6. QUANTUM PHYSICS

The repeated contradictions between classical laws and experimental results concerning black-body radiation, stability of atoms, atomic spectra and wave-particle duality gave birth to modern quantum physics.

6.1 BLACK-BODY RADIATION

A body that would absorb all the radiation falling on it is called a black body. In 1890 there existed two theoretical laws describing the distribution of the intensity of radiation of a black body versus wavelength. These laws were based on classical ideas but neither of them was in accord with experimental findings. A law which fitted the experimental data nicely was proposed by **Planck**:

$$I(\lambda, T) = \frac{2\pi hc^2}{\lambda^5\left(e^{\frac{hc}{\lambda kT}} - 1\right)}$$

where $I(\lambda, T)$ is radiation intensity as a function of wavelength λ at temperature T, k is Boltzmann's constant, c is the speed of light and h is Planck's constant

$$h = 6.626 \times 10^{-34}\ J.s$$

Planck assumed that the atoms that make up a black body behave like electromagnetic oscillators that can have energies given by the formula

$$E = nhf$$

where f is the oscillator frequency and n is a quantum number. The oscillators do not emit energy continuously but only in **quanta**

$$\Delta E = \Delta nhf.$$

A graph of the intensity of radiation from the black body versus wavelength is a smooth curve falling to zero for long as well as for short wavelengths, and with a maximum at a wavelength λ_{max} which depends on temperature T. This dependence is expressed by **Wien's displacement law**, or

$$\lambda_{\max} T = c_0$$

where constant $c_0 = 2.898x10^{-3}\ m.K.$

The total energy emitted per unit of time per unit of area from a black body at temperature T is called the radiancy R_T. **Stefan's law** expresses the fact that radiancy R_T increases rapidly with the increasing temperature T, or

$$R_T = \sigma T^4$$

where $\sigma = 5.67x10^{-8}\ W.m^{-2}K^{-4}$ is called the Stefan-Boltzmann constant.

Problem 6-1. Assuming that the intensity of radiation from the sun has its maximum for the wavelength $\lambda_{max} = 5.1x\,10^{-7}\ m$ at particular temperature T and the sun's surface behaves like a black body, estimate the surface temperature of the sun. Determine the power radiated from $1\ m^2$ of the surface of the sun.

Solution: To determine the surface temperature T of the sun we use Wien's displacement law:

$$\lambda_{max} T = c_0$$

Thus we obtain

$$T = \frac{2.898x\,10^{-3}}{5.1x\,10^{-7}} = 5700\ K$$

The power radiated from $1\ m^2$ of the surface of the sun can be determined using Stefan's law and the temperature which we have just obtained, or

$$R_T = \sigma T^4 = 5.67x\,10^{-8}\,x\,(5700)^4 = 5.9x\,10^7\ W.m^{-2}$$

Problem 6-2. Temperature T of a metallic wire of a light bulb is $2500\ K$, and diameter d of the wire is $0.1\ mm$. Calculate the current I through the wire, supposing that the wire radiates energy like a black body. Losses of heat due to conduction can be disregarded. The resistivity of the wire material is $\rho = 2.5x\,10^{-4}\ \Omega.cm$.

Solution: Since the wire radiates energy like a black body, the energy radiated from $1\ m^2$ per one second can be determined from Stefan's law, or

$$R_T = \sigma T^4$$

The total energy irradiated by a wire of surface S per 1 second is

$$W = R_T\,S = \sigma\ T^4 \pi\ d\ l$$

where l is the length of the wire. To keep the temperature of the wire constant, the loss of energy per one second caused by radiation of the wire must be equal to the amount of energy produced by Joule's heating, or

$$W = RI^2$$

Thus we have

$$RI^2 = \sigma\ T^4 \pi\ d\ l$$

The resistance of a wire of diameter d is

$$R = \rho \frac{l}{\pi \frac{d^2}{4}}$$

Substituting for R into the equation for the balance of energies we obtain for current

$$I = \frac{\pi\ d\,T^2}{2}\sqrt{\frac{\sigma\ d}{\rho}}$$

Finally we have numerically for current:

$$I = \frac{\pi\ 10^{-4}(2500)^2}{2}\sqrt{\frac{5.7x10^{-8}.10^{-4}}{2.5x10^{-6}}} = 1.47A$$

Problem 6-3. The average rate of solar radiation incident per unit area on the earth is *1355 W/m²* . The distance between the earth and the sun is $d=149.5x10^6$ *km,* and the radius of the sun is *R=695 550 km.* Estimate the surface temperature of the sun, assuming that the sun's surface behaves like a black body.

$$[T \cong 5700\ K]$$

Problem 6-4. Determine the rate of energy radiation from a human body of area *1.8 m²* and temperature *31 ℃.* Explain why people do not glow in the dark.

$$[P = 872\,W]$$

Problem 6-5. Sensitive infrared detectors allow anti-aircraft missiles to respond to the low-intensity radiation emitted by the target aircraft's airframe and not to the hot exhaust. This makes attack from any angle feasible. To what wavelength should a missile seeker be most sensitive, if the target temperature is *17 ℃.* Disregard atmospheric absorption.

$$[\lambda = 9.99\ \mu\, m]$$

6.2 STABILITY OF ATOMS - ATOMIC SPECTRA

According to classical physics, atoms are not stable particles. Furthermore, the continuous spectrum of the radiation that would be emitted following classical physics considerations is not in agreement with the discrete spectrum which is known to be emitted by atoms The problem of stability of atoms and their spectra led to the simple model of atomic structure proposed by Niels Bohr. This model is based on the following postulates:

1. Atoms can exist only in certain **stationary** states of discrete energies. When in such a state the atom is stable and emits no radiation.
2. Stationary states are those for which the 2π multiple of the electron's angular momentum is **quantized** as

$$2\pi\ mvr_n = nh$$

   where m is mass of electron, v is its velocity, r_n is radius of the *n-th* orbit, n is a principal quantum number and h is Planck's constant.
3. The radiation emitted by the atom is produced when the electron undergoes a **transition** from a higher-energy stationary state W_m to a lower-energy state W_n. The frequency f of the emitted photon is given by the equation

$$W_m - W_n = hf$$

Using Bohr's postulates, the expression for the total energy of an atomic electron moving in the orbit described by the principal quantum number n is

$$W_n = -\left(\frac{Z^2 e^4 m}{8\varepsilon_0^2 h^2}\right)\frac{1}{n^2}$$

where Z is the number proportional to the charge Ze of the nucleus (for a neutral hydrogen atom $Z=1$, for a helium atom $Z=2$ etc.), e is a charge of an electron and ε_0 is a permittivity of a free space.
The quantum number n that labels the orbit radii also labels the energy levels. The lowest energy level or energy state, characterised by $n=1$, is called the **ground state**. Higher states with $n>1$ are called **excited states**.
The energy required to remove the electron from the ground state to a state of zero total energy is called **ionisation energy** The energy of the hydrogen atom in its ground state is -13.6 eV. The negative sign indicates that the electron is bound to the nucleus and that the energy 13.6 eV must be provided from outside to remove the electron from the atom, or to **ionise** the atom. Hence 13.6 eV is the ionisation energy for atomic hydrogen.
Frequencies of the spectral lines emitted by hydrogen atoms is given by the expression

$$f = \frac{me^4}{8\varepsilon_0 h^3}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

Problem 6-6. Calculate the radius of the first circular orbit and velocity of an electron on this orbit in Bohr's model of a hydrogen atom. The permittivity of a free space $\varepsilon_0 = 8.85\ x\, 10^{-12}\ F.m^{-1}$, charge of electron $e = 1.602\ x\, 10^{-19}\ C$, mass of electron $m_e = 9.1\ x\, 10^{-31}\ kg$ and Planck's constant $h = 6.626\ x\, 10^{-34}\ J.s.$

Solution. The motion of an electron around a proton represents a central motion. In this case the centripetal force needed to hold the electron in an *n-th* circular orbit is balanced by Coulomb's force, or

$$m_e \frac{v^2}{r_n} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_n^2}$$

where n is a quantum number.
From Bohr's second postulate for stationary states $2\pi\, m v r_n = nh$ we can express the velocity of an electron. Substituting for velocity into the expression for balance of forces we obtain for the radius of the *n-th* quantum orbit

$$r_n = \frac{\varepsilon_0 h^2}{\pi\, m_e e^2} n^2$$

Substituting numerical values we obtain for the radius of the first orbit $(n=1)$ $r_1 = 0.53\ x\, 10^{-10}\ m$. Finally, for the velocity of an electron on this orbit we obtain

$$v_1 = \frac{\varepsilon_0 h}{2\pi\, r_1\, m_e} = \frac{e^2}{2\varepsilon_0 h} = 2.18\ x\, 10^6\ m.s^{-1}$$

Problem 6-7. Compare the gravitational attraction of an electron and proton in the ground state of a hydrogen atom with Coulomb's attraction. The radius of the first orbit $r_1 = 0.53 \, x \, 10^{-10} \, m$, permittivity of a free space $\varepsilon_0 = 8.85 \, x \, 10^{-12} \, F.m^{-1}$, charge of electron $e = 1.602 \, x \, 10^{-19} \, C$, mass of electron $m_e = 9.1 \, x \, 10^{-31} \, kg$, mass of proton $m_p = 1837 \, m_e$, and universal gravitational constant $\kappa = 6.67 \, x \, 10^{-11} \, N.m^2.kg^{-2}$.

