CHAPTER 1 BASIC CONCEPTS

In 1895 Wilhelm Röentgen discovered rays, which he called x rays, that could penetrate matter. Since then, scientists have been concerned with the interaction of radiation with matter. Radiation can be energetic charged particles such as electrons, protons, alpha particles, or heavy ions; energetic neutral particles such as neutrons; and parts of the electromagnetic spectrum such as x rays and gamma rays. Radiation can alter the atomic and molecular structure of a medium by interacting with its atomic electrons and nuclei. The mechanisms of these interactions and methods to measure the radiation and its effects are the subjects of radiation dosimetry, which is of interest in fields such as biology, medicine, and instrumentation. Properties of some particles of interest in radiation dosimetry are given in Table 1.1.

Table 1.1
Mass and charge of particles of interest in radiation dosimetry.

Particle	Charge (C)	Mass (kg)	m/m_e
Electron	-1.6022×10^{-19}	9.109383×10^{-31}	1
Proton	$+1.6022 \times 10^{-19}$	1.672622×10^{-27}	1836
Neutron	0	1.674927×10^{-27}	1839
Photon	0	0	0
Positron	Same values as electron but with + charge		

One aspect of radiation dosimetry is the calculation and measurement of energy absorbed by an irradiated medium. In general, energy absorbed is not calculable. However, when a projectile interacts with a target, it is almost always possible to calculate the energy lost by the projectile and transferred to the target. The simplest example of this, and one used extensively in radiation dosimetry, is the collision of two particles.

1.1 NON-RELATIVISTIC ELASTIC COLLISIONS OF TWO PARTICLES

Consider a projectile particle of mass m_1, velocity v, and kinetic energy T incident on a target of mass m_2 initially at rest. As in Fig. 1.1, the projectile scatters at an angle θ_1 with velocity v_1 and energy T_1, and the target scatters at an angle θ_2 with velocity v_2 and energy T_2. The energy T_2 given to the target is the energy lost by the projectile, T_{lost}, and is also called the energy transferred to the target, T_{tr}.

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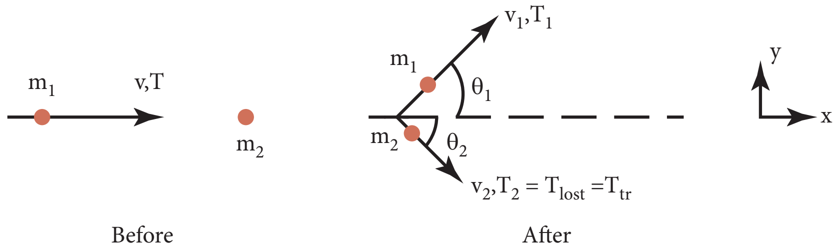


FIG. 1.1
Collision of two particles. Before the collision the target is at rest.

Conservation of momentum gives:

$$\text{for the x direction,}\quad m_1 v = m_1 v_1 \cos\theta_1 + m_2 v_2 \cos\theta_2, \tag{1.1}$$

$$\text{for the y direction,}\quad 0 = m_1 v_1 \sin\theta_1 - m_2 v_2 \sin\theta_2. \tag{1.2}$$

If the collision is elastic, kinetic energy is conserved. That is, the initial kinetic energy of the system equals the final kinetic energy. So, for an elastic collision,

$$\frac{1}{2} m_1 v^2 = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2 \quad \text{or,}\quad m_1 v^2 = m_1 v_1^2 + m_2 v_2^2. \tag{1.3}$$

Generally, the masses are known as well as the initial velocity, v, of the projectile. There are four unknowns (v_1, v_2, θ_1, θ_2) and three equations that can be solved relating the unknowns to each other. Energy lost by the projectile and transferred to the target is determined from v_2, which, on solving the equations, is

$$v_2 = 2\frac{m_1}{m_1 + m_2} v \cos\theta_2. \tag{1.4}$$

The kinetic energy lost by the projectile and transferred to the target is then

$$T_2 = T_{lost} = T_{tr} = \frac{1}{2} m_2 v_2^2 = m_2 \frac{2 m_1^2 v^2}{(m_1 + m_2)^2} \cos^2\theta_2 = 4T \frac{m_1 m_2}{(m_1 + m_2)^2} \cos^2\theta_2. \tag{1.5}$$

To obtain the relation between the two scattering angles, substitute (1.4) into (1.3) to obtain an expression for v_1^2. Substituting this and Eq. (1.4) into (1.2) gives

$$\sin\theta_1 = \frac{2m_2}{m_1 + m_2} \frac{\sin\theta_2 \cos\theta_2}{\left(1 - \frac{4 m_1 m_2}{(m_1 + m_2)^2} \cos^2\theta_2\right)^{1/2}}. \tag{1.6}$$

1.1.1 Head-on collision: maximum energy lost

The maximum energy lost by the projectile occurs for a head-on collision. The target is projected forward ($\theta_2 = 0$) and Eq. (1.5) has a maximum value of

$$T_{\text{lost max}} = T_{\text{tr max}} = 4T\frac{m_1 m_2}{(m_1 + m_2)^2}. \tag{1.7}$$

For $m_1 \gg m_2$, $T_{\text{lost max}}$ is small and given by $T_{\text{lost max}} \approx 4(m_2/m_1)T$.
For $m_1 = m_2$, $T_{\text{lost max}} = T$. The projectile transfers all its energy to the target and comes to rest.
For $m_1 = m_2$, $T_{\text{lost max}}$ is small and given by $T_{\text{lost max}} \approx 4(m_1/m_2)T$.

For head-on collisions the greatest energy lost or transferred occurs for two equal masses. The greater the difference between the masses the smaller the energy lost. For example, in a head-on collision between a proton and an electron the projectile loses only about 0.22% of its energy.

There is no condition for which the target can backscatter by which is meant that it cannot scatter at angles greater than $\pi/2$.

