CHAPTER 3

Nuclear Processes and Neutron Physics

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Summary:

In this section, we first describe the nucleus, including its composition and the fundamental forces that affect its behaviour. Then, after introducing the concepts of radioactivity and nuclear decay, we discuss the various interactions between radiation and matter that can take place in and around a nuclear reactor. We finish with a presentation of neutron physics for fission reactors.

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1 Introduction

Energy production in an operating nuclear reactor is mainly the result of fission reactions initiated by neutrons. Following these reactions, radiation is produced in the form of alpha particles, electrons (β-particles), photons, and neutrons, as well as a large number of unstable nuclei (including actinides and fission products) that may decay, thereby producing additional radiation and energy. The neutrons generated directly in the fission reaction as well as those resulting from fission product decay are a key factor in maintaining and controlling the chain reaction as discussed in Chapters 4 and 5. Radiation also has an impact on the properties of the various materials in the core as well as on living cells. It is therefore important to understand how radiation interacts with matter if one needs, for example, to evaluate the radio-toxicity of burned fuel (Chapter 19) or to determine the kind of barrier that must be put in place to protect the public, the environment, or the personnel in a nuclear power plant (Chapter 12). Moreover, the energy produced by these decays contributes to heating the fuel, whether it is still in the reactor or in the spent fuel pools. The aim of this chapter is to provide the reader with an overview of the nuclear processes that take place in and around a reactor.

1.1 Overview

Several very important processes take place simultaneously in a nuclear reactor, including neutron slowdown as a result of collisions with nuclei, nuclear fission, and decay of radioactive nuclei with radiation emissions that subsequently lose energy or are absorbed.

To understand how all these physical processes take place, it is important to possess a general knowledge of the physics of the nucleus, including its composition and the fundamental forces that affect its behaviour. Although one rarely uses a description of the nucleus in terms of elementary particles and their interaction in power-reactor applications, such a description provides a practical background for a study of nuclear structure. In fact, the nucleus is such a complex object that it can be described only through simplified models that provide useful information. For example, the liquid drop model (Section 2.4) gives an empirical description of how one can extract energy from a nucleus by breaking it into smaller components (fission or decay) or by combining nuclei (fusion). These models are also used to predict the stability of a nucleus under various decay processes, the energy associated with its excited states, and the associated gamma-ray spectrum. In Section 2, an overview of the structure of the nucleus is provided, starting from a fundamental description and progressing to more practical models. We will also introduce some language specific to nuclear physics that will be useful throughout this book.

The majority of the fission reactions taking place in a reactor are initiated following the absorption of a neutron by a heavy nucleus. Radioprotection also involves the interaction between radiation, in the form of alpha particles, electrons, photons, and neutrons, and matter. Two important points must then be addressed before describing the physics of neutrons in a nuclear reactor: the source of this radiation and its behaviour over time, and the interaction of the emitted particles with matter. Therefore, Section 3 is divided into three parts: it starts with a description of radioactivity and the decay of nuclei, continues with a description of the interaction of ionizing radiation with matter (everything but neutrons), which is a very important topic for radiation protection studies, and ends with a brief discussion of the interaction of neutrons with matter.

The last section of this chapter is dedicated to the nuclear chain reaction. It starts by giving an extensive description of the fission reaction and discusses the need to slow down neutrons. This is followed by a description of the neutron transport equation that can be used to characterize the behaviour of neutrons inside a reactor.

1.2   Learning Outcomes

The goal of this chapter is for the reader to:

* Understand the fundamental forces in nature and the structure of the nucleus;
* Learn how to compute the mass of a nucleus based on the liquid drop model and to evaluate the energy released by the fission and fusion processes;
* Understand how to evaluate the activity and radio-toxicity of spent fuel;
* Become familiar with nuclear cross-section databases for neutrons and ionization radiation and the computation of reaction rates between particles and matter;
* Recognize the need to slow down neutrons in thermal reactors and to evaluate the effectiveness of a moderator.