Solution: The attractive force between a proton and an electron is expressed by Coulomb's law

$$F_C = \frac{1}{4\pi \varepsilon_0} \frac{e^2}{r_1^2}$$

Substituting numerical values we obtain $F_C = 8.21 \, x \, 10^{-8} \, N$. The attractive gravitational force between a proton and an electron is expressed by Newton's law of universal gravitation

$$F_g = \kappa \frac{m_e \, m_p}{r_1^2}$$

Substituting numerical values we obtain $F_g = 3.63 \, x \, 10^{-47} \, N$. From the ratio of these two forces

$$\frac{F_C}{F_g} = 2.26 \, x \, 10^{39}$$

we can conclude that in Bohr's model of a hydrogen atom the gravitational force can be disregarded with respect to Coulomb's attractive force.

Problem 6-8. Calculate the ionisation energy of an electron in a ground state of a hydrogen atom.

Solution: The energy required to remove the electron from the ground state to a state of zero total energy is called ionisation energy. To determine this energy it is therefore necessary to calculate the total energy of an electron in a ground state. The total energy W of an electron is equal to the sum of its potential $W(p)$ and kinetic $W(k)$, or

$$W = W(p) + W(k)$$

Let us define the potential energy of an electron to be zero when the electron is infinitely distant from a proton. Then the potential energy at any finite distance r_n is equal to the work required to move the electron from infinity to the point r_n, or

$$W(p) = -\int_{\infty}^{r_n} \vec{F}_C . d\vec{r} = -\int_{\infty}^{r_n} \left(-\frac{e^2}{4\pi \varepsilon_0 r^2} \right) dr = -\frac{e^2}{4\pi \varepsilon_0 r_n}$$

The negative sign in the expression for Coulomb's force in the integrand is caused by the fact that a proton has a positive charge and an electron has a negative charge of the same magnitude.

The kinetic energy of an electron is

$$W(k) = \frac{1}{2} m v^2$$

The term ($m v^2$) can be expressed from the balance of Coulomb's force and centripetal force

$$m_e \frac{v^2}{r_n} = \frac{1}{4\pi \varepsilon_0} \frac{e^2}{r_n^2}$$

Solving for ($m v^2$) and substituting into the expression for kinetic energy we obtain

$$W(k) = \frac{e^2}{8\pi \varepsilon_0 r_n}$$

The total energy of an electron on the *n-th* orbit is therefore

$$W_n = -\left(\frac{e^4 m}{8\varepsilon_0^2 h^2} \right) \frac{1}{n^2}$$

The ground state is characterised by the quantum number $n=1$. Thus after substituting numerical values into the previous expression for total or ionisation energy of an electron we obtain

$$W_{n=1} = -2.17 \, x \, 10^{-18} \, J = -13.6 \, eV$$

The conversion between electronvolts and Joules is $1 \, eV = 1.602 \, x \, 10^{-19} \, J$.

Problem 6-9. Calculate the wavelength of the radiation emitted by a hydrogen atom during the transition of an electron from the quantum orbit $m=4$ to the quantum orbit $s=2$. The speed of light is $c=3 \, x \, 10^8 \, m/s$.

Solution: The radiation which is emitted by the hydrogen atom is produced when the electron undergoes a transition from a higher-energy stationary state to a lower-energy state . The frequency f of the emitted photon is given by the equation

$$W_m - W_s = h f$$

Substituting from problem 6-8 for the total energy of an electron on an *n-th* orbit the expression

$$W_n = -\left(\frac{e^4 m}{8\varepsilon_0^2 h^2} \right) \frac{1}{n^2}$$

we can obtain for the frequency of the emitted radiation the following formula

$$f = \frac{m_e e^4}{8\varepsilon_0^2 h^3} \left(\frac{1}{s^2} - \frac{1}{m^2} \right)$$

Substituting numerical values we obtain for frequency $f = 6.178 \, x \, 10^{14} \, s^{-1}$.

Taking into account that $\lambda = \frac{c}{f}$ we finally obtain for the wavelength of the emitted radiation $\lambda = 0.485 \times 10^{-6}\ m$.

Problem 6-10. Calculate the period of revolution and the velocity of an electron in Bohr's model of a hydrogen atom for $n=3$.

$$\left[T = 4.1 \times 10^{-5}\ s,\ v = 729\ km.s^{-1}\right]$$

Problem 6-11. A hydrogen atom is excited from a state with $n=1$ to a state with $n=2$. Calculate the energy that must be absorbed by the atom.

$$[W = 10.2\ eV]$$

Problem 6-12. In the ground state of a hydrogen atom, according to Bohr's theory, what are the angular momentum b, linear momentum p, angular velocity ω and acceleration a of the electron.

$$\left[\ b = 1.1 \times 10^{-34}\ J.s,\ p = 2 \times 10^{-24} kg.m.s^{-1},\ \omega = 4.1 \times 10^{16}\ s^{-1},\ a = 9.0 \times 10^{22}\ m.s^{-2}\right]$$

Problem 6-13. How much energy is required to remove an electron from a hydrogen atom in a state with a quantum number $n=2$?

$$[W = 3.4\ eV]$$

6.3 WAVE-PARTICLE DUALITY

In classical physics it is assumed that energy is transported either by waves or by particles. The concept of waves cannot be mixed with the concept of particles.
However the situation becomes more complicated when treating atomic systems and radiation. The wave model of electromagnetic radiation provides a good description of phenomena such as interference and diffraction. However, to explain the photoelectric effect or Compton's effect a photon or particle model is needed. Similarly, the Newtonian particle model is inadequate to describe some behaviour of atomic particles such as electrons or neutrons. We need the idea of matter waves to explain electron and neutron diffraction.

Photoelectric effect

The photoelectric effect is the name given to the release of electrons from a clean metal surface when electromagnetic radiation of the proper frequency shines on it. This effect was explained in 1905 by Albert Einstein. He assumed that the incident light consisted of **photons.** A photon is a massless bundle of electromagnetic radiation which behaves like a particle. Its energy is

$$E = hf = \hbar\omega$$

where $\hbar = \frac{h}{2\pi}$ is the so called reduced Planck's constant, and $\omega = 2\pi f$.

The individual photons collide with individual electrons in the metal and knock them out of the metal by giving up to the electrons their entire energy. Einstein's equation for the photoelectric effect, i.e. conservation of energy law for this collision of a photon and electron, is

$$hf = E_{K,\max} + \Phi$$

where $E_{K,max}$ is the kinetic energy of an electron escaping from a metal surface and Φ is the energy required to remove an electron from themetal. This energy is called the **work function**.

The cutoff frequency f_0 of the photoelectric effect is the frequency for which the ejected photoelectrons have zero value of kinetic energy:

$$hf_0 = \Phi$$

Compton's effect

Compton's effect is the name given to the increase in the wavelength of x-rays when scattered by free electrons.

This effect could not be explained within the framework of classical physics. Compton therefore assumed that x-rays of the wavelength λ can be treated as a stream of photons carrying energy and momentum. The momentum of a photon is

$$p = \frac{h}{\lambda} = \hbar \vec{k}$$

where $\vec{k}$ is a wave vector ($k = \frac{2\pi}{\lambda}$). An elastic collision between an x-ray photon and a free electron caused the photon to have its energy and hence its frequency decreased, and its wavelength therefore increased. Compton then applied the laws of conservation of energy and momentum in a relativistic form to the collision process and obtained a formula for the shift in wavelength between incident and scattered photons:

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0 c}(1 - \cos\varphi)$$

where λ is the wavelength of the incident x-ray photon, λ' is the wavelength of the scattered x-ray photon, φ is the scattering angle, m_0 is the mass of an electron and c is the speed of light. Provided the values predicted by this equation fit perfectly with experiental values the particle properties of electromagnetic radiation were proved.

Diffraction of particles

Just as a photon has a light wave associated with it that governs its motion, so a material particle (e.g. an electron) has an associated wave that governs its motion. This fact was proved by the experiments of Davisson-Germer (scattering of electrons on a crystal of nickel) and G.P. Thomson (diffraction of an electron beam passing through a thin film).

Problem 6-14. a) What is the energy associated with a photon in the radio-frequency region with *f=100kHz?* b) What is the energy associated with a photon for the wavelength λ*=500 nm?* c) What is the energy associated with a gamma ray of frequency $f = 10^{20}\ Hz$.

Solution: ad a). $E = hf = 6.6.10^{-34} x 10^{5} = 6.6^{-29}\ J$

ad b).

$$f = \frac{c}{\lambda} = \frac{3x10^{8}}{500x10^{-9}} = 6\ x\ 10^{14}\ Hz$$

$$E = hf = 6.6.10^{-34} x 6x10^{14} = 4\ x10^{-19}\ J$$

ad c). $E = hf = 6.6.10^{-34} x 10^{20} = 6.6\ x\ 10^{-14}\ J$

Notice that the energy of a photon differs by 15 orders of magnitude between the radio-frequency and gamma rays regions of the spectrum. This explains why radio waves and gamma rays interact so differently with matter.

Problem 6-15. Electromagnetic radiation of wavelength *436 nm* falls on a piece of lithium metal in a vacuum. If the work function Φ of lithium is $3.8x10^{-19}\ J$, what is the maximum kinetic energy of the emitted electrons? What is the maximum speed of the emitted electrons? What is the longest wavelength which will eject electrons from the metal?