1.1.2 Scattering angles: $m_1 \gg m_2$

The projectile much more massive than the target applies; for example, to protons incident on electrons. It is physically impossible for the projectile to backscatter. That is, there will be no scattering for $\theta_1 > \pi/2$. For $m_1 \gg m_2$, Eq. (1.6) becomes

$$\sin\theta_1 \approx 2\frac{m_2}{m_1}\sin\theta_2\cos\theta_2 = \frac{m_2}{m_1}\sin 2\theta_2.$$

θ_1 is a maximum when $\sin 2\theta_2 = 1$ ($\theta_2 = \pi/4$), giving

$$\theta_{1\,\text{max}} \approx \sin^{-1}\frac{m_2}{m_1}. \tag{1.8}$$

Since $m_1 \gg m_2$, the scattering angle of the projectile is very small. Intuitively it is expected that a massive particle colliding with a much lighter one will be deflected very little. Specifically, for a proton incident on an electron the maximum proton scattering angle is only $\theta_{1\,\text{max}} \approx \sin^{-1}(0.00054) = 0.03^\circ$. *When a proton or other massive particle is incident on an electron, the projectile travels in essentially a straight line and the electron scatters between 0° and 90°.*

1.1.3 Scattering angles: $m_1 = m_2$ and $m_1 \ll m_2$

Target and projectile of equal mass applies, for example, to electron–electron, proton–proton, and neutron–proton interactions. There can be no backscattering. In a head-on collision the projectile comes to rest and transfers all its energy to the target. With $m_1 = m_2$ Eq. (1.6) gives

$$\theta_1 + \theta_2 = \pi/2 \tag{1.9}$$

showing that equal masses scatter at 90° to each other.

The projectile much less massive than the target applies, for example, to protons incident on much heavier nuclei and for electrons incident on any nucleus including a single proton. With $m_1 \ll m_2$ Eq. (1.6) reduces to $\sin\theta_1 \approx 2\sin\theta_2\cos\theta_2$. For a head-on collision, $\theta_2 = 0$ and the physically meaningful value of θ_1 is $\theta_1 = \pi$, showing that the lighter projectile backscatters.

1.2 WAVES

A disturbance at a point generates a wave that propagates spherically from the source. A *wavefront* is a surface connecting points of waves of the same phase. For a point source the wavefronts are surfaces of spheres as illustrated in Fig. 1.2 where the fronts connect crests and troughs.

Far from the source the wavefronts are approximately planes. In a non-dissipative medium (no frictional forces) the waves propagate with constant amplitude. A description of a plane wave travelling in the +x direction could be

$$y = y_0 \sin(kx - \omega t), \tag{1.10}$$

where y_0 is the amplitude, $k = 2\pi/\lambda$ so that the wave repeats in a distance equal to the wavelength λ, and $\omega = 2\pi\nu = 2\pi/T$ so that the wave repeats after a time equal to the period $T = 1/\nu$ where ν is the frequency. The wave travels (propagates) a distance of one λ in a time T giving a propagation speed $v = \lambda/T = \lambda\nu$.

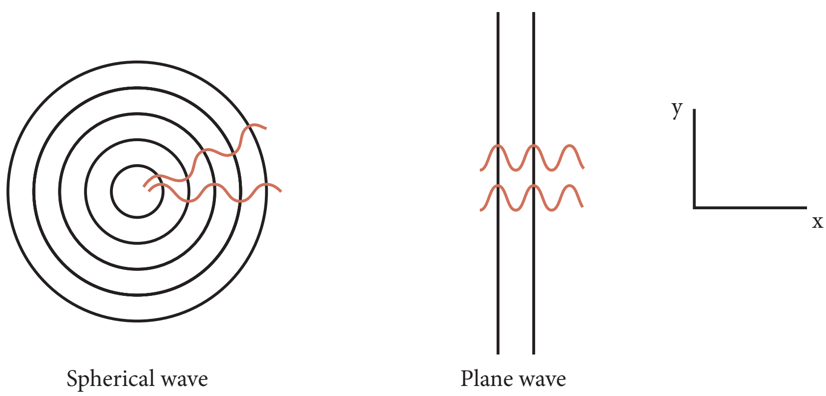


FIG. 1.2
Spherical wavefronts approaching plane wavefronts at large distance.

1.3 ELECTROMAGNETIC WAVES

The magnitude and direction of an electric field, $\boldsymbol{\mathcal{E}}$, is defined in terms of the force $\mathbf{F} = q\boldsymbol{\mathcal{E}}$ it produces on a charge. The units of $\mathcal{E}$ are N/C. The magnitude and direction of a magnetic field, $\boldsymbol{\mathcal{B}}$, are defined in terms of the force $\mathbf{F} = q(\mathbf{v} \times \boldsymbol{\mathcal{B}})$ it produces on a moving charge. The units of $\mathcal{B}$ are (N/C)/(m/s) which is defined to be a tesla, T. That is, 1 T = 1 N s/C m = 1 N/A m. An older unit of magnetic field is the gauss (G) with 1 T = 10^4 G.

The belief that electromagnetic radiation is a wave was supported by the work of Maxwell who reformulated the work of Gauss, Faraday, and Ampere to arrive at a set of equations for electrodynamics. Maxwell's equations in free space show that there is a class of waves composed of an alternating electric field and an alternating magnetic field that propagates in vacuum at speed $c = 2.9979 \times 10^8$ m/s ($\approx 3 \times 10^8$ m/s). Far from any source, the plane wave solutions for the electric and magnetic fields are

$$\boldsymbol{\mathcal{E}} = \mathcal{E}_0 \sin(kx - \omega t)\hat{1}_x \quad \text{and} \quad \boldsymbol{\mathcal{B}} = \mathcal{B}_0 \sin(kx - \omega t)\hat{1}_y \tag{1.11}$$

with the two fields perpendicular to each other and mutually perpendicular to the direction of propagation as depicted in Fig. 1.3.

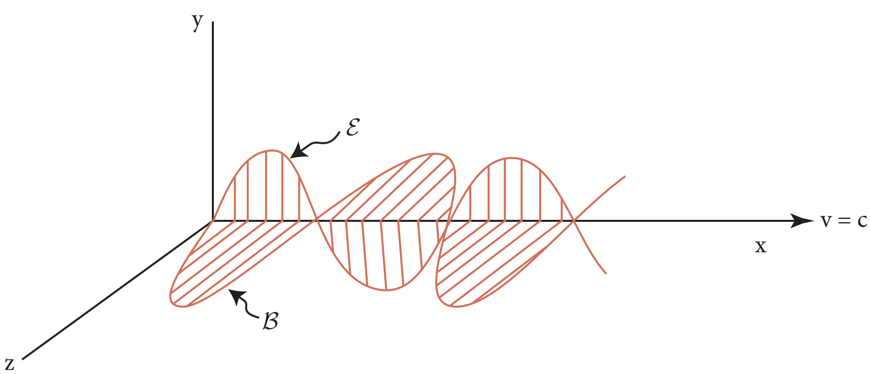


FIG. 1.3
Polarized plane electromagnetic wave.