2   Structure of the Nucleus

2.1   Fundamental Interactions and Elementary Particles

Four forces, or interactions, are currently sufficient to understand and explain nature from particle physics to astrophysics, including chemical and biological processes. These forces are classified relative to their intensity at the nuclear level (distances of the order of 1 fm) as follows:

* The strong force: responsible for the cohesion of the proton as well as the nucleus. This force is always attractive.
* The electromagnetic force: governs the physics of the atom and the associated chemical and biological processes. This force can be both attractive and repulsive.
* The weak force: responsible for the existence of the neutron as well as many other radioactive nuclei. This force is always attractive.
* The gravitational force: governs the large-scale structure of the universe. This force ensures the stability of the solar system as well as the fact that people can keep their feet on the ground. This force is always attractive.

From the point of view of physics, these forces arise from the specific intrinsic properties of the particles on which they act. For example, the electromagnetic force arises between two particles that have electric charges, while the gravitational force appears between two particles with masses (or more generally, between two particles with energy). For the strong force, the so-called "colour" of the particle plays a role equivalent to that of electric charge in electromagnetic interactions, while the weak force is the result of the interaction of two particles having a "weak" charge. **Table 1** provides a brief description of the general properties of the four fundamental forces, where the α's are dimensionless coupling constants related to the intensity of the interaction and the spatial dependence of the force is expressed in powers of r, the distance between the two interacting particles [Halzen1984]. For example, the electromagnetic force between two particles of charge ze and Ze is given by:

$$| \vec{F}(\vec{r}) | = \left(\frac{e^2}{4\pi\varepsilon_0} \right) \frac{zZ}{|r|^2} = (\alpha_e \hbar c) \frac{zZ}{|r|^2},$$ (1)

where $e = 1.6 \times 10^{-19}$ C is the charge of an electron, $\varepsilon_0 = 8.854 \times 10^{-12}$ F/m is the electric permittivity of vacuum, $\hbar = 1.0546 \times 10^{-34}$ J × s is the reduced Planck constant, and $c = 2.9979 \times 10^8$ m/s is the speed of light. For the gravitational force, the coupling constant is expressed in terms of proton masses. One can immediately see that the range of the gravitational and electromagnetic forces is substantially larger than that of the weak force due to their $\frac{1}{r^2}$ dependence. Accordingly, the weak force is important only when two particles with weak charges are in close contact. On the other hand, the strong (colour) force remains significant irrespective of the distance between particles with colour charge. This observation led to the concept of colour confinement, meaning that it is impossible to isolate a particle having a net colour charge different from zero [Halzen1984].

Table 1 Properties of the four fundamental forces

Force	Equivalent charge	Coupling constant	Spatial dependence
Strong	Colour charge	$\alpha_S \approx 1$	$\approx r^0$
Electromagnetic	Electric charge	$\alpha_e \approx 1/137$	r^{-2}
Weak	Weak charge	$\alpha_w \approx 10^{-6}$	r^{-5} to r^{-7}
Gravitational	Mass	$\alpha_G \approx 10^{-39}$	r^{-2}

In the standard model of particle physics [Halzen1984, Le Sech2010], these forces are repre-sented by 12 virtual particles of spin 1 called "gauge bosons":

- the massless photon that carries the electromagnetic interaction;
- eight massless gluons that carry the strong (colour) force;
- three massive bosons ($W^{\pm}$ and Z^0) that mediate the weak interaction.

These bosons are exchanged between the 12 "physical fermions" (spin 1/2 particles) that make up all the matter in the universe:

- six light fermions or leptons that have a weak charge. Three of these have no electric charge (the neutrinos), while three are charged (electron, muon, and tau);
- six heavy fermions or quarks that have colour, weak, and electric charges. These fermions cannot exist freely in nature because of colour confinement and must be combined in trip-lets of quarks or quark-antiquark pairs to form respectively baryons (protons, neutrons) and mesons (pion, kaon) that have no net colour charge.