Solution: From Einstein's equation for photoelectric effect

$$hf = E_{K,\max} + \Phi$$

we can express the maximum kinetic energy of emitted electrons

$$E_{K,\max} = hf - \Phi = \frac{hc}{\lambda} - \Phi = \frac{\left(6.6^{26}\,x\,10^{-34}\right)\left(3\,x\,10^{8}\right)}{436\,x\,10^{-9}} - \Phi = \cancel{7\,x\,10^{-18}}\ J \quad 7{,}6\cdot10^{-20}\ J$$

The maximum speed of the emitted electrons is

$$v_{\max} = \sqrt{\frac{2\,E_{K,\max}}{m_e}} = 3.9\,x\,10^{5} m.s^{-1} \quad 4{,}08\cdot10^{5}\ m/s$$

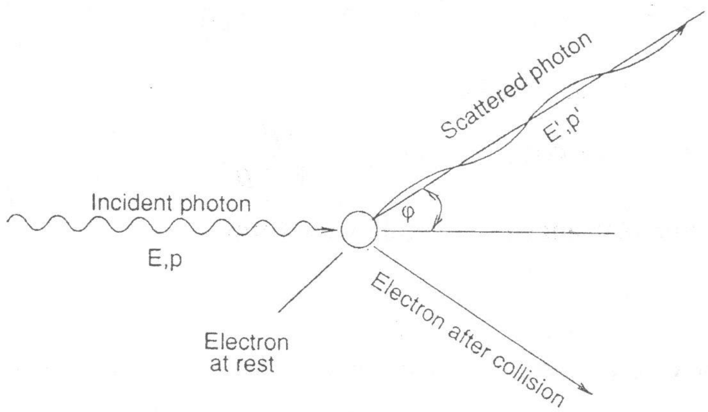
The longest wavelength of radiation which will eject electrons from the metal is found from condition $\frac{hc}{\lambda} = \Phi$. Thus, for the wavelength we obtain

$$\lambda = \frac{\left(6.6\,x\,10^{-34}\right)\left(3\,x\,10^{8}\right)}{3.8\,x\,10^{-19}} = 5.2\,x\,10^{-7}\ m \quad V$$

Hence only light of a wavelength less than $5.2x10^{-7}\,m$ has photons with enough energy to eject electrons from lithium.

Problem 6-16. Calculate the shift $\Delta\lambda$ in the wavelength of x-rays on free stationary electrons as a function of the scattering angle φ.

<u>Solution:</u> The collision process is shown in the diagram. A photon of energy $\hbar\omega$ and momentum $\hbar\vec{k}$ is incident on a stationary electron with rest energy $W_0 = m_0\, c^2$.
The photon is scattered at an angle φ and moves off with energy $\hbar\omega'$ and momentum $\hbar\vec{k}'$. The electron recoils with a certain kinetic energy and momentum p_e. Compton applied the conservation of momentum and relativistic energy laws to solve this collision problem. Relativistic equations must be used since the photon always moves at relativistic velocities, as does recoiling electron under most circumstances.



The conservation of total relativistic energy law:

The energy of the incident photon = energy of the scattered photon + kinetic energy of an electron:

$$\hbar\omega = \hbar\omega + m_0\, c^2 \left[\frac{1}{\sqrt{1-\beta^2}} \right] \qquad \text{where } \beta = \frac{v}{c}$$

Substituting for

$$\frac{\hbar}{m_0\, c^2} = a \tag{1}$$

we obtain, after a little rearrangement,

$$a\left(\omega - \omega'\right) = \frac{1}{\sqrt{1-\beta^2}} - 1 \tag{2}$$

For the square of this equation we have

$$a^2\left(\omega^2 - 2\omega\omega' + \omega'^2\right) = \frac{1}{1-\beta^2} - \frac{2}{\sqrt{1-\beta^2}} + 1 \tag{3}$$

For the recoiling electron the relativistic expression for the linear momentum is

$$\vec{p}_e = \frac{m_0\, \vec{v}}{\sqrt{1-\beta^2}} \tag{4}$$

The conservation of linear momentum law for this collision is

$$\hbar\vec{k} = \hbar\vec{k}' + \frac{m_0\, \vec{v}}{\sqrt{1-\beta^2}}$$

For linear momentum we can also write

$$p^2 = (\hbar k)^2 + (\hbar k')^2 - 2\hbar^2 kk'\cos\varphi$$

Substituting for p from Eq.4 and for $|\vec{k}| = \frac{\omega}{c}$ we have

$$\left(\frac{m_0 v}{\sqrt{1-\beta^2}}\right)^2 = \hbar^2\frac{\omega^2}{c^2} + \hbar^2\frac{\omega'^2}{c^2} - 2\hbar^2\frac{\omega\omega'}{c^2}\cos\varphi$$

Taking into account the substitution which is expressed by Eq. 1 we obtain

$$\frac{\beta^2}{1-\beta^2} = a^2\left(\omega^2 - \omega'^2 - 2\omega\,\omega'\cos\varphi\right) \qquad (5)$$

Substracting Eq.3 from Eq. 5 we have

$$a^2(-2\omega\,\omega'\cos\varphi + 2\omega\,\omega') = \frac{\beta^2}{1-\beta^2} - \frac{1}{1-\beta^2} + \frac{2}{\sqrt{1-\beta^2}} - 1$$

This equation can be rearranged to the following form

$$2a^2\omega\,\omega'\sin^2\frac{\varphi}{2} = \frac{1}{\sqrt{1-\beta^2}} - 1 \qquad (6)$$

From comparison of Eq. 6 and Eq. 2 we can see that

$$2a^2\omega\,\omega'\sin^2\frac{\varphi}{2} = a(\omega - \omega')$$

Taking into account Eq.1 we obtain

$$\omega - \omega' = 2\frac{\hbar}{m_0c^2}\omega\,\omega'\sin^2\frac{\varphi}{2}$$

With respect to the fact that $\omega = 2\pi\frac{c}{\lambda}$ we finally obtain for the shift $\Delta\lambda$ in the wavelength

$$\Delta\lambda = \lambda' - \lambda = \frac{4\pi\hbar}{m_0c}\sin^2\frac{\varphi}{2} = \frac{h}{m_0c}(1-\cos\varphi)$$

Notice that $\Delta\lambda$ depends only on the scattering angle φ and not on the initial wavelength λ. The quantity $\lambda_C = \frac{h}{m_0c} = 2.43x10^{-12}\ m$ is known as Compton's wavelength.

Problem 6-17. The energy required to remove an electron from sodium is *2.3 eV*. What is the cutoff wavelength for a photoelectric emission from sodium.

$$\left[\lambda = 5.4x10^{-7}\ m\right]$$

Problem 6-18. The maximum wavelength of light capable of causing photoelectric emission from tungsten is $\lambda = 2750.10^{-10} m$. Calculate the work function of tungsten and the maximum velocity of the emitted electrons.

$$\left[\Phi = 4.5\,eV,\ v = 9.1x10^5\ m.s^{-1}\right]$$

Problem 6-19. An x-ray photon of the wavelength $\lambda = 1x10^{-10}\ m$ is incident on a free electron at rest and is scattered at right angles from the initial direction. Find the energy of the recoiled electron.

$$\left[W_e = 4.8x10^{-17}\ J \right]$$

Problem 6-20. An electron which is scattered by an x-ray photon gains energy $50\ keV$ during the Compton's collision. Find the minimum energy of an x-ray photon.

$$\left[W_{ph} = 23.3x10^{-15}\ J \right]$$

Problem 6-21. The wavelength of yellow light is 589 nm. What is the energy of the corresponding photons?

$$\left[E = 2.11\ eV \right]$$

Problem 6-22. A light bulb emits light at a wavelength of $630\ nm$. The bulb is rated at $60\ W$, and is $93\ \%$ efficient in converting electrical energy to light. How many photons will the bulb emit over 730 hours.

$$\left[4.66x10^{26} \right]$$

Problem 6-23. Find the maximum kinetic energy of photoelectrons if the work function of metallic sodium is $2.3\ eV$ and the frequency of the light producing the photoeffect is $3x10^{15}\ Hz$.

$$\left[10.1\ eV \right]$$

Problem 6-24. An x-ray photon of wavelength $0.01\ nm$ strikes an electron head on $(\alpha = 180°)$. Calculate: a) the change in wavelength of the incident photon,

b) the change in energy of the photon, and

c) the kinetic energy imparted to the electron.

$$\left[a)\ 4.8\ pm,\ b) - 41 keV,\ c)\ 41\ keV \right]$$

6.4 WAVE NATURE OF MATTER

According to Louis de Broglie's hypothesis not only electrons, but all material objects, charged or uncharged, show wavelike properties. The wave which is associated with every particle having a momentum $p = mv$ is called the **de Broglie matter wave.** The wavelength of matter waves is

$$\lambda = \frac{h}{m\,v}$$

Principle of complementarity:
The wave and particle description of reality are complementary; both models are required to describe the behaviour of electromagnetic radiation and atomic particles, but the two are never applied at the same time to the same physical measurement.

Problem 6-25. Calculate the wavelength of the de Broglie matter wave associated with an electron which is accelerated by a potential difference $U=100V$.

Solution: The speed of an electron can be found from its kinetic energy or

$$\frac{1}{2} m_e v^2 = e.U$$

Thus we have

$$v = \sqrt{\frac{2eU}{m_e}} = \sqrt{\frac{2x1.6x10^{-19}x100}{9.1x10^{-31}}} = 5.9 \ x \ 10^6 \ m.s^{-1}$$

The momentum follows from

$$p = m.\ v = 5.4 \ x \ 10^{-24} \ kg.m/s$$

The wavelength of the associated de Broglie matter wave is

$$\lambda = \frac{h}{m\,v} = \frac{6.6x10^{-34}}{5.4x10^{-24}} = 1.2 \ x \ 10^{-10} \ m$$

Note that this wavelength is of the same order as the size of an atom.