The waves of Eq. (1.11) and Fig. 1.3 are linearly polarized. That is, the electric and magnetic fields oscillate in only one direction (y and z respectively). For the more general case of unpolarized waves the field vectors are at any orientation in the yz plane. From Maxwell's equations, the magnitudes of the fields are related by $\mathcal{E}_0 = c\mathcal{B}_0$ and the intensity (energy per unit area per unit time) of the wave is $I = \varepsilon_0 c\mathcal{E}_0^2/2$.

1.3.1 How electromagnetic radiation interacts with charged particles

In the wave theory, electromagnetic radiation interacts with charged particles through forces exerted by the electric and magnetic fields. Because the electric field is much greater than the magnetic field, interactions with charged particles are primarily via the electric field. Consider an electromagnetic wave incident on a particle of charge q and velocity **v**. The ratio of the magnetic force, $F_B = qv\mathcal{B}$, to the electric force, $F_E = q\mathcal{E}$, is

$$\frac{F_B}{F_E} = \frac{v\mathcal{B}_0}{\mathcal{E}_0} = \frac{v}{c},$$

showing that for non-relativistic particles, the magnetic force is much smaller than the electric force.

1.4 PHOTONS

When electromagnetic radiation is incident on matter electrons are sometimes liberated. This is called the photoelectric effect. The wave theory of light predicts that the effect should occur for any frequency of sufficient intensity. However, experiment showed that there is a cutoff frequency below which the photoelectric effect does not occur regardless of the light intensity.

To explain the photoelectric effect Einstein postulated that the energy of an electromagnetic wave is not continuously distributed in space but rather is transported as discrete packets, or quanta, called photons with each photon having energy

$$E = h\nu,$$

where ν is the light frequency. Planck's constant, $h = 6.6262 \times 10^{-34}$ J s, had already been determined from Planck's theory of blackbody radiation. The intensity of light is then determined by the number of photons. Einstein treated photons as particles to describe the photoelectric effect. When a photon strikes a metallic surface, conservation of energy gives the maximum kinetic energy of a photoelectron to be

$$T_{max} = h\nu - W,$$

where W is the energy required to free an electron from the surface. In this particle treatment there is a threshold energy and frequency. When $h\nu < W$ the effect cannot occur.

Einstein's resolution of the photoelectric effect introduced a wave–particle duality to electromagnetic radiation. Some interactions of electromagnetic radiation, such as diffraction, are explained by the wave theory. Other interactions, such as the photoelectric effect, can only be explained by the particle theory in which photons interact with matter as do particles by conservation of energy and momentum.

1.5 THE ELECTROMAGNETIC SPECTRUM

Electromagnetic waves can be of any frequency. Since $\lambda\nu = c$ is constant in vacuum, high-frequency waves have short wavelengths and low-frequency waves have long wavelengths. Electromagnetic radiation, therefore, covers a wide spectrum of wavelengths and energies. Photons of waves with very short wavelengths have correspondingly very high frequency and energy. These γ rays and x rays have more than enough energy to ionize atoms and to break molecular bonds. This part of the spectrum is therefore referred to as *ionizing radiation*. At the other end of the spectrum are waves with very long wavelengths and correspondingly very low frequency, such as microwaves and radio waves. Photons of these waves have energies orders of magnitude less than atomic binding energies. This part of the spectrum is therefore referred to as *non-ionizing radiation*.

1.6 ELECTRON VOLT

Compared to macroscopic particles the kinetic energy of atomic particles is very small. The unit of energy used on the atomic scale is the electron volt (eV).

Electric potential is measured in volts, V, where 1 V = 1 J/C. Potential difference, ΔV, is the difference between the potentials at two points as established, for example, by a battery. When a particle of charge q accelerates across a potential difference of ΔV it gains a kinetic energy $\Delta T = q\,\Delta V$. An electron volt is defined to be the energy gained by an electron accelerating across a potential difference of one volt. Here, $q = e$ and $\Delta V = 1$ V. Then,

$$\Delta T = q\Delta V = (1e)(1\ \text{V}) = 1\ \text{eV} = (1.6022 \times 10^{-19}\ \text{C})(1\ \text{V}) = 1.6022 \times 10^{-19}\ \text{J}.$$

The eV to joule conversion is therefore 1.6022×10^{-19} J/eV. So, for example, if an electron accelerates from rest across 100 kV its final kinetic energy is $T = 100\ \text{keV} = 1.6 \times 10^{-14}$ J.

1.7 SPECIAL RELATIVITY

An inertial frame of reference is a non-accelerating frame. Consider two inertial frames S and S' whose axes are parallel. Let S' have speed u relative to S in the common +x direction. The relation between the motion of an object in S to its motion as observed in S' is given by the Galilean transformation that relates x to x', etc. If an object of mass m moves in S with speed v in the +x direction then its speed as measured by an observer in S' is $v' = v - u$. The momentum of the object in S is $p = mv$ and in S' is $p' = m(v - u)$. Time is the same in all Galilean inertial frames. If a force **F** is applied to object in S then the force as observed in S' is $F' = dp'/dt = md(v - u)/dt = mdv/dt = dp/dt = F$. Force and change in momentum are the same in each frame. Therefore, if momentum is conserved in frame S it is also conserved as observed in S'. Similarly for conservation of energy.

The laws of mechanics, Newton's laws of motion, are the same in all inertial frames. Another way to say this is that the laws of mechanics are invariant under a Galilean transformation. For example, a person playing billiards on a ship observes conservation of momentum when two balls collide. An observer on the ground records different velocities for the balls but also sees momentum to be conserved.

All electromagnetic effects resulting from Maxwell's equations depend on the speed of light, c. But, with the Galilean transformation, if an electromagnetic wave is observed in frame S with speed c then an observer in S' sees the wave to be travelling at speed $c' = c - u$. Maxwell's equations and subsequent effects are then dependent on the frame of reference. That is, they are not invariant under a Galilean transformation.

The postulates of special relativity are: (1) the laws of physics are the same in all inertial frames; (2) the speed of light in free space, c, is the same in all inertial frames. The Galilean transformation is replaced by the Lorentz transformation which leads to distance and time being observer (frame) dependent. Maxwell's equations are invariant under the Lorentz transformation. Under this transformation an object moving in S with speed v in the +x direction has speed, as measured in S', of

$$v' = \frac{v - u}{1 - vu/c^2}. \tag{1.12}$$

Note that if $v \ll c$ this reduces to the Galilean result $v' = v - u$. Also note that if the object's speed is c in one frame it is c in all frames. That is, if $v = c$ then $v' = c$.