Table 2 Properties of leptons and quarks

Leptons			Quarks		
Particle	Mass (GeV/c^2)	Charge	Particle	Mass (GeV/c^2)	Charge
e	0.000511	-1	u	≈ 0.003	2/3
ν_e	$< 2.5 \times 10^{-9}$	0	d	≈ 0.006	$-1/3$
μ	0.1057	-1	c	≈ 1.2	2/3
ν_μ	< 0.000170	0	s	≈ 0.1	$-1/3$
τ	1.7777	-1	t	≈ 173	2/3
ν_τ	< 0.018	0	b	≈ 4.1	$-1/3$

Table 2 provides a description of the main properties of leptons and quarks with the masses given in GeV/c^2, with 1 GeV/c$^2 \approx 1.782661 \times 10^{-27}$ kg, and the charges in terms of the charge of one electron [Le Sech2010].

2.2   Protons, Neutrons, and the Nuclear Force

The two lightest baryons that can be created out of a quark triplet are the positively charged proton, which is composed of two u quarks and one d quark, and the neutral neutron, made up of two d quarks and one u quark. These are present in the nucleus of all the elements present naturally in the universe. The main properties of the proton and the neutron are provided in **Table 3** [Basdevant2005]. One can immediately see that the masses of the proton and neutron are very large compared with those of the u and d quarks. In fact, most of their mass is a result of the strong colour force (gluon interaction). One can also observe that protons are stable, while neutrons are unstable and decay relatively rapidly into protons through the weak interaction. A second observation is that the magnetic moment, which is created by the movement of charged particles, is negative for the neutron. This confirms, at least partially, the theory that neutrons are made of quarks because even though the neutron is neutral, the distribution of charge inside it is not uniform.

Table 3 Main properties of protons and neutrons.

Property	Proton	Neutron
Mass (GeV/c^2)	$m_p = 0.938272$	$m_n = 0.939565$
Charge (electron charge)	1	0
Magnetic moment (μ_N)	$\mu_p = 2.792847$	$\mu_n = -1.913042$
Spin	1/2	1/2
Mean-life (s)	$\tau_p > 10^{36}$	$\tau_n = 881.5$

Although the proton and neutron have a neutral colour, they interact through the nuclear force, which is a residual of the strong colour force. However, instead of exchanging gluons directly, as do the quarks inside the proton or neutron, they interact by exchanging of virtual pion. As a result, the nuclear force is much weaker than the strong force in the same way that

the Van der Waals force between neutral atoms is weaker than the electromagnetic force. Moreover, in contrast to the strong colour force, the magnitude of the nuclear force decreases rapidly with distance, the nuclear interaction being given approximately by the Yukawa potential:

$$V_{Yukawa}(r) = -\alpha_N \hbar c \frac{e^{-\frac{m_\pi c r}{\hbar}}}{r}, \tag{2}$$

where m_π is the mass of the pion (140 MeV/c^2) and $\alpha_N \approx 14.5$ is a constant that controls the strength of the nuclear interactions between baryons (protons or neutrons). The minus sign here indicates that the resulting force ($\vec{F} = -\vec{\nabla}V$) is always attractive. This potential is identical for proton-proton, proton-neutron, and neutron-neutron interactions.

The strength of this force at short distances is so intense that it can compensate for the repulsive electromagnetic force between protons, leading to the formation of bonded nuclei as well as inhibiting neutron decay. For example, the helium nucleus, which is composed of two protons and two neutrons, is stable. Similarly, the stable deuteron is composed of one proton and one neutron. The absence in nature of a nucleus composed of two protons is not a result of the fact that the electromagnetic force is greater than the strong force, but rather due to the exact structure of the nuclear force. In addition to having a spatial behaviour provided by the Yukawa potential, this potential is also spin-dependent and repulsive between particles with anti-parallel spins (a nucleus with two protons having parallel spins is not permitted because of Pauli's exclusion principle). This also explains why stable nuclei containing only neutrons are not seen in nature.