Problem 6-26. Helium atoms move at a speed of $1.63 \ x \ 10^3 \ m/s$. Calculate the wavelength of the associated de Broglie matter wave. The molar mass of helium is 4.0 g/mole, Avogadro's number is $6.02 \ x \ 10^{23} \ mol^{-1}$.

$$\left[\lambda = 0.609 \ x \ 10^{-10} \ m\right]$$

6.5 WAVE FUNCTION

Microscopic particles act as if certain aspects of their behaviour are governed by the behaviour of an associated de Broglie wave which is described by the **wave function** $\Psi(x,y,z,t)$. The wave function may be real as well as complex. The basic connection between the properties of the wave function and the behaviour of the associated particle is expressed in terms of the probability density $dP(x,y,z,t)$, which tells us that the probability that the particle will be found in the volume dV at a certain instant of time is

$$dP(x,y,z,t) = \left|\Psi(x,y,z,t)\right|^2 dV$$

where

$$\left|\Psi(x,y,z,t)\right|^2 = \Psi(x,z,y,t).\Psi^*(x,z,y,t).$$

In this expression Ψ^* is the imaginary conjugated function to Ψ. Thus for **probability density** we obtain

$$\left|\Psi(x,y,z,t)\right|^2 = \frac{dP(x,y,z,t)}{dV}$$

The total probability of finding the particle somewhere in the volume V is necessarily equal to one, if the particle exists. This fact is expressed by the **normalisation condition**:

$$\int_V \left|\Psi(x,y,z,t)\right|^2 dV = 1$$

Problem 6-27. Normalise the wave function $\Psi(x)$)=A $\sin kx$ by determining the value of the arbitrary constant A in that wave function for $-a \leq x \leq +a$.

Solution: The probability of finding the particle somewhere in the interval $-a \leq x \leq +a$ equals one if the particle exists. This fact is expressed by the normalisation condition

$$\int_{-a}^{+a} \Psi(x)\,\Psi^*(x)\,dx = 1$$

Inserting wave function into the normalisation condition we obtain

$$A^2 \int_{-a}^{+a} \sin^2 kx\,dx = 1$$

Solving this integral we obtain

$$A = \pm\frac{1}{\sqrt{a}}$$

Thus for the wave function we finally have

$$\Psi(x) = \pm\frac{1}{\sqrt{a}}\sin kx$$

6.6 UNCERTAINTY PRINCIPLE

It is impossible to measure simultaneously both the position and the corresponding momentum of a particle with complete accuracy:

$$\Delta x\,\Delta p \geq h$$

where Δx and Δp are inaccuracies in the position and momentum of the particle, respectively. The uncertainties in energy and time are related in the same way as are the uncertainties in position and momentum, or

$$\Delta E\,\Delta t \geq h$$

Problem 6-28. An electron is accelerated by voltage U=$12V$. Assume that you can measure its speed with a precision of $1.5\ \%$. With what precision can you simultaneously measure the position of the electron?

Solution: The velocity of an electron can be found from its kinetic energy

$$v = \sqrt{\frac{2eU}{m_e}} = \sqrt{\frac{2x1.6x10^{-19}x12}{9.1x10^{-31}}} = 2.05\ x\ 10^{6}\ m.s^{-1}$$

The uncertainty in its velocity is therefore

$$\Delta v = 1.5\%\ v = 3.07\ x\ 10^{4}\ m/s$$

We can find the uncertainty in the linear momentum of the electron as

$$\Delta p = m\ \Delta v = \ 9.1x10^{-31}\ x\ \ 3.07x10^{4} = 2.79\ x\ 10^{-26}\ kg.m/s$$

Thus from the uncertainty principle $\Delta x\, \Delta p \geq h$ we have for the uncertainty in the position of the electron

$$\Delta x = \frac{h}{\Delta p} = \frac{6.6x10^{-34}}{2.79x10^{-26}} = 2.35\ x\ 10^{-8}\ m$$

Problem 6-29. Calculate the uncertainty in the energy of a π-meson. The lifetime of this particle is $\tau = 2.5\ x\ 10^{-8}\ s$.

$$\left[\Delta E = 2.6\ x\ 10^{-26}\ J\right]$$

Problem 6-30. A bullet of mass 50 g travels at a speed of 300 m/s. The uncertainty in the velocity is 0.01%. Calculate the uncertainty in the position of the bullet if the position is measured simultaneously with the speed.

$$\left[\Delta x = 3\ x\ 10^{-32}\ m\right]$$

6.7 SCHROEDINGER'S EQUATION

Postulate: **To every wave function corresponds a unique state of motion of the particle**. In fact the wave function contains all the information that the uncertainty principle allows us to learn about the associated particle. Schroedinger's equation allows us to find the wave function $\Psi(x,y,z,t)$ if we know the force acting on the associated particle by specifying the potential energy V corresponding to this force. In other words the wave function is a solution to Schrodinger's equation for that potential energy.

Time-dependent Schroedinger's equation:

$$i\hbar\frac{\partial\Psi(x,y,z,t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi(x,y,z,t) + V(x,y,z,t)\,\Psi(x,y,z,t)$$

Provided that the potential energy V does not depend explicitly on the time t the wave function can be written as

$$\Psi(\vec{r},t) = \psi(\vec{r})\ \Omega(t)$$

For this case we obtain the so called **time-independent Schroedinger's equation**:

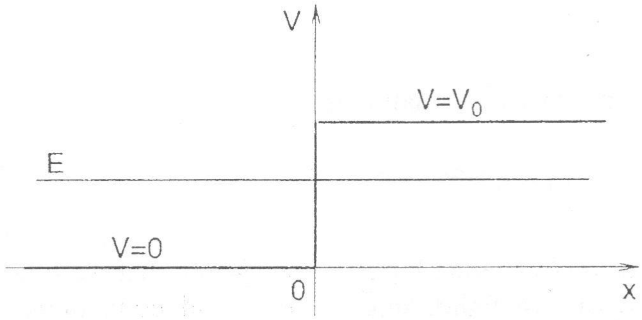
$$\Delta\psi(\vec{r}) + \frac{2m}{\hbar^2}(E - V)\,\psi(\vec{r}) = 0$$

The functions $\psi(\vec{r})$ are called **eigenfunctions.** Wave functions are always represented by a capital letter $\Psi(\vec{r},t)$, eigenfunctions are represented by a lower case letter $\psi(\vec{r})$. To be an acceptable solution (in the one dimensional case) an eigenfunction and its derivative are required to have the following properties:

$\psi(x)$ must be finite	$\frac{d\psi(x)}{dx}$ must be finite
$\psi(x)$ must be single valued	$\frac{d\psi(x)}{dx}$ must be single valued
$\psi(x)$ must be continuous	$\frac{d\psi(x)}{dx}$ must be continuous

Acceptable solutions to the time-independent Schroedinger's equation exist only for certain values of energy which are called **eigenvalues** of potential. A particular potential has a particular set of eigenvalues.

Problem 6-31. Consider a particle of mass m and total energy E which is moving from the region $x<0$ toward the point $x=0$ at which the potential $V(x)$ abruptly changes from 0 to V_0 (see Figure). Find the probability density distribution. The energy of the particle is less than the potential height.



Solution: According to classical mechanics, the particle will move freely in the region $x<0$ until it reaches point $x=0$, where it is subjected to a force of infinite magnitude:

$$F_x = -\frac{dV}{dx} \qquad \lim_{x=0} F_x \to \infty$$

Thus, according to classical mechanics, the particle cannot enter the region $x > 0$. To find the probability density distribution we must find the eigenfunction of the time-independent Schroedinger's equation.

This equation is solved separately for each region of variable x. Then the eigenfunction valid for the entire range of x is constructed by joining the two solutions together at $x = 0$ in such a way that the eigenfunction and its first derivative are everywhere finite, single valued and continuous.

For the step potential, which is shown in the Figure, the x axis breaks up into two regions:

$$V = 0 \qquad \text{for} \qquad x < 0$$

and

$$V = V_0 \qquad \text{for} \qquad x \geq 0$$

In the region where $\boldsymbol{x < 0}$ (left of the step) the eigenfunction is a solution to the time-independent Schroedinger's equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\,\psi = 0$$

Denoting $$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

the solution of the Schroedinger's equation is

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \tag{1}$$

In the region where $\boldsymbol{x \geq 0}$ (right of the step) the eigenfunction is a solution to the time-independent Schroedinger's equation:

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\,\psi = 0$$

Denoting $$k_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

the solution of the Schroedinger's equation is

$$\psi(x) = Ce^{k_2x} + De^{-k_2x} \tag{2}$$

The arbitrary constants A, B, C and D must be so chosen that the total eigenfunction and its derivative are everywhere finite, single valued and continuous. Consider first the behaviour of $\psi(x)$ as $x \to +\infty$. In this region of the x axis the general form of $\psi(x)$ is given by Eq. 2. Inspection shows that it will generally increase without limit as $x \to +\infty$, because of the presence of the first term Ce^{k_2x}. In order to prevent this, and keep $\psi(x)$ finite, we must set the constant in the first term equal to zero. Thus we have $C = 0$. Single valuedness is satisfied automatically by these functions. To assure the continuity of $\psi(x)$ we have to consider the point $x=0$. At this point the forms of $\psi(x)$, given by Eqs. 1 and 2, must join in such a way that $\psi(x)$ and $\dfrac{d\psi}{dx}$ are continuous.

Thus we obtain

$$A+B=D \tag{3}$$

$$A-B=\frac{ik_2}{k_1}D \tag{4}$$

Adding and subtracting Eqs.3 and 4 gives

$$A=\frac{D}{2}\left(1+\frac{ik_2}{k_1}\right) \qquad B=\frac{D}{2}\left(1-\frac{ik_2}{k_1}\right)$$

Thus the eigenfunction for the step potential and for energy of the particle $E<V_0$ is:

$x<0$

$$\psi(x)=\frac{D}{2}\left(1+\frac{ik_2}{k_1}\right)e^{ik_1x}+\frac{D}{2}\left(1-\frac{ik_2}{k_1}\right)e^{-ik_1x} \tag{5}$$

$x\geq 0$

$$\psi(x)=De^{-k_2x}$$

The presence of the one remaining constant D reflects the fact that the time-independent Schroedinger's equation is linear in $\psi(x)$, and so solutions of any amplitude are allowed by the equation.