Special relativity retains the Newtonian definition of force as $\mathbf{F} = d\mathbf{p}/dt$. If the momentum of a particle is conserved in one inertial frame it should be conserved in all inertial frames. For this to be true, momentum has to be redefined as

$$\mathbf{p} = \gamma m \mathbf{v}, \tag{1.13}$$

where

$$\gamma = 1/\sqrt{1 - \beta^2} \quad \text{with } \beta = v/c. \tag{1.14}$$

In the non-relativistic limit of $\beta \ll 1$, $\gamma \approx 1$ and the relativistic momentum approaches the non-relativistic $p = mv$.

The change in kinetic energy of an object of mass m is the work done by an applied force. This is one way to arrive at an expression for the energy of a free object. For simplicity the derivation is given for one dimension. Then,

$$\Delta T = W = \int F dx = \int \frac{dp}{dt} dx = \int v dp.$$

Table 1.2
Rest energy of some particles.

Particle	$E_0 = mc^2$ (MeV)
Electron	0.511
Proton	938.3
Neutron	939.6
Photon	0

From Eq. (1.13), $dp = m(\gamma dv + v d\gamma)$. If the object started at rest its kinetic energy at speed v is

$$T = m\int_0^v v(\gamma dv + v d\gamma).$$

Substituting $dv = (c^2/v\gamma^3)d\gamma$ obtained from Eq. (1.14) the integral gives

$$T = \gamma mc^2 - mc^2. \tag{1.15}$$

The first term of this equation is velocity dependent. But the second term is a constant called the rest energy, E_0. It is the energy an object has just by virtue of having mass. This gives the famous equivalency of mass and energy

$$E_0 = mc^2. \tag{1.16}$$

The total energy of an object, E, is then

$$E = T + E_0 = \gamma mc^2 = \gamma E_0. \tag{1.17}$$

Rest energies are generally expressed in MeV as in Table 1.2.

When the energy of an object is given it is always the kinetic energy. Total energy is then kinetic plus rest energy. For example, a 3 MeV electron has a total energy of $E = T + E_0 = 3.511$ MeV.

The relation between kinetic energy and speed, obtained by rewriting Eq. (1.15), is

$$T = (\gamma - 1)E_0 = \left(\frac{1}{\sqrt{1-\beta^2}} - 1\right)E_0. \tag{1.18}$$

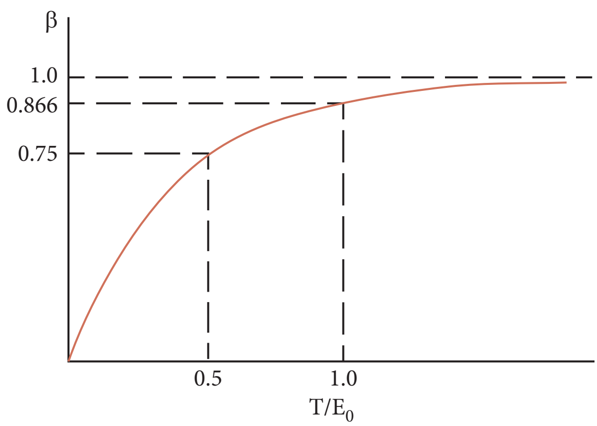


FIG. 1.4
β as a function of kinetic energy.

The speed of an object in vacuum cannot exceed c for as $v \rightarrow c$, $T \rightarrow \infty$, which means that an infinite amount of work would have to done. The relation between T and β is shown in Fig. 1.4.

For $T/E_0 > 1$, the speed is so close to the speed of light that further increases in kinetic energy do not increase speed appreciably. This corresponds approximately to $T > 0.5$ MeV for electrons and to $T > 938$ MeV for protons. A consequence of this is that interaction times do not vary much for energies $T > E_0$.

An expression for momentum is obtained by substituting (1.13) into (1.17) which gives $E = \gamma mc^2 = pc^2/v$. Then $p = Ev/c^2$ which, for *photons* ($v = c$), becomes

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}. \tag{1.19}$$

When can an object be treated as non-relativistic? The immediate answer to this is whenever $\beta \ll 1$. However, it is often more convenient to express this in terms of kinetic energy. When β is much less than 1, γ is slightly greater than 1 and $T = (\gamma - 1)E_0 \ll E_0$. Thus, an object is non-relativistic when $T \ll E_0$.

1.7.1 Relativistic elastic collisions of two particles

Conservation of relativistic energy and momentum can be applied as done for non-relativistic particles. The result gives the maximum energy lost, which occurs for a head-on collision, as

$$T_{\text{lost max}} = T_{2\text{max}} \begin{cases} \nearrow T \quad \text{for } m_1 = m_2 \\ \searrow \approx 2m_2c^2 \dfrac{\beta^2}{1-\beta^2} \quad \text{for } m_1 \gg m_2 \end{cases}. \tag{1.20}$$

1.8 RUTHERFORD–BOHR ATOMIC MODEL

By 1902 it was established that α-radiation emanating from uranium was actually a particle of positive charge. In 1911 Rutherford analyzed the results of experiments done by Geiger and Marsden for the scattering of α-particles incident on a thin gold foil with the intent of gaining insight into the nature of atoms. Some α-particles reversed direction. Rutherford concluded that these must have encountered a massive object and experienced a large force. He proposed that an atom consists of a small nucleus containing all the positive charge and virtually all the mass. The much lighter electrons he postulated are distributed around this nucleus. When an α-particle is incident on an atom its path is unaffected by the much lighter electrons. But the repulsive Coulomb force exerted by the nuclear charge causes a change in direction (scatter). Rutherford calculated the fraction of α-particles that should be scattered in particular angular directions. The results of the experiment were in agreement with this calculation, leading to acceptance of Rutherford’s model.

With the discovery of the neutron by Chadwick in 1939 came the realization that nuclei contain both protons and neutrons which are collectively referred to as nucleons. Nuclei are characterized by an atomic number Z which is the number of protons and by a mass number A which is the total number of nucleons. Since atoms are electrically neutral, Z is also the number of electrons distributed around the nucleus. Symbolically, an atom is described as ${}^{A}_{Z}X$ where X is the chemical symbol. Different masses of an element, called *isotopes*, exist in nature. Isotopes of an element have the same Z but different A due to a different number of neutrons. For example, two stable isotopes of hydrogen are found in nature, ${}^1_1H$(hydrogen) and ${}^2_1H$(deuterium), with abundances of about 99.985% and 0.015% respectively.

1.8.1 Electron distribution in atoms: Bohr's model

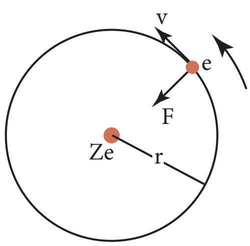


FIG. 1.5
Bohr's model of one electron in circular orbit around Z protons.