2.3 Nuclear Chart

As indicated in the previous section, not all combinations of neutrons and protons can lead to bonded states. **Figure 1** provides a list of all bonded nuclei [Brookhaven2013, KAERI2013]. The points in red represent stable nuclei, while those in green indicate radioactive nuclei. The straight black line indicates nuclei having the same number of neutrons and protons. Note that this chart is quite different from the periodic table, where the classification of the elements is based on the number of electrons surrounding the nucleus. Because the number of electrons surrounding the nucleus is identical to Z, the number of protons inside the nucleus, each element corresponds to a combination of the nuclei that are found on a horizontal line of the nuclear chart. The nomenclature used to classify these nuclei is the following:

- The number of protons in the nucleus is used to identify the element. For example, all nuclei with $Z = 8$ are known as oxygen (atomic symbol O), independently of the number of neutrons present in the nucleus.

- For a given element, the specific isotope is identified by $A = Z + N$, where A is known as the mass number and N is the number of neutrons in the nucleus. For example, oxygen-17, denoted by ^{17}O, corresponds to an oxygen atom where the nucleus has eight protons and nine neutrons. Instead of the notation $^{N+Z}$X, with X the element associated with Z, the notation $^{N+Z}_{Z}$X is also found in the literature.
- Two other terms are less frequently used: isobars, corresponding to nuclei having the same mass numbers, but different values for Z and N; and isotones, corresponding to nuclei having the same number of neutrons, but a different number of protons.

Several conclusions can be reached from **Figure 1**:

- Isotopes containing a small number of protons ($Z < 20$) will generally be stable only if N and Z are nearly equal. If the difference $|N - Z|$ is slightly too large, the nucleus becomes unstable. For combination of protons and neutrons with large values of $|N - Z|$, no nuclei can be formed.
- For nuclei with values of Z ranging from 20 to 82, the number of excess neutrons ($N - Z$) required to create bonded nuclei increases steadily. One can also observe that for a specific value of Z, several stable nuclei can be produced with different numbers of neutrons.
- No stable nucleus exists with $Z > 83$, although some radioactive nuclides with $Z < 93$ can still be found in nature because they decay at a very slow rate. No isotope with Z above 92 remains in nature.

Approximately 3200 bonded nuclei have been identified, out of which 266 are stable. The stability of a nucleus is ensured by the presence of a sufficient number of neutrons to compensate for the effect of the Coulomb force between protons. Because the nuclear force acts only at short distances, while the Coulomb force has a longer range, additional neutrons are required when the radius R of the nucleus increases because of the presence of more nucleons (protons and neutrons):

$$R \propto A^{1/3} R_0, \tag{3}$$

where R_o is the average radius of a single nucleon.
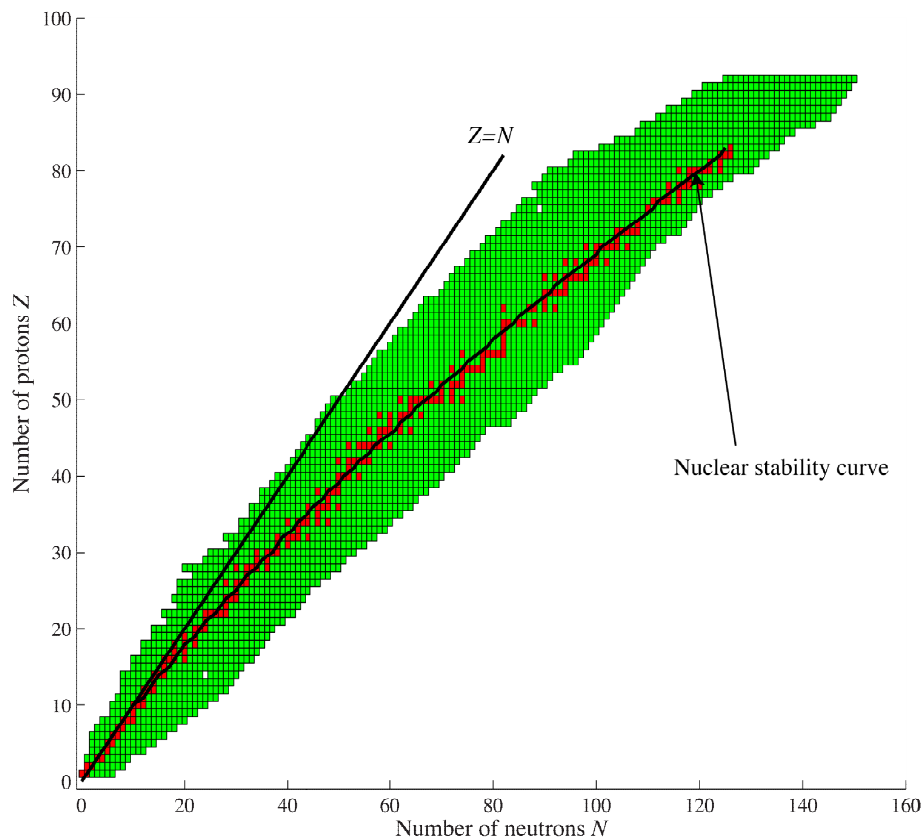
Figure 1 Nuclear chart, where N represents the number of neutrons and Z the number of protons in a nucleus. The points in red and green represent respectively stable and unstable nuclei. The nuclear stability curve is also illustrated.