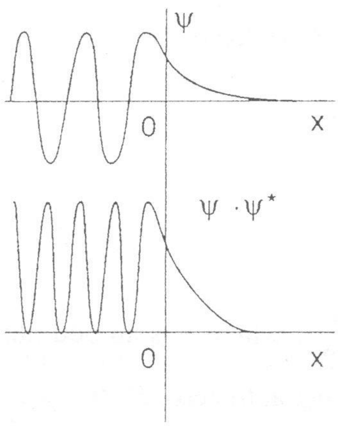
Consider now the eigenfunction of Eq.5. Using the formula

$$e^{ikx}=\cos kx+i\sin kx$$

the eigenfunction given by the Eq.5 can easily be rewritten into the form

$$\psi(x)=D\cos k_1x+D\frac{k_2}{k_1}\sin k_1x$$

The eigenfunction is a real function of x if we take D real. In the top part of the figure the eigenfunctions are illustrated. The bottom part shows the probability density distribution. This part of the figure reveals a feature which is in sharp contrast to predictions based on classical physics.



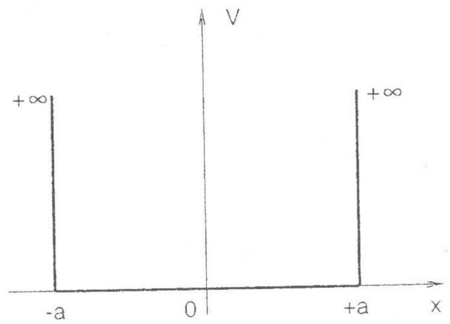
Although in the region $x\geq 0$ the probability density

$$\psi\,\psi^*=De^{-k_2x}\;De^{-k_2x}=D^2e^{-2k_2x}$$

decreases rapidly with increasing x, there is a finite probability of finding the particle in the region $x>0$. In classical mechanics it would be absolutely impossible to find the particle in this region. This phenomenon, called penetration into the classically forbidden region, is one of the most striking predictions of quantum mechanics.

Problem 6-32. Consider a particle of mass m inside an infinite square potential well, see Figure. Find the eigenfunctions and probability density distribution for quantum numbers $n = 1, 2$ and 3.

Solution:



The infinite square well potential is written as

$$\text{for } |x| \geq a \qquad V \to \infty$$

$$\text{for } |x| < a \qquad V = 0$$

This well has the feature that it will bind a particle with any finite total energy. In classical mechanics, any of these energies are possible, but in quantum mechanics only certain discrete eigenvalues are allowed. In the region inside the well the behaviour of the particle is described by Schroedinger's equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\,\psi = 0$$

Denoting $k = \sqrt{\dfrac{2mE}{\hbar^2}}$ (1)

the solution of the Schroedinger's differential equation is

$$\psi(x) = A \sin kx + B \cos kx \tag{2}$$

To find the value of the eigenfunction for $x = \pm a$ we use the fact that in this case the potential V goes to infinity. We can write Schroedinger's equation in the following form

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2} E\,\psi + \frac{2m}{\hbar^2} V\psi$$

Dividing by ψ and denoting $\dfrac{d^2\psi}{dx^2} = \psi''$ we have

$$\frac{\psi''}{\psi} = -\frac{2m}{\hbar^2} E + \frac{2m}{\hbar^2} V$$

Since for $x = \pm a$ the right side of this equation goes to infinity

$$\psi(a) = \psi(-a) = 0$$

Applying this boundary condition to eigenfunctions of Eq.6 we have for

$$x = -a \qquad 0 = -A \sin ka + B \cos ka \tag{3}$$

and for

$$x = a \qquad 0 = A \sin ka + B \cos ka \tag{4}$$

Addition of Eqs. 3 and 4 gives

$$2\,B \cos ka = 0 \tag{5}$$

Since $ka \neq 0$ we see that $\cos ka \neq 0$ (supposing that $ka \neq \dfrac{n\pi}{2}$, where n is an odd number).

Consequently from Eq. 5 we see that constant B must be equal to zero, $B=0$.
However, constants A and B in the expression for eigenfunction cannot both equal zero, for then the eigenfunction vanishes everywhere and the eigenfunction would be of no interest, because the particle would not be in the box. Therefore A must be different from zero, or $A \neq 0$. Thus for the points $x = \pm a$ the eigenfunction is

$$\psi = A \sin ka = 0 \tag{6}$$

Since $A \neq 0$ we have

$$sinka = 0$$

and consequently we obtain for allowed values of k

$$k = \frac{n\pi}{2a} \qquad \text{where } n \text{ is an even number.} \qquad (7)$$

Finally we can write for eigenfunction

$$\psi_{even} = A\sin\frac{n\pi}{2a}x \qquad (8)$$

where n is called the quantum number.

We can now substract Eq.3 from Eq. 4. Thus we obtain

$$2A\sin ka = 0 \qquad (9)$$

Since $ka \neq 0$ we see that $\sin ka \neq 0$ (supposing that $ka \neq \frac{n\pi}{2}$, where n is an even number).

Consequently from Eq. 9 we see that constant A must be equal to zero, $A=0$.
However, constants A and B in the expression for eigenfunction cannot both equal zero, for then the eigenfunction vanishes everywhere and the eigenfunction would be of no interest because the particle would not be in the box. Therefore B must be different from zero, or $B \neq 0$. Thus for the points $x = \pm a$ the eigenfunction is

$$\psi = B\cos ka = 0 \qquad (10)$$

Since $B \neq 0$ we have $coska = 0$ and consequently we obtain for allowed values of k

$$k = \frac{n\pi}{2a} \qquad \text{where } n \text{ is an odd number} \qquad (11)$$

Finally we can write for the eigenfunction

$$\psi_{odd} = B\cos\frac{n\pi}{2a}x. \qquad (12)$$

Thus we see that we have obtained two classes of allowed solutions of the time-independent Schroeinger equation for particle confined in the well. To find the constants A and B which figure in the expression for the eigenfunctions we have to use a normalisation condition. Thus for the eigenfunction given by Eq. 8 we have

$$A^2 \int_{-a}^{+a} \sin^2 kx\, dx = 1$$

Solving this integral we have

$$A = \pm \frac{1}{\sqrt{a}}$$

The constant B, for the eigenfunction which is expressed by Eq.12, is obtained in the same way, or

$$B^2 \int_{-a}^{+a} \cos^2 kx\, dx = 1$$

Solving this integral we have

$$B = \pm \frac{1}{\sqrt{a}}$$

Since the probability density is equal to the product of the wave function times the imaginary conjugated wave function we can choose the positive sign in the expression for constants A and B. Substituting for A and B into Eqs.8 and 12 we finally obtain for the eigenfunctions

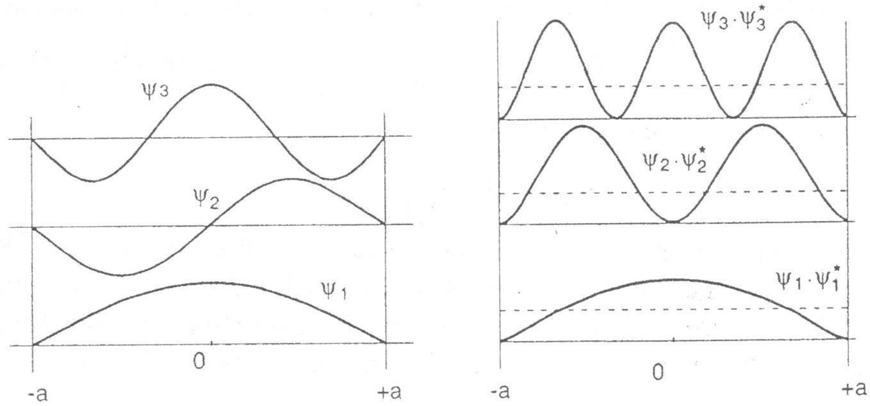
$$\psi_{even} = \frac{1}{\sqrt{a}}\sin\frac{n\pi}{2a}x \qquad n=2,4,6,... \qquad (13)$$

$$\psi_{odd} = \frac{1}{\sqrt{a}}\cos\frac{n\pi}{2a}x \qquad n=1,3,5,... \qquad (14)$$

The probability density is therefore

$$\psi_{even}\psi^*_{even} = \frac{1}{a}\sin^2\frac{n\pi}{2a}x \qquad \psi_{odd}\psi^*_{odd} = \frac{1}{a}\cos^2\frac{n\pi}{2a}x$$

The eigenfunctions of the particle in the infinite square potential well for the quantum numbers $n=1,2$ and 3 are shown on the left side of the following figure, and the corresponding probability distributions are shown on the right. It is seen that the probability distribution differs for different quantum numbers. Thus, for example for the state described by the eigenfunction ψ_1 the particle will with the gratest probability be found in the centre of the well. Conversely for the state described by the eigenfunction ψ_2 the probability of finding the particle in the centre of the well equals zero. These conclusions are in a sharp contradiction with presumptions made by classical mechanics. The dashed curves in the right side picture are the predictions of classical mechanics.



Problem 6-33. Find the allowed values of energy for quantum numbers $n=1,2$ and 3 for an electron which is confined in an infinite square potential well for the case when the well has: 1.) microscopic dimensions $a=10^{-10}$ m and
2.) macroscopic dimensions $a=10^{-2}$ m.
The mass of an electron is $9.1x10^{-31}$ kg, Planck's constant is $6.6x10^{-34}$ $J.s$.