The nature of the distribution of atomic electrons was proposed by Bohr as a planetary model in which the electrons orbit the nucleus. The Coulomb force of attraction on each electron toward the nucleus keeps the electrons in their orbits. The simplest orbital shape, and the first proposed by Bohr, is a circle. Consider *hydrogen-like atoms* of *one* electron in circular orbit around a nucleus of Z protons as in Fig. 1.5.

A relation between v and r is obtained from Coulomb's force and centripetal acceleration:

$$F = \frac{kZe^2}{r^2} = m_e a = m_e \frac{v^2}{r},$$

from which

$$v^2 = \frac{kZe^2}{m_e r}. \qquad (1.21)$$

The total energy of the electron is

$$E = \frac{1}{2} m_e v^2 - k\frac{Ze^2}{r},$$

where the negative term is the potential energy. Substituting (1.21) gives

$$E = -\frac{1}{2} k \frac{Ze^2}{r}. \qquad (1.22)$$

The negative energy simply means that the electron is bound. To free it requires an input of the same magnitude energy.

Since the electron is accelerating it should, according to classical electromagnetic theory, radiate energy. The electron would quickly radiate away all its energy and the atom would collapse. A stable atom as proposed by Rutherford would be impossible. To circumvent this Bohr proposed that atomic electrons exist in certain allowed and stable orbits and that while in these orbits no radiation occurs. In a circular orbit the electron has angular momentum $L = rp$. This has the same units as Planck's constant, namely J s. Bohr proposed that angular momentum is quantized (that is, can take on only certain discrete values) according to the rule $L = n\hbar$ where n is any positive integer and $\hbar = h/2\pi$. Therefore, for a circular orbit of radius r,

$$L = rp = m_e v r = n\hbar, \qquad (1.23)$$

from which $v = n\hbar/m_e r$. Substituting this into (1.21) gives the allowed orbital radii, which, on substituting into (1.22), gives the corresponding quantized energy levels of hydrogen-like atoms. The results are

$$r_n = \frac{\hbar^2}{ke^2 m_e}\frac{n^2}{Z} \quad \text{and} \quad E_n = -\frac{k^2 e^4 m_e}{2\hbar^2}\frac{Z^2}{n^2}, \tag{1.24}$$

where $n = 1, 2, 3, \ldots$. Substituting values for the constants and converting to eV gives:

$$r_n = a_0 \frac{n^2}{Z} \quad \text{and} \quad E_n = -13.6\frac{Z^2}{n^2} \text{ eV}, \tag{1.25}$$

where $a_0 = \hbar^2/m_e ke^2 = 0.53 \times 10^{-8}$ cm is called the *Bohr radius*.

Substituting the first of Eqs. (1.25) into (1.21) gives the speed of the electron, which can be written as

$$\beta_n = \frac{v_n}{c} = 0.0073\frac{Z}{n}. \tag{1.26}$$

The lowest energy state, or ground state, of hydrogen is for $n = 1$, which is called the K-shell. Successively higher energy states are called the L-shell, M-shell, N-shell, etc. Absorption of energy by a H atom can result in excitation to a higher energy state or to ionization (ejection of an electron). The absolute value of E_n is called the binding energy, BE_n, or ionization energy, I_n, of shell n. That is, $I_n = BE_n = |E_n|$.

In the Bohr model the ground state of H is one electron in the K-shell ($n = 1$) around one proton ($Z = 1$). The K-shell has a binding or ionization energy of 13.6 eV, an orbital radius of $r = a_0 = 0.53 \times 10^{-8}$ cm. The dimension of a H atom is two Bohr radii or about 10^{-8} cm. The electron has an orbital speed of 0.0073c and period $T = 2\pi r/v = 1.52 \times 10^{-16}$ s. The first excited state ($n = 2$) has a binding energy $BE_2 = 3.4$ eV. To be excited to this level the atom must absorb 13.6 eV − 3.4 eV = 10.2 eV.

1.9 PARTICLES AS WAVES

In 1924 de Broglie extended the wave–particle duality of electromagnetic radiation proposed by Einstein by postulating that particles at times exhibit properties of waves of length:

$$\lambda = \frac{h}{p}. \tag{1.27}$$

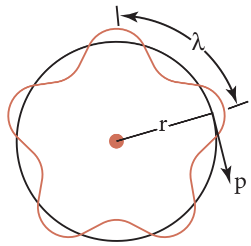


FIG. 1.6
An electron as a wave in an atomic orbit of radius r.

This is the same relation between wavelength and momentum for photons given in Eq. (1.19).

Bohr's quantization of angular momentum is derivable from the de Broglie wavelength. Consider an electron of momentum p in a circular orbit of radius r. Only those standing waves are allowed for which the circumference of the orbit is a multiple of a wavelength as illustrated Fig. 1.6.

Then, $2\pi r = n\lambda = nh/p$. This gives $pr = L = n\hbar$ which is Bohr's quantization rule in Eq. (1.23). Thus, the de Broglie hypothesis leads to Bohr's quantized orbits.

1.10 QUANTUM THEORY: SCHRÖDINGER EQUATION

The form of quantum theory most commonly used was developed by Erwin Schrödinger in 1925. The success of de Broglie in obtaining quantized atomic orbits by treating an electron as a wave prompted the search for a wave theory of particles. The equation arrived at by Schrödinger cannot be derived from first principles but various justifications have been offered.

The non-relativistic *Schrödinger equation* for stationary states of a particle in a force field in which the potential energy is U is

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - U)\psi = 0, \tag{1.28}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{1.29}$$

and Ψ, called a *wave function*, is a mathematical description of the particle.

1.10.1 Interpretation of Ψ

Unlike the electric field in the electromagnetic wave equation or the displacement of a medium in the physical wave equation, the wave function has no measurable property. But Ψ has information about the energy and spatial distribution of a particle. The meaning of Ψ, proposed by Born, is that $|\Psi|^2$ is a probability density. That is, it is the probability, dP, of finding a particle per unit volume, dV. The absolute value is used because Ψ can have an imaginary component. So, according to this:

$$\frac{dP}{dV} = \left|\Psi^2\right| = \Psi\Psi^*,$$

where Ψ^* is the complex conjugate of Ψ. Solutions to Schrödinger's equation must satisfy the *normalization condition*:

$$\int_{-\infty}^{\infty} dP = \int_{-\infty}^{\infty} \Psi\Psi^* dV = 1,$$

which simply says that the probability of finding the particle somewhere is 100%.