The stability of a nucleus does not only depend on the number of nucleons it contains but also on how these protons and neutrons are paired. For example, out of the 266 stable nuclei:

- 159 contain an even number of protons and of neutrons,
- 53 have an even number of protons, but an odd number of neutrons,
- 50 have an odd number of protons and an even number of neutrons, and
- only 4 are made up of an odd number of protons and of neutrons.

In addition, for values of Z or N equal to 8, 20, 50, 82, and 126, the number of stable nuclei is very high. These numbers are known as "magic numbers". They suggest that the neutrons and protons, just like electrons in atoms, are more tightly bonded when they fill a quantum energy shell (see Section 2.5).

The mass m_{N+Z_X} of a nucleus produced by combining Z protons and N neutrons is less than the sum of the masses of its constituents:

$$m_{N+Z\,X} = Z\,m_p + Nm_n - AB/c^2,\tag{4}$$

where $B > 0$, the average binding energy per nucleon, is the result of the negative potential that binds the nucleons inside the nuclei. As can be seen in **Figure 2**, where a plot of B as a function of A is provided for stable nuclei, B first increases rapidly for low mass numbers, reaching a maximum around $A = 60$, and then decreases slowly with A. This means that, on the average, nucleons are more tightly bonded inside nuclei having intermediate values of A ($20 < A < 120$) than for very low or very high values.
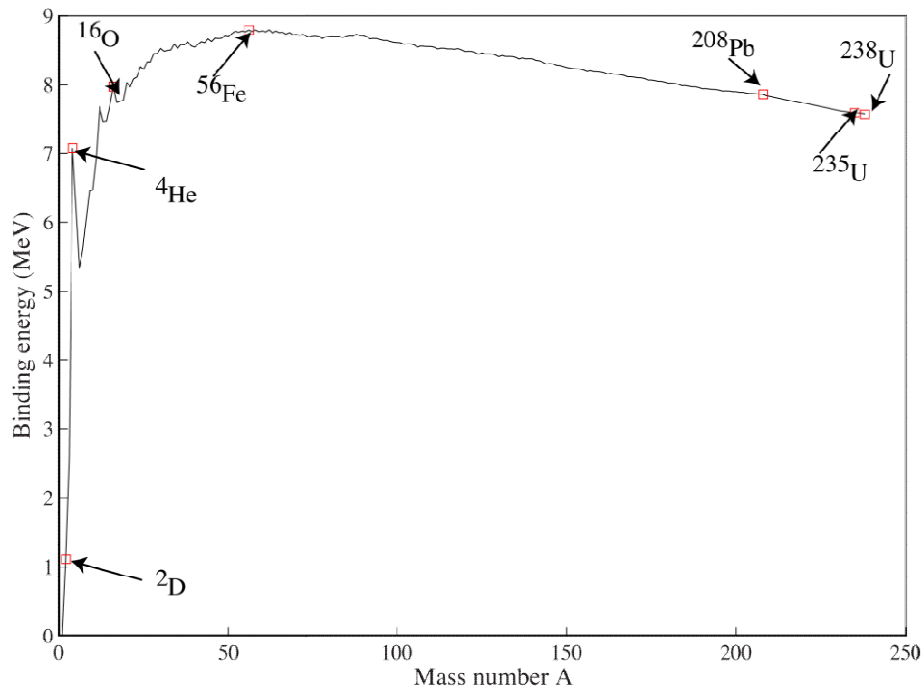
Figure 2 Average binding energy per nucleon (MeV) as a function of the mass number (number of nucleons in the nucleus).