Solution: To find the allowed values of energy for an electron which is confined in an infinite square potential well we can use the results obtained in Problem 6-27. When solving Schroedinger's equation we denoted $k = \sqrt{\frac{2mE}{\hbar^2}}$ .For k we have also obtained

$$k = \frac{n\pi}{2a} \qquad \text{where } n \text{ is a quantum number.}$$

Combining these two equations we obtain for the allowed values (eigenvalues) of energy

$$E = \frac{n^2 \pi^2 \hbar^2}{8ma^2}$$

Substituting for $\hbar = \dfrac{h}{2\pi}$ and using the conversion relation $1\ eV = 10^{-19}\ J$ we obtain for the allowed values (eigenvalues) of energy for:

1.) a well of microscopic dimensions:

$E_1 = 8.5\ eV$ $\qquad E_2 = 34\ eV$ $\qquad E_3 = 76.5\ eV$

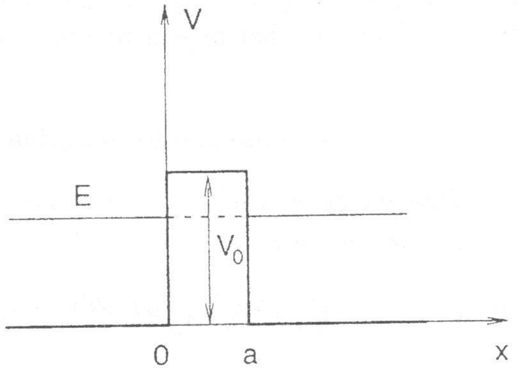
2.) a well of macroscopic dimensions:

$E_1 = 8.5x10^{-16}\ eV$ $\qquad E_2 = 34x10^{-16}\ eV$ $\qquad E_3 = 76.5x10^{-16}\ eV.$

It is seen that if the dimensions of the well are macroscopic in comparison with the dimensions of the region where the electron is likely to be, then the difference between the energies of the two adjacent energetic levels is so small that it can be hardly detected (in our example of the order $10^{-16}\ eV$). We can therefore suppose that the energy of an electron changes continuously. We can also say that the energy is not quantised. On the other hand, if the dimensions of the well are comparable with the dimensions of the region in which the electron is likely to be (say $10^{-10}\ m$) then the changes of energy on two adjacent levels are detectable (electronvolts) and thus we see that the energy is quantised.

Problem 6-34. Consider a particle of a mass m tunnelling through the potential barrier, see Figure. The energy E of the particle is less than the height V_0 of the barrier. Find the eigenfunctions in the different regions of the potential and plot the probability density distribution. Evaluate the transmission coefficient T through the barrier.

Solution: The potential barrier can be written as follows:



$V = V_0$ $\qquad$ for $\quad 0 < x < a$

$V = 0$ $\qquad$ for $\quad x < 0$ or $x > a$.

We suppose that a particle is in the region $x < 0$ and it is moving along the x axis to the right. The height of the barrier is greater than the energy of the particle. According to classical mechanics the particle cannot reach the region $x > a$. However quantum mechanics predicts that there is a certain probability that the particle will be transmitted into the classically forbidden region $x > a$.

To find the eigenfunction, Schroedinger's equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - V_0\right)\psi = 0 \qquad (1)$$

breaks up into three separate equations for three regions:

x < 0	left of the barrier
0 < x < a	within the barrier, and
x > a.	right of the barrier.

In the regions to the left and to the right of the barrier, Eq.1 changes into the equation for a free particle of total energy *E:*

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\,\psi = 0 \qquad (2)$$

The solutions of this differential equation of the second order with constant coefficients are

$$\psi_I = A_1 e^{ik_1x} + B_1 e^{-ik_1x} \qquad \text{for} \qquad x < 0 \qquad (3)$$

and

$$\psi_{III} = A_3 e^{ik_1x} + B_3 e^{-ik_1x} \qquad \text{for} \qquad x > a \qquad (4)$$

where

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad (5)$$

In the region inside the barrier (0 < x < a) Eq.1 can be rewritten (because $E < V_0$) into the following form:

$$\frac{d^2\psi_{II}}{dx^2} - \frac{2m}{\hbar^2}\left(V_0 - E\right)\psi_{II} = 0 \qquad (6)$$

Denoting $$k_2 = \sqrt{\frac{2m}{\hbar^2}\left(V_0 - E\right)} \qquad (7)$$

the solution of Schroedinger's equation is

$$\psi_{II} = A_2 e^{-k_2x} + B_2 e^{k_2x} \qquad (8)$$

The arbitrary constants A_1, A_2, A_3, B_1, B_2 and B_3 must be so chosen that they make $\psi(x)$ and $\frac{d\psi(x)}{dx}$ continuous at points $x=0$ and $x=a$. Since we are considering the case of a particle incident on a barrier from the left, in the region to the right of the barrier there can be only a transmitted wave, as there is nothing in that region to produce a reflection. Thus we can set $B_3=0$.

In matching $\psi(x)$ and $\frac{d\psi(x)}{dx}$ at points $x=0$ and $x=a$, four equations for the arbitrary constants A_1, A_2, A_3, B_1, and B_2 will be obtained. Thus we have:

$\psi_I(0) = \psi_{II}(0)$ $\qquad$ $\psi_{II}(a) = \psi_{III}(a)$

$$1 + B_1 = A_2 + B_2 \qquad (9) \qquad\qquad A_2 e^{-k_2a} + B_2 e^{k_2a} = A_3 e^{ik_1a} \qquad (10)$$

$$\frac{d\psi_I(0)}{dx} = \frac{d\psi_{II}(0)}{dx} \qquad\qquad \frac{d\psi_{II}(a)}{dx} = \frac{d\psi_{III}(a)}{dx}$$

$$k_1(1 - B_1) = k_2(A_2 - B_2) \quad (11) \qquad -A_2e^{-k_2a} + B_2e^{k_2a} = \frac{ik_1}{k_2}A_3e^{ik_1a} \quad (12)$$

Equations 9-11 can be used to evaluate A_2, A_3, B_1, and B_2 in terms of A_1. The value of A_1 determines the amplitude of the eigenfunction and it can be left arbitrary. We can therefore assume that $A_1 = 1$.

Transmission coefficient T through the barrier is defined as the ratio of a probability flux transmitted through the barrrier into the region $x > a$ to the probability flux incident upon the barrier. The probability flux incident on the barrier is defined as

$$I_{inc} = \frac{\hbar k_1}{m}|A_1|^2$$

Similarly the probability flux transmitted through the barrier is

$$I_{trans} = \frac{\hbar k_1}{m}|A_3|^2$$

Thus for the transmission coefficient we have

$$T = \frac{I_{inc}}{I_{trans}} = |A_3|^2$$

It is therefore seen that to determine transmission coefficient T it is necessary to determine constant A_3. This constant can be determined from Eqs 9-12 using Cramer's rule. To do this we rewrite Eqs. 9-12 into the following form

$$\begin{array}{ccccccccc}
B_1 & - & A_2 & - & B_2 & + & 0 & = & -1 \\
-k_1 B_1 & - & k_2 A_2 & + & k_2 B_2 & + & 0 & = & -k_1 \\
0 & + & e^{-k_2a}A_2 & + & e^{k_2a}B_2 & - & e^{ik_1a}A_3 & = & 0 \\
0 & + & e^{-k_2a}A_2 & - & e^{k_2a}B_2 & + & \frac{ik_1}{k_2}e^{ik_1a}A_3 & = & 0
\end{array} \quad (13)$$

The determinant of the system is the fourth-order determinant

$$D_S = \begin{vmatrix} 1 & -1 & -1 & 0 \\ -k_1 & -k_2 & +k_2 & 0 \\ 0 & e^{-k_2a} & e^{k_2a} & -e^{ik_1a} \\ 0 & e^{-k_2a} & -e^{k_2a} & \frac{ik_1}{k_2}e^{ik_1a} \end{vmatrix}$$

Evaluation of this determinant gives

$$D_S = e^{ik_1a}\left[2k_1\left(e^{k_2a} + e^{-k_2a}\right) + i\left(e^{k_2a} - e^{-k_2a}\right)\left(\frac{k_2^2 - k_1^2}{k_2}\right)\right]$$

To determine the constant A_3 we have to evaluate the determinant in which the fourth column in the D_S is substituted by the right side of the system of equations 13, or

$$D_{A3} = \begin{vmatrix} 1 & -1 & -1 & -1 \\ -k_1 & -k_2 & +k_2 & -k_1 \\ 0 & e^{-k_2 a} & e^{k_2 a} & 0 \\ 0 & e^{-k_2 a} & -e^{k_2 a} & 0 \end{vmatrix} = 4k_1$$

Thus for constant A_3 we have

$$A_3 = \frac{D_{A3}}{D_S} = \frac{4k_1 ik_2 e^{-ik_1 a}}{e^{k_2 a}(k_1 + ik_2)^2 - e^{-k_2 a}(k_1 - ik_2)^2}$$

The transmission coefficient through the barrier is therefore

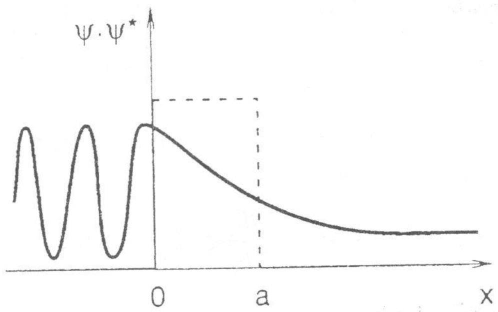
$$T = |A_3|^2 = \frac{4k_1^2 k_2^2}{\left(k_1^2 + k_2^2\right)^2 \sinh^2 k_2 a + 4k_1^2 k_2^2}$$

Since for most situations $k_2 a \rangle\rangle 1$ the expression for T may be simplified to the following form

$$T = \frac{16\, k_1^2 k_2^2}{\left(k_1^2 + k_2^2\right)^2} e^{-2k_2 a} = T_0\, e^{-\frac{2}{\hbar}\sqrt{2m(V_0 - E)}} \tag{14}$$

The expression for T makes a prediction which is very remarkable from the point of view of classical mechanics. It is seen that a particle of mass m and total energy E, incident on a potential barrier of height V_0 and finite thickness a has a certain probability of penetrating the barrier and appearing on the other side. This phenomenon is called a *tunnel effect* and the particle is said to *tunnel* through the barrier. An inspection of Eq. 14 shows that the probability that the particle penetrates through the barrier is nonzero only in the case of microscopic dimensions of the barrier $\left(a \approx 10^{-15}\, m\right)$ and for microscopic particles.