1.10.2 Hydrogen-like atoms

The potential energy of an electron in the field of Z protons of a nucleus is

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

Because of the spherical symmetry of the potential energy Schrödinger's equation is best solved in spherical coordinates. Expressing x, y, and z in terms of the spherical coordinates r, θ, and ϕ, Eqs. (1.28) and (1.29) become

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2m_e}{\hbar^2}\left(\frac{kZe^2}{r} + E\right)\psi = 0. \tag{1.30}$$

The solution to this equation can be found in any text on quantum theory and is only outlined here. The equation can be solved by separation of variables. That is, let Ψ be the product of a function of r, a function of θ and a function of ϕ as

$$\psi = R(r)\Theta(\theta)\Phi(\phi).$$

Substituting this into (1.30) leads to the three ordinary differential equations, one for r, one for θ, and one for ϕ. The equation for r has solutions only for specific values of energy in agreement with Bohr's quantized energy levels:

$$E_n = -\frac{k^2e^4m_e}{2\hbar^2}\frac{Z^2}{n^2}, \tag{1.31}$$

where n, called the *principal quantum number*, is any positive integer. As in the Bohr model, an atomic shell is defined by n. For example, $n = 1$ is the K-shell.

The equations for θ and ϕ have solutions only for specific (quantized) values orbital angular momentum, **L**, and quantized values of its projection, L_z, along the direction of an applied magnetic field. The magnitude of the angular moment is $L = \sqrt{\ell(\ell+1)}\hbar$ where $\ell = 0, 1, 2, 3, \ldots, (n-1)$ is called the *orbital angular momentum quantum number*. Note the difference between the quantization of angular momentum from Schrödinger's equation and that proposed by Bohr. Each ℓ of a principal quantum number is a *sub-shell*. So each n has n sub-shells. For example, the L-shell ($n = 2$) has two sub-shells, namely $\ell = 0$ and $\ell = 1$. The quantized projections of **L** along an applied magnetic field are $L_z = m_\ell\hbar$ where m_ℓ, called the *magnetic quantum number*, can have values $m_\ell = -\ell, -\ell+1, \ldots, 1, \ldots, (\ell-1), \ell$. The values of ℓ are given letter designations of s, p, d, f for $\ell = 0, 1, 2, 3$, respectively.

In summary, the three atomic quantum numbers satisfy the restrictions

$$n = 1, 2, 3, \ldots,$$

$$\ell = 0(s), 1(p), 2(d), 3(f), \ldots, (n-1),$$

$$m_\ell = -\ell, \ -\ell+1, \ldots, 0, \ldots, (\ell-1), \ell.$$

1.10.3 Ground state of hydrogen

Wave functions for quantized states of atoms are symbolized by Ψ_{nlm}. The solution to Schrödinger's equation for the ground state of H ($Z=1$, $n=1$, $\ell=0$, $m_\ell=0$) is

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\frac{1}{a_0^{3/2}} e^{-r/a_0},$$

and the probability of finding the electron in a volume element dV is

$$\frac{dP}{dV} = |\Psi^2| = |\psi_{100}^2| = \frac{1}{\pi}\frac{1}{a_0^3} e^{-2r/a_0}.$$

Note that the wave function and probability density are spherically symmetric. There is equal probability of finding the K-shell electron at any θ and ϕ. Since $dV = r^2\, dr \sin\theta\, d\theta d\phi$, integration over the angles gives 4π and the radial probability density is

$$\frac{dP}{dr} = 4r^2 \frac{1}{a_0^3} e^{-2r/a_0},$$

which has a maximum value at $r = a_0$. Thus, the electron is most likely to be found at a radius of a_0 which is the Bohr radius of the ground state of hydrogen.

1.11 INTRINSIC ANGULAR MOMENTUM: SPIN

Atoms in excited states quickly return to the ground state with the emission of energy frequently in the form of light. For example, if the electron of hydrogen is excited to the L-shell it quickly makes a transition back to the K-shell. The electron becomes more bound and loses energy equal to the difference in the shell binding energies of 13.6 eV − 3.4 eV = 10.2 eV which is given to a photon. This ultraviolet spectral line is actually split in two lines very close in energy. This is called *fine structure*. An orbiting electron is a current and a current sets up a magnetic field. This orbital magnetic field interacts other magnetic fields altering the energy of shells. To explain the observed split it was postulated that an electron has an intrinsic magnetic field produced by an angular momentum called spin, S, that has only two possible orientations to the orbital magnetic field. Mimicking the orbital angular momentum, the spin angular momentum is $S = \sqrt{s(s+1)}$ and $S_z = m_s\hbar$ with

$m_s = s, s+1, \ldots, 0, \ldots, s$. For there to be only two values of m_s it must be that $s = 1/2$. Then, $m_s = -1/2, 1/2$. There are, therefore, four quantum numbers to completely describe atomic states, namely, n, ℓ, m_ℓ, and m_s.

1.12 PAULI EXCLUSION PRINCIPLE

Each shell n of an atom has n^2 sub-shells. For example, shell $n = 2$ has four sub-shells, one with $\ell = 0 (m_\ell = 0)$ and three with $\ell = 1 (m_\ell = -1, 0, 1)$. To explain the chemical properties of atoms and the structure of the Periodic Table, Pauli proposed that no two electrons can have the same set of the four quantum numbers n, ℓ, m_ℓ, and m_s. Since m_s has two values, each sub-shell of n can have two electrons and the maximum possible number of electrons that can be in a shell n is $2n^2$. The K-shell ($n = 1$) can hold a maximum of 2 electrons, the L-shell ($n = 2$) can hold a maximum of 8, etc.

The ground state of an atom is the most tightly bound configuration in which all electrons are in their lowest allowed energy shells. The description of the ground state of some elements is given in Table 1.3.

The electronic configuration of atoms arrived at from quantum theory explains many features of the Periodic Table. Columns of the table, called groups, list atoms that have similar chemical behavior. The combination of atoms to form molecules is controlled by the outermost, or valence, electrons. For example, two atoms can share valence electrons to form a covalent bond or a valence electron can be transferred from one atom to another to form an ionic bond. Hydrogen, lithium, and sodium are three atoms listed in group 1 of the Periodic Table. As seen in Table 1.3, the configuration of lithium and sodium is one valence electron outside a filled inner shell which explains their chemical similarity to hydrogen. All elements in group 1 have one valence electron; all elements in group 2 have two valence electrons; etc.

Table 1.3
Ground state configuration of some atoms.