Information on the atomic mass of over 3000 isotopes is available in [Livermore2013]. Note that the atomic mass is different from the nuclear mass of an isotope because it includes both the mass and the binding energy of the Z electrons gravitating around the nucleus. One simple way to compute the atomic mass is using

$$M_{N+Z}X \approx Z\,M_{^1H} + Nm_n - AB/c^2, \tag{5}$$

where the mass of the proton has been replaced by that of the hydrogen atom, which includes the electron mass as well as its binding energy. The approximation sign comes from the fact that the binding energy of each of the Z electrons around a heavy nucleus is different from that of a single electron attached to a proton in the hydrogen atom.

Finally, the natural composition of a given element will include stable as well as some radioactive isotopes. Assuming that the relative atomic abundance of isotope i of atomic mass M_i in the natural element is γ_i, then the mass of the natural element is given by:

$$M_X = \sum_i \gamma_i M_i. \tag{6}$$

In reactor physics, one often works with the mass (or weight) fraction for the abundance of an isotope, defined as:

$$w_i = \frac{\gamma_i M_i}{M_X}. \tag{7}$$

For completeness, one can compute the isotopic concentration N_X of an element (atoms/cm^3) with atomic mass M_X (g/moles) and density ρ (g/cm^3) using:

$$N_X = \frac{\rho}{M_X}\,\mathbb{N}_A, \tag{8}$$

where $\mathbb{N}_A = 6.022 \times 10^{23}$ atoms/moles is the Avogadro number. The concentration of isotope i is then given by:

$$N_i = \gamma_i\,\frac{\rho}{M_X}\,\mathbb{N}_A = \gamma_i N_X. \tag{9}$$

More information related to the isotopic contents of natural elements can be found in [KAERI2013, WebElements2013].

2.4 Nuclear Mass and the Liquid Drop Model

As discussed in Section 2.3, the mass of the nucleus is smaller than its classical mass (the mass of its constituents) because the strong force linking the nucleons reduces the global energy of the nuclear system, the binding energy being related to the missing mass Δm_X according to

$$\Delta m_X c^2 \approx AB. \tag{10}$$

This missing mass is very difficult to compute based on theoretical models because the form of the nuclear potential is known only approximately and because quantum models involving more than two particles in interaction cannot be solved exactly. For evaluation of the missing mass, one generally relies on a semi-empirical model known as the liquid drop model. The main assumption used in this model is that the nuclear force is identical for protons and neutrons.

The liquid drop model first assumes that each of the A nucleons in the nucleus sees the same nuclear potential [Basdevant2005]. Moreover, this potential is independent of the number of nucleons in the nucleus. This second assumption can be justified by the fact that the range of the nuclear force is small, and therefore each nucleon feels the effect of only the limited

number of nucleons that are close by. Accordingly, the contribution to the missing mass from the A nucleons is given by:

$$\Delta m_V c^2 = a_V A, \tag{11}$$

where the constant $a_V \approx 15.753$ MeV has been determined experimentally. This contribution is known as the volume effect because the volume of a nucleus can be assumed to be proportional to the number of nucleons it contains. This term would be sufficient if the nucleus had an infinite size. However, this is not the case, and the protons and neutrons that are located near the boundary of the nucleus will interact with a smaller number of nucleons. If the surface of the nucleus is given by $4\pi R^2 \propto A^{2/3}$, one can assume that the $A^{2/3}$ nucleons near the outer surface of the nucleus see a reduced uniform potential. This leads to a negative surface contribution to the mass defect of the form:

$$\Delta m_S c^2 = -a_S A^{2/3}, \tag{12}$$

where $a_S \approx 17.804$ MeV.