The tunnel effect is responsible for the emission of α particles in the decay of radioactive nuclei, for nuclear fusion, for the functioning of the tunnel diode, etc. The probability density distribution may be drawn using the eigenfunctions which are expressed by Eqs. 3,4 and 8. This distribution is shown in the following figure.



Problem 6-35. Find allowed values of energy and probability distribution for a free electron.

[All values of energy are allowed]

[ψ ψ•=const]

6.8 OPERATORS - EXPECTATION VALUES

An operator maps a function onto a function, or

$$\Phi = \hat{A}\,\psi$$

If an operator acting on a certain function produces a scalar multiple of the same function, or

$$\hat{A}\psi_n = A_n \psi_n$$

we call the function ψ_n an **eigenfunction** and the scalar A_n an **eigenvalue** of the operator $\hat{A}$.

Postulate: **To each dynamical variable there corresponds a Hermitian operator whose eigenvalues are possible values of the dynamic variable.**

The set of eigenvalues A_n of operator $\hat{A}$ is called the **spectrum** of this operator. This spectrum can be purely discrete, or continuous.

As an operator of coordinate $\hat{x}$ we take the multiplication by the coordinate, or

$$\hat{x}\psi_n = x_n \psi_n$$

An operator of linear momentum $\hat{p}$ is

$$\hat{p} = -\,i\hbar\nabla$$

where i is an imaginary unit, ∇ is a del operator and h is Planck's constant.

An operator of kinetic energy $\hat{E}$ is

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

An operator of total energy, or a so called Hamiltonian operator, is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla + V$$

The time-independent Schroedinger equation in the operator form is

$$\hat{H}\psi = E\psi$$

The expectation value is the average of the observed values which characterize, for example, the position at time t of a particle associated with the wave function $\Psi(x,t)$, or

$$\overline{x} = \int_{-\infty}^{\infty} \Psi^*(x,t)\,\hat{x}\,\Psi(x,t)\,dx$$

The same expression would be appropriate for evaluating the expectation value of any physical quantity, if we substitute operator $\hat{x}$ by an operator of this quantity.

Problem 6-36. Find an operator $\hat{\vec{b}}$ of the angular momentum of a particle.

Solution: The vector of angular momentum $\vec{b}$ in classical physics is defined as $\vec{b} = \vec{r}\ x\ \vec{p}$. In quantum mechanics the operator of angular momentum is expressed by an operator which is defined in the same way as angular momentum in classical physics, or

$$\hat{\vec{b}} = \left[\vec{r} \; x \; \hat{\vec{p}} \right]$$

where $\hat{p}$ is an operator of linear momentum

$$\hat{p} = -i\hbar\nabla$$

and $\vec{r}$ is a position vector with coordinates x, y and z. Since for an operator of coordinate $\hat{x}$ we take the multiplication by the coordinate x (and similarly for operators $\hat{y}$ and $\hat{z}$ we take the multiplication by the coordinates y and z respectively) we can write

$$\hat{\vec{b}} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ -i\hbar\dfrac{\partial}{\partial x} & -i\hbar\dfrac{\partial}{\partial y} & -i\hbar\dfrac{\partial}{\partial z} \end{vmatrix}$$

Thus for the components of the angular momentum operator we have

$$\hat{b}_x = i\hbar\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z} \right)$$

$$\hat{b}_y = i\hbar\left(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x} \right)$$

$$\hat{b}_z = i\hbar\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right)$$

Problem 6-37. Consider a particle of mass m inside an infinite square potential well, see problem 6-32. Evaluate the expectation value of co-ordinate $\bar{x}$ using the eigenfunction

$$\psi = \frac{1}{\sqrt{a}}\cos\frac{n\pi}{2a}x$$

Solution: To evaluate $\bar{x}$ we have to apply the equation for expectations values

$$\bar{x} = \int_{-\infty}^{\infty} \Psi^*(x,t)\,\hat{x}\,\Psi(x,t)\,dx$$

to our case, i.e., to a situation where a particle is confined in an infinite square potential well $-a \leq x \leq a$. Thus we obtain

$$\bar{x} = \int_{-a}^{a} \frac{1}{\sqrt{a}}\left(\cos\frac{n\pi}{2a}x\right) x \frac{1}{\sqrt{a}}\left(\cos\frac{n\pi}{2a}x\right) dx = \frac{1}{a}\int_{-a}^{a} x\cos^2\frac{n\pi}{2a}x.dx$$

Note that the integrand is the product of $\cos^2\left(\frac{n\pi}{2a}x\right)$, which is an even function of x, times x itself, which is an odd function of x. The integrand is therefore an odd function of x. From this conclusion it follows that

$$\overline{x} = \frac{1}{a}\int_{-a}^{a} x\cos^2\frac{n\pi}{2a}x.\,dx = 0$$

because the integral of an integrand which is an odd function of the variable of integration is zero, if the integration is taken over a range which is centred about its origin.

Problem 6-38. Find the operator $\hat{b}^2$ of a square of angular momentum of a particle.

$$\left[\ \hat{b}^2 = -\hbar^2\left\{\left(z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right)^2 + \left(x\frac{\partial}{\partial z} - z\frac{\partial}{\partial x}\right)^2 + \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)^2\right\}\right]$$

Problem 6-39. Consider a particle of mass m inside an infinite square potential well, see problem 6-32. Evaluate the expectation value of momentum $\overline{p}$ using the eigenfunction

$$\psi = \frac{1}{\sqrt{a}}\left(\cos\frac{n\pi}{2a}x\right)e^{\frac{iEt}{\hbar}}$$

$[\ \overline{p} = 0]$

7. NUCLEAR PHYSICS

The nucleus of any nuclide consists of nucleons. **Nucleon** is the generic name given to the protons and neutrons in the nucleus.
The mass number A gives the total number of neutrons and protons in a nucleus.
The atomic number Z gives the number of protons in a nucleus.
The neutron number N gives the total number of neutrons in a nucleus.
In agreement with these definitions we can write

$$A = Z + N$$

Nuclides can be represented by the following symbols:

$${}^{A}_{Z}X \qquad X^{A}_{Z} \qquad {}_{Z}X^{A} \qquad XA$$

where X stays for a chemical symbol.
The isotopes of a given element have the same number of protons in the nucleus but different numbers of neutrons.
The radius of the nucleus of mass number A:

$$R \cong 1.5\,x\,10^{-15}\,A^{1/3}\ m$$

Nuclear masses are given in atomic mass units u,

$$1\ u = 1.661x10^{-27}\,kg.$$

One atomic mass unit is a mass equal to one-twelfth of the mass of a carbon C^{12}_{6} atom.

Nuclear binding energy is the energy required to tear a nucleus apart into its constituent separate protons and neutrons

$$E = \Delta m\, c^2$$

where

$$\Delta m = [\, Z\, m_p \; + (A\text{-}Z)\; m_n \,] - M_{nucleus}$$

A strong nuclear force is a short range, charge independent force which holds the nucleus together, despite the strong electrostatic repulsion between the protons in the nucleus.

Natural radioactivity is a process in which some atoms existing naturally on the earth spontaneously emit alpha, beta and gamma rays and change into other kinds of nuclei. Alpha particles are nuclei of helium He_2^4, beta particles are electrons, and gamma rays are extremely high-frequency electromagnetic waves.

The exponential decay law expresses the number N of radioactive nuclei present at time t as a function of the number of radioactive nuclei present at time $t=0$

$$N = N_0\; e^{-\lambda t}$$

where λ is the so called decay constant.

The half-life τ is the time required for half the nuclei in a sample of a particular species to decay radioactively. The relationship between the decay constant and half-life is

$$\lambda = \frac{0.693}{\tau}$$

A radioactive series is a set of radioactive nuclides decaying successively into each other by alpha decay (and/or other decay processes). The equilibrium condition for the number of nuclei N_2 of the parent and the number of nuclei N_1 of the daughter is

$$\frac{N_2}{N_1} = \frac{\tau_2}{\tau_1},$$

where τ_1 and τ_2 are the respective half-lives.

Nuclear activity is defined as the number of disintegrations of a particular species per second. The unit of activity is 1 becquerel (abbr. Bq):

1 Bq = 1 nuclear disintegration per second.

The absorbed dose is the energy absorbed by a given mass of material. It is measured in grays (abbr. Gy):

1 Gy = 1 J/kg.

Relative biological effectiveness RBE is a measure of the relative biological damage produced by equal doses of different kinds of ionising radiation.

The standard unit for measuring the **actual biological damage** to be expected from radiation is 1 sievert (abbr. Sv):

absorbed dose in sieverts = (absorbed dose in grays) x (RBE).

Alpha decay is the process of emission of alpha particles from a nucleus. As a result of this process the atomic number Z is reduced by 2 and the mass number A is reduced by 4. This nuclear reaction is described by the equation:

$$X_Z^A \rightarrow Y_{Z-2}^{A-4} + He_2^4$$

Beta decay is the process of emission of electrons from a nucleus which is described by the following equation

$$X_Z^A \rightarrow Y_{Z+1}^A + e_{-1}^0$$

During this process the mass number A stays the same and the atomic number Z is increased by one.