Element	Symbol	Z	Ground state
Hydrogen	H	1	1s
Helium	He	2	$1s^2$
Lithium	Li	3	$1s^2 2s$
Carbon	C	6	$1s^2 2s^2 2p^2$
Sodium	Na	11	$1s^2 2s^2 2p^6 3s$

where, for example, $2p^6$ means six electrons in the 2p ($n = 2$, $\ell = 1$) sub-shell.

1.13 MULTI-ELECTRON ATOMS

In multi-electron atoms the repulsive force on an electron from other electrons counteracts the attractive force of the nucleus thereby reducing the binding energy of a shell from the value given for hydrogen-like atoms. This can be thought of as a shielding (or screening) effect. That is, each electron partially shields other electrons from the full positive charge of the nucleus. Consider, for example, the hydrogen-like atom of one electron in the K-shell around the 82 protons of lead. Equation (1.25) gives the binding energy to be $13.6(82)^2$ eV = 91.4 keV and the orbit radius to be $a_0/82$. The actual binding energy of a K-shell electron of lead is about 88 keV. The effective nuclear charge experienced by this electron, obtained by substituting the actual binding energy into the second of equations (1.25), is $Z_{eff} \approx 80.4$ and the corresponding orbital radius is $a_0/80.4$.

In a single-electron atom the energy of shells is independent of the angular momentum quantum number ℓ. This is not the case for multi-electron atoms. Solutions to hydrogen-like atoms show that for electrons in the same shell those with smaller angular momentum are more likely to be found closer to the nucleus than those with larger angular momentum and are, therefore, more tightly bound.

1.14 RELATIVE ATOMIC MASS

Well before anything was known about atomic structure, atoms were accepted as the fundamental units of matter. A table of *relative atomic mass*, A_r was established based on how elements combined. For example, 0.6485 g of Na combines with 1 g of Cl to form NaCl with no sodium or chlorine left over. This means that every atom of Na and Cl combined. So, 0.6485 g of Na has the same number of atoms as 1 g of Cl. Therefore, the relative atomic mass of Na to Cl is 0.6485. From chemical combinations of other elements, the relative atomic mass of the known elements was established. ^{12}C, which is assigned $A_r = 12$, is taken as the reference for the relative masses. Table 1.4 gives the relative atomic masses of some elements. A sample of any element contains the various stable isotopes of that element and the resulting relative mass is the abundance weighted average of the relative masses of the isotopes.

Table 1.4
Relative atomic masses of some elements.

Element	Symbol	Z	A_r
Hydrogen	H	1	1.008
Helium	He	2	4.003
Boron	B	5	10.81
Carbon-12	^{12}C	6	12.00
Carbon	C	6	12.01
Sodium	Na	11	22.99
Chlorine	Cl	17	35.45
Cobalt	Co	27	58.93

Note that, as stated above, the relative atomic mass of Na to Cl is 22.99/35.45 = 0.6485.

1.15 AVOGADRO'S NUMBER AND ATOMIC MASS

The quantity mole is defined to be a gram atomic (or molecular) weight. That is, a mole is the mass in grams numerically equal to A_r. Thus, 1 mol of ^{12}C is 12 g of ^{12}C. A mole of anything contains as many objects as a mole of anything else. For example, 4 g of an element $A_r = 4$ contains as many atoms as 2 g of an element of $A_r = 2$ since both the mass and relative mass (per atom) are doubled. The number of atoms in a mole is called Avogadro's number, N_A, whose currently accepted value is $N_A = 6.022140857 \times 10^{23}\ mol^{-1}$. The mass of a ^{12}C atom can be determined from Avogadro's number. Since 1 mol of ^{12}C contains N_A atoms and has a mass of 12 g,

$$1\ mol_{^{12}C} = 12\ g = N_A m_{^{12}C},$$

giving

$$m_{^{12}C} = \frac{12\ g}{6.022140857 \times 10^{23}} = 1.99264685 \times 10^{-23}\ g.$$

The mass of any atom can be obtained from its relative mass and the mass of ^{12}C.

The mass of ^{12}C is less than the sum of the masses of its six neutrons, six protons, and six electrons, which adds up to 2.0096×10^{-23} g. This is called a *mass defect*. When free protons and neutrons combine to form a nucleus they become more tightly bound and energy is liberated. This binding energy of the nucleus originates from a conversion of mass into energy according to $E_0 = mc^2$. Consequently, the mass of a nucleus is less than the sum of the masses of its individual nucleons. Only ^1H has no mass defect. As a result of mass defect, relative atomic masses of atoms are not whole numbers.

Atomic masses are given in terms of the *unified mass unit*, u, which is defined to be 1/12 the mass of a ^{12}C atom. Therefore,

$$1\ u = m_{^{12}C}/12 = 0.1660539 \times 10^{-23}\ g.$$

Due to the mass defect, 1 u is somewhat less than the mass of a nucleon. Therefore, the mass of ^1H is greater than 1 u. By definition, the mass of ^{12}C is 12 u. Since ^1H has no mass defect, its mass can be calculated from the mass a proton and an electron as

$$m_{^1H} = m_p + m_e = 0.1673533 \times 10^{-23}\ g = 1.0078\ u.$$

A more convenient definition of u is 1/12 the rest energy of ^{12}C. Then, $1\ u = m_{^{12}C}c^2/12 \approx 931.5$ MeV. Table 1.5 gives the atomic mass and rest energy of some isotopes.

The atomic mass of an element can be obtained from the abundances of its isotopes. For example, hydrogen has two stable isotopes, ^1H and ^2H, with abundances of about 0.99985 and 0.00015 respectively. The atomic mass of H is then $1.0078(0.99985) + 2.0141(0.00015) = 1.008$ u.

Table 1.5
Atomic mass and rest energy of some isotopes.

Element	Isotope	Z	A	Rest mass/energy (u)[a]
Hydrogen (deuterium)	$^{1}_{1}H$	1	1	1.0078
	$^{2}_{1}H$	1	2	2.0141
Helium	$^{4}_{2}He$	2	4	4.0026
	$^{5}_{2}He$	2	5	5.0121
Boron	$^{10}_{5}B$	5	10	10.0129
	$^{11}_{5}B$	5	11	11.0093
Carbon	$^{12}_{6}C$	6	12	12.0000
	$^{13}_{6}C$	6	13	13.0034
Cobalt	$^{59}_{27}Co$	27	59	58.9332
	$^{60}_{27}Co$	27	60	59.9338

[a] For mass: $1\ u = 0.1660539 \times 10^{-23}$ g; for energy: $1\ u = 931.5$ MeV.