Until now, only the nuclear force has been taken into account. However, the protons present inside the nucleus repel each other through the Coulomb force, thereby decreasing the binding energy. Because the potential associated with this force is long-range ($V(R) \propto 1/R \propto 1/A^{1/3}$), each of the Z protons will interact with the remaining $Z-1$ protons, leading to a contribution of the form:

$$\Delta m_C c^2 = -a_C \frac{Z(Z-1)}{A^{1/3}} \approx -a_C \frac{Z^2}{A^{1/3}}, \tag{13}$$

where only the dominant term in Z has been preserved, and $a_C \approx 0.7103$ MeV.

It can be observed in the nuclear chart that stable nuclei with a low mass number generally contain an equal number of protons and neutrons. As the number of excess neutrons or protons in a nucleus increases, it becomes more and more unstable until no bonded state can be produced. This means that nuclear binding should decrease as a function of $|N - Z| = |A - 2Z|$, the form of the contribution being

$$\Delta m_A c^2 = -a_A \frac{(A-2Z)^2}{A}, \tag{14}$$

where $a_A \approx 23.69$ MeV is known as the asymmetry term. The nuclear chart also shows that few stable nuclei with an odd number of neutrons and protons (odd-odd nuclei) can be found in nature, while the number of isotopes with an even number of protons and neutrons (even-even nuclei) dominates. This means that the binding energy should be large for even-even and small for odd-odd nuclei. Assuming that the contribution to the missing mass presented previously remains valid only for odd-even or even-odd nuclei (A odd), an additional empirical correction of the form

$$\Delta m_P c^2 = (-1)^Z a_P \frac{\left(1+\left(-1\right)^A\right)}{2A^{3/4}} \tag{15}$$

is required. Here, $a_P \approx 33.6$ MeV is known as the pairing term.

The final formula for the missing mass is therefore

$$\Delta m_X c^2 \approx a_V A - a_S A^{\frac{2}{3}} - a_C \frac{Z^2}{A^{\frac{1}{3}}} - a_A \frac{(A-2Z)^2}{A} + (-1)^Z a_P \frac{\left(1+(-1)^A\right)}{2A^{3/4}}, \tag{16}$$

which is known as the Bethe-Weizsäcker or semi-empirical mass formula (SEMF). Even if this mechanistic model is relatively simple, it provides a very good approximation to the mass of the nuclei found in nature. It can also be used to determine the value of A that minimizes the mass of a nucleus for a specific value of Z, thereby maximizing the probability that it is stable. Neglecting the pairing term, one then obtains

$$Z(A) = \frac{4Aa_A + A\left(m_n - m_p\right)c^2}{8a_A + 2a_C A^{\frac{2}{3}}}. \tag{17}$$

This equation, which is also illustrated in **Figure 1** (the nuclear stability curve), closely follows the nuclear stability profile.

The main weakness of the liquid drop model is its lack of predictive power. For example, it neither explains the presence of "magic numbers", nor the gamma-ray absorption spectrum, nor the decay characteristics of different nuclei. These explanations can be obtained only by looking at the interactions between protons and neutrons using quantum theory, as explained in the next section.

2.5 Excitation Energy and Advanced Nuclear Models

All chemists and physicists are familiar with atomic "magic numbers", even though the explicit term is rarely used. For example, the number of electrons in noble gases could be considered "magic" because these gases are odourless, colourless, and have very low chemical reactivity. For such atoms, all the states associated with principal quantum energy levels 1 to n are occupied by electrons (closed or filled shells). In addition, the absorption (emission) spectrum of light by different atoms is the result of electrons being excited (de-excited) from one electronic shell to another. One can therefore expect nuclear magic numbers to have a similar nature, namely, that only specific energy levels are permitted for the protons and neutrons when they are bonded inside a nucleus (which would explain also the photon emission and absorption spectra). These energy levels are not uniformly distributed, but occur in bands called *shells*. The fact that all the quantum states in a shell (a neutron or proton shell) are occupied by a nucleon increases the stability of the nucleus compared to nuclides with partially filled shells.