Since a gamma ray has no mass or electric charge, **gamma decay** has no effect on the mass number A or on the atomic number Z of a nucleus.

In any **nuclear reaction** the following quantities must be conserved:

a) number of nucleons
b) charge
c) total relativistic energy
d) linear momentum
e) angular momentum
f) parity.

Nuclear fission is a nuclear reaction which consists in breaking up a heavy nucleus into two nuclei of intermediate masses, together with the release of two or more neutrons and large amounts of energy.

Nuclear fusion is a nuclear reaction in which two light nuclei are combined to form a heavier nucleus, accompanied by the release of large amounts of energy.

A chain reaction is a reaction which results in the rapid build-up of energy which occurs in a nuclear bomb when the multiplication factor exceeds unity and the number of neutrons producing fission at successive stages of the reaction increases exponentially.

Problem 7-1. Compare the size of a uranium nucleus with that of a hydrogen nucleus.

Solution: Since the radius of a nucleus is given by the following expression

$$R \cong 1.5 \times 10^{-15} A^{1/3}$$

we have for the ratio of the radii of the two commonest isotopes of uranium and hydrogen

$$\frac{R\left(U_{92}^{238}\right)}{R\left(H_1^1\right)} = \frac{1.5 \times 10^{-15} \times (238)^{1/3}}{1.5 \times 10^{-15} \times (1)^{1/3}} = 6.2$$

Hence the uranium nucleus has a radius about six times that of a hydrogen nucleus. The volume of a uranium nucleus is 238 times larger than the volume of a hydrogen nucleus, since the volume depends directly on the mass number A.

Problem 7-2. An alpha particle He_2^4 with kinetic energy E_K=5.3 *MeV* heads directly toward a nucleus of gold Au_{79}^{197} at rest. How close does the alpha get to the centre of the gold nucleus before it momentarily comes to rest and reverses its course. Neglect the recoil of the massive gold nucleus.

Solution: To solve this problem we use the conservation of energy law. Initially the total mechanical energy of the system of two interacting particles is equal to the kinetic energy of the alpha particle E_K=5.3 *MeV*. At the moment when the alpha particle comes to rest, the total mechanical energy of the system is equal to the electrostatic potential energy E_p. Since total energy is a conserved quantity we can write

$$E_K = E_p$$

or

$$E_K = \frac{1}{4\pi\,\varepsilon_0}\frac{Q_\alpha\,Q_{Au}}{d}$$

where the charges of the alpha particle and the gold nucleus are $Q_\alpha = 2e$ and $Q_{Au} = 79e$ respectively, and d is the distance between the centres of the two particles. Solving the previous equation for distance we obtain

$$d = \frac{Q_\alpha\,Q_{Au}}{4\pi\,\varepsilon_0\,E_K} = \frac{2\ x\ 79\ x\left(1.6\ x\ 10^{-19}\right)^2}{4\pi\ 8.89\ x\ 10^{-12}\ x\ 5.3\ x\ 10^{6}\ x\ 1.6\ x\ 10^{-19}} = 4.29\ x\ 10^{-14}\ m$$

Problem 7-3. Calculate the binding energy of a deuterium atom. The mass of a deuterium atom is *2.014102 u*, the mass of a hydrogen atom is *1.007825 u*, and the mass of the neutron is *1.008665 u*.

Solution: The total mass of the nucleons of the deuterium atom is

$$1.008665u + 1.007825u = 2.016490u$$

The mass defect which is given as the difference between the sum of the masses of the nucleons forming a nucleus and the nucleus itself is therefore

$$\Delta m = 2.016490u - 2.014102u = 0.002388u$$

The binding energy is

$$E = \Delta m\ c^2 = 0.002388\ x\ 1.66053\ x\ 10^{-27}\ x\ (3\ x\ 10^{8})^2 = 3.5688\ x\ 10^{-13}\ J$$

Problem 7-4. A sample of Kr gas contains *2.00 x 10*^{20} atoms of Kr_{36}^{88}. What is the decay constant for Kr_{36}^{88}. At a time $t=11.2$ hours later, how many Kr_{36}^{88} remain? [The half-life of Kr_{36}^{88} is *2.8* hours].

Solution: The decay constant is

$$\lambda = \frac{0.693}{\tau} = \frac{0.693}{2.8 \times 3600} = 6.88 \times 10^{-5}\ s^{-1}$$

The number of atoms present after *11.2* hours is

$$N = N_0\, e^{-\lambda t} = 2.00 \times 10^{20} \times e^{-6.88 \times 10^{-5} \times 11.2 \times 3600} = 1.24 \times 10^{19}\ atoms.$$

Problem 7-5. Calculate which amount of radium Ra_{88}^{226} and radon Rn_{86}^{222} is in equilibrium with one gram of uranium U_{92}^{238}. The half-life of uranium $\tau_1 = 4.4x10^9$ years, the half-life of radium is $\tau_2 = 1590$ years and the half-life of radon is $\tau_3 = 3.825$ days.

Solution: Radium Ra_{88}^{226} and radon Rn_{86}^{222} are daughters in the radioactive series which begins with parent uranium U_{92}^{238}. The equilibrium condition for the number of nuclei N_2 of the parent and the number of nuclei N_1 of the daughter is

$$\frac{N_2}{N_1} = \frac{\tau_2}{\tau_1},$$

where τ_1 and τ_2 are the respective half-lives. Thus for the number of radium atoms we can write

$$N_2 = N_1 \frac{\tau_2}{\tau_1}$$

and for the number of radon atoms we have

$$N_3 = N_1 \frac{\tau_3}{\tau_1}.$$

The mass m of n atoms of a given element can be expressed as

$$m = \frac{M}{N} n$$

where M is the molar mass of this element and N is the Avogadro number. Consequently each kilogram of U_{92}^{238} contains

$$n_1 = \frac{6.02}{238} \times 10^{26} \text{ atoms.}$$

Finally for the mass of radium in equilibrium we obtain

$$m_2 = \frac{M_2}{N} n_1 \frac{\tau_2}{\tau_1} = \frac{226}{6.02 \times 10^{26}} \frac{6.02 \times 10^{26}}{238} \frac{1590}{4.4 \times 10^9} = 3.4 \times 10^{-7}\ kg$$

For the mass of radon in equilibrium we have

$$m_3 = \frac{M_3}{N} n_1 \frac{\tau_3}{\tau_1} = \frac{222}{6.02 \times 10^{26}} \frac{6.02 \times 10^{26}}{238} \frac{3.825}{4.4 \times 10^9 \times 365} = 2.2 \times 10^{-12} \, kg .$$

Problem 7-6. The isotope radium-*226* undergoes alpha decay. Write the reaction equation and determine the identity of the daughter nucleus.

Solution: From the periodic table of the elements (see appendix) we find that the atomic number of radium is 88. So the reaction will appear as follows:

$$Ra_{88}^{226} \rightarrow ? + He_2^4$$

The atomic number A of the daughter nucleus must be *222*, since the mass numbers must be equal on both sides of the arrow. By the same reasoning, the atomic number Z must be *86*. From the periodic table we find the element radon (*Rn*) has $Z=86$. The daughter nucleus is radon *Rn222* and the reaction is therefore:

$$Ra_{88}^{226} \rightarrow Rn_{86}^{222} + He_2^4$$

Problem 7-7. The isotope iodine-*131* undergoes beta decay. Write the reaction equation and determine the identity of the daughter nucleus.

Solution: From the periodic table we find that the atomic number Z of iodine is *53*. Therefore we have

$$I_{53}^{131} \rightarrow ? + e_{-1}^{0}$$

Since during this process the mass number A stays the same and the atomic number Z is increased by one we find that the daughter nucleus is xenon *Xe131*:

$$I_{53}^{131} \rightarrow Xe_{54}^{131} + e_{-1}^{0}$$

Problem 7-8. The isotope U_{92}^{238} undergoes 4 alpha decays and 2 beta decays. Write the reaction equation and determine the identity of the daughter nucleus.

Solution: The reaction can be described by the following equation:

$$U_{92}^{238} \rightarrow 4 \times He_2^4 + 2 \times e_{-1}^{0} + X_Z^A$$

From the conservation of mass law we have

$$238 = 4x4 + 0 + A$$

and from the conservation of an electric charge law we obtain

$$92 = 8 - 2 + Z$$

Thus we obtain for the mass number A of the unknown daughter nucleus $A=222$, and for the atomic number $Z=86$. From the periodic table we find that the daughter nucleus is radon Rn_{86}^{222}.

Problem 7-9. If a nuclear power plant generates power of *5 000 kW* how many kilograms of pure uranium *235* would be needed to produce electricity at this rate for a day, assuming that the power plant produces electricity with an efficiency of *16.7 %*. The fission of a uranium *235* nucleus releases about *200* MeV.

Solution: The energy contained in *1* kg of uranium is:

$$E = \frac{6.02 \; x \; 10^{26}}{235} 200 \; x \; 1.6 \; x \; 10^{-13} = 8.2 \; x \; 10^{13} \; J$$

The energy released by a power plant per one day is

$$E' = 5 \; x \; 10^{6} \; x \; 3600 \; x \; 24 = 4.3 \; 10^{11} \; J$$

Finally for one day's consumption of uranium we obtain

$$\frac{E' \; 100}{E \; 16.7} = 32 \; g$$

Problem 7-10. Calculate the binding energy per nucleon of a sodium Na_{11}^{23} nucleus. The mass of this atom is *22.98977u*.

$\left[8.11 \; MeV \; per \; nucleon \right]$

Problem 7-11. Identify the unknown particles in the following nuclear reactions:

a). The beta decay of cesium Cs_{55}^{137}.

b). The alpha decay of fermium Fm_{100}^{255}.

$\left[a) \; Ba_{56}^{137}, \; b) \; Cf_{98}^{251} \right]$