1.16 ATOMIC DIMENSIONS

The size of all atoms is approximately of the order 10^{-8} cm which is the dimension of the ground state of hydrogen as given by Bohr's model. This is because in higher Z atoms K-shell electrons are more tightly bound and have radii less than a_0. Inner shell electrons partially shield outer ones from the full nuclear charge. So, for example, the single L-shell electron of lithium is closer to experiencing the force of one proton than the full nuclear charge of three protons and therefore has a radius approximately that of H.

1.17 NUCLEAR DIMENSIONS AND THE NUCLEAR FORCE

With the acceptance that the nucleus contains all the positive charge of an atom it was realized that there must exist a hitherto unknown force. The repulsive Coulomb force between protons would make nuclei unstable and the Rutherford nucleus would not exist. To counter this repulsion there must be a strongly attractive force exerted between protons. It was later recognized that this nuclear force is exerted between all nucleons (protons and neutrons).

It is possible to estimate the range of the nuclear force and the size of a nucleus from scattering experiments. For example, in the scattering of 5.5 MeV α-particles by gold analyzed by Rutherford the Coulomb force correctly predicts the scattering pattern. Therefore, it must be that α-particles did not make contact with the nucleus; otherwise the scattering would be affected by the nuclear force. Direct backscatter occurs in a head-on collision. As the α-particle approaches the nucleus it slows down due to the repulsive force. At the turning point, which is the minimum separation, the kinetic energy is zero and the total energy is the potential energy $kZ_1Z_2e^2/r$ where Z_1e and Z_2e are the charges of the α-particle and nucleus. Equating this with the initial 5.5 MeV and setting $Z_1 = 2$ and $Z_2 = 79$ for the α-particle and gold gives the minimum separation of $r = 4 \times 10^{-12}$ cm. Since there was no contact, this is an overestimate of the size of the nucleus and the range of the nuclear force. To get a more accurate estimate requires a closer distance of approach using either higher energy α-particles or lower Z nuclei. Such experiments give the nuclear size and range of the nuclear force to be approximately

$$r = 1.2 \times 10^{-13}\ A^{1/3}\ \text{cm}. \tag{1.32}$$

Nuclear sizes are approximately 10^4 to 10^5 times smaller than atomic sizes.

Nuclei, like atoms, have energy levels with spacing in the order of MeV. When a nucleus in an excited state makes a transition to a lower state, the decrease in energy appears as an energetic photon called a γ ray.

1.18 NUMBER OF ELECTRONS AND ATOMS PER GRAM

When radiation enters matter it can interact with atomic electrons and nuclei. It is therefore informative to know the number of such targets per cc or the number of targets per gram. One mole of an element of relative mass A_r has mass A_r grams and N_A atoms. Therefore,

$$\#\text{at/g} = \frac{\#\text{at/mol}}{\text{g/mol}} = \frac{N_A}{A_r}.$$

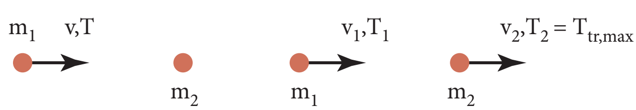
Multiplying this by Z electrons per atom gives

$$\#\text{e/g} = N_A Z/A_r.$$

For H $A_r \approx A = 1 = Z$ and the number of electrons per gram is $\approx N_A$. For all other elements $A_r \approx A \approx 2Z$ and the number of electrons per gram is $\approx N_A/2$. Thus, except for H, all elements have approximately the same number of electrons per gram. This will be a very useful result. To be more exact, elements of $Z > 20$ have $A_r > 2Z$ because they have more neutrons than protons in their nuclei. Therefore, for $Z > 20$ the number of electrons per gram is somewhat less than $N_A/2$.

PROBLEMS

1. Maximum energy lost by particles occurs in a head-on elastic collision.



A projectile of mass m_1, velocity v, and kinetic energy T makes a head-on elastic collision with a target particle of mass m_2 initially at rest. Note that there are no angles involved. Apply conservation of kinetic energy and momentum for this one-dimensional motion to show that after collision:

a. the kinetic energy lost to the target is $T_{max\ lost} = 4T\ m_1 m_2/(m_1 + m_2)^2$
b. in the case where target mass ≫ projectile mass, $T_{max\ lost} \approx 4T\ m_1/m_2$
c. in the case where projectile mass ≫ target mass, $T_{max\ lost} \approx 4T\ m_2/m_1$
d. if $m_1 = m_2$, $T_{max\ lost} = T$

2. Nuclear mass is approximately Am_p where A is the mass number (number of neutrons + protons) and m_p is the mass of a proton. In a head-on collision a proton loses (or transfers) more energy to a heavy nucleus than to an electron. Use the results of problem 3 above to show that in a head-on collision a proton loses about:
   a. 0.2% of its energy to an electron
   b. 5% of its energy to a nucleus of A = 80

3. Electrons start from rest from the heated filament (metal coil) of an electron gun, accelerate across a potential difference of 100 kV and emerge from a hole in the anode as a beam.
   a. What is the energy of electrons in the beam? (Ans. 100 keV)
   b. What is the speed of electrons in the beam in terms of c using relativistic physics? (Ans. 0.548c)

4. a. What are the energies of the K-, L-, M-shells of hydrogen? (Ans. −13.6, −3.4, −1.5 eV)
   b. What are the radii of these shells in terms of a_0 and cm? (Ans. a_0, $4a_0$, $9a_0$)
   c. What is the binding energy of the ground state of hydrogen? (Ans. 13.6 eV)
   d. Electrons from an electron gun excite some atoms in a H gas to the L-shell. How much energy is absorbed by the atoms? This is the first excitation. (Ans. 10.2 eV)

5. For the electron in the ground state of hydrogen:
   a. what is the orbital time? (Ans. 1.52×10^{-16} s)
   b. what is the orbital frequency? (Ans. 6.6×10^{15} rev/s)
   c. how many orbits are made in 10^{-8} s? (the answer is in millions)

6. The atomic number of lead is 82 and its K-shell binding energy is 88 keV.
   a. What is the effective nuclear charge felt by a K electron of lead? (Ans. 80.4)
   b. What is the orbital time of a K electron of lead? (2.4×10^{-20} s)

7. For Al: $Z = 13$, $A \approx 27$, $\rho = 2.7$ g/cc:
   a. use Avogadro's number to show that aluminum has 2.23×10^{22} at/g
   b. show that aluminum has 2.9×10^{23} e/g
   c. show that aluminum has 6.02×10^{22} at/cc.