of the n th state of an electron in hydrogen atom, write the equation describing the frequency of light given off when an electron makes a transition from an initial to a final state. From there derive the value for Rydberg constant.

2.7 Calculate the largest velocity, the lowest energy level and the smallest orbit radius for the electron in hydrogen-like atoms. When the orbit becomes infinite what is the value of energy?

2.8 Calculate how many times in a second an electron in hydrogen atom orbiting at the level $n = 30$ goes around the nucleus?

2.9 What is the excited state of sodium atom? What is the excited state of hydrogen atom?

2.10 Knowing that the first excited state of sodium atom is at 2.1 eV above 3s level, determine the wavelength and frequency of the photon emitted in the $3p \rightarrow 3s$ transition.

2.11 The ground state of hydrogen atom has one electron in the 1s level with its spin pointing either way. Calculate the energy of the electron in this orbit using Bohr's theory. What is the value of the ionizing energy?

2.12 The ground state of a helium atom has two electrons and both in 1s level. How are their spins oriented? The first ionization potential is found experimentally to be 24.6 eV. Calculate the effective charge, Z_{eff} .

2.13 Calculate the value of Rydberg constant for the hydrogen atom taking into account the effect of reduced mass.

2.14 For heavy hydrogenic ions how does the reduced mass change and consequently what is the value of Rydberg constant?

2.15 Calculate the wavelengths of Balmer lines in hydrogen atom.

2.16 Explain departure from Rutherford formula. Give an example.

2.17 Calculate the first ionization potential of hydrogen helium atom.

2.18 Draw possible trajectories of an α particle in Rutherford experiment for different impact parameters and scattering angles.

2.19 For a gold (assuming to have a nuclear radius about 7 fm and an atomic radius of about 0.13 nm) thin foil used in Rutherford experiment estimate its maximum thickness that would not produce the multiple scattering of α particles.

2.20 For an ion of ^{23}Mg write the number of protons, neutrons and electrons.

2.21 Study the Millikan's experiment. Knowing that the oil droplets were produced such to have a radius of 1 μm , and that the voltage between plates positioned at the distance of 0.042 m was recorded whenever the droplets become stationary, using data provided, show that the charge difference is always the integral multiples of 1.602×10^{-19} C. Assume that the density of oil is 900 kg/m^3 . The voltage as measured in Millikan's experiment is 391.49 V, 407.80 V, 376.43 V, 337.49 V, 362.49 V, 376.43 V.

2.22 What is the difference between the atomic weight and atomic mass? Give an example.

2.23 Show that the mass of the hydrogen atom is 1.6735×10^{-24} g and that of the oxygen atom is 2.6561×10^{-23} g.

2.24 If naturally occurring carbon consists of 98.892% ^{12}C and 1.108% ^{13}C what is the average mass (in amu) of carbon?

2.25 Calculate the molecular mass of methane (CH_4). What is the percentage by mass of the elements in this compound?

2.26 Using Eq. (2-3) write the computer code to plot the 7.7 MeV α particle's trajectories as a function of impact parameters and angles of deflection. Indicate the points of closest approach.

2.27 Use the Bohr's atomic model and write the computer code to calculate the orbiting velocity of the electron in hydrogen atom (see Example 2.5), helium ion, lithium ion and boron ion. Comment on the results.

2.28 To the computer code developed for Problem 2.27 add the calculation of the time it takes for an electron to complete one revolution in hydrogen atom and ions of helium, lithium and boron. How does the time change, with the orbits moving further away from the nucleus? Comment on the results.

2.29 Write the computer code to reproduce the spectral lines shown in Fig. 2-19.

2.30 Plot the Rydberg energy for hydrogen atom, and first 11 ions from the table of elements. Comment on the results.

2.31 Calculate the ratio of the allowed energies in the helium and lithium ions to that in the hydrogen atom, taking into account the effect of nuclear motion (see Example 2.9).

2.32 Calculate how much energy (in J and eV) does one electron with a principle quantum number of $n = 2$ have.

2.33 Write the electron configuration by explaining the filling of the shells and draw the complete orbital diagram (using the style of Fig. 2-23) for iron Fe.

2.34 In the Rutherford experiment replace the gold foil with the copper foil. For the α particle with the velocity of 1.6×10^9 cm/sec, what is the closest approach to the foil?

2.35 Calculate the ground state hydrogen atom diameter based on Bohr atomic model.

2.36. Demonstrate the Bohr correspondence principle by showing that the frequency of the radiation emitted f_{cl} (classical physics) is equal to the orbital frequency f_{orb} of the electron around the nucleus (Bohr theory).

2.37. Assume the transition from the state n_1 to state n_2 in the Problem 2.37 such that $n_1 - n_2 = 1$ or $= 2$ or $= 3$. What is the frequency of the emitted radiation? Comment.



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