To obtain the energy levels permitted for protons and neutrons inside the nucleus, one needs to solve the quantum-mechanics Schrödinger equation for A strongly coupled nucleons [Griffiths2005]. However, when trying to solve this equation, two problems arise:

* the Schrödinger equation has no analytic solution for problems where three or more particles are coupled;
* the interaction potential between nucleons is not known exactly.

As a result, this many-body problem is generally simplified using the following assumptions that are inherent to the shell model [Basdevant2005]:

* each nucleon in the nucleus is assumed to move independently without being affected by the displacement of other nucleons;

- a nucleon moves in a potential $V(r)$ that is relatively uniform inside the nucleus and increases sharply near its outer surface, namely when $r \approx R$ (mean field approximation).

Note that in this model, there are no one-to-one interactions between the nucleons. This means that instead of solving the Schrödinger equation for A strongly coupled nucleons, the problem is reduced to the solution of A independent Schrödinger equations for a single nucleon with an averaged potential. The conventional nuclear potential used in the shell model is the Saxon-Wood potential (see **Figure 3**), which has the form [Basdevant2005]:

$$V(r) = -V_0 \left(\frac{1}{1 + e^{(r-R)/R}} \right), \tag{18}$$

where $V_0 \approx 30$ MeV is the potential depth and $R \propto A^{1/3}$ is the radius of the nucleus in fm.
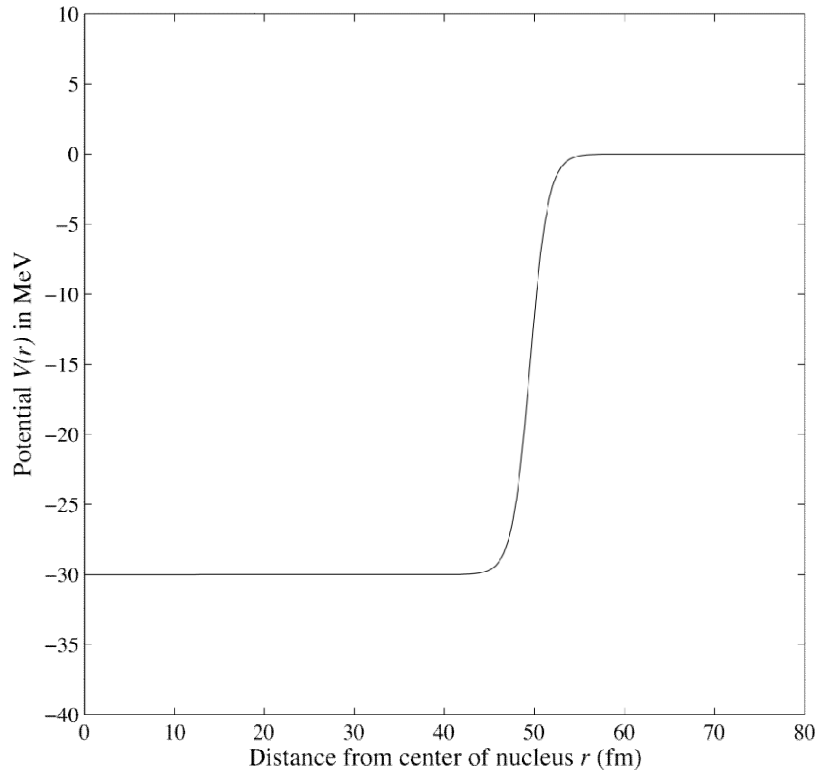
Figure 3 Saxon-Wood potential seen by nucleons inside the uranium-235 nucleus.

The energy levels are then very similar to those associated with the harmonic potential, namely

$$E_N = \frac{\hbar \sqrt{2V_0}}{R \sqrt{m_n}} \left(N + \frac{3}{2} \right), \tag{19}$$

where m_n is the mass of a nucleon (proton or neutron), $N = (2n + l - 2) = 0,1,2,\cdots$ with $n = 1,2,\cdots$ the principal quantum number, and $l = 0,1,2,\cdots$ the angular momentum quantum number that takes into account spin-orbit coupling. In general, one assumes that the energy is independent of the magnetic quantum number m. The spin j of each of the nucleons, which is important when determining the probability of interaction between a nucleus (spin J) and other particles, is a combination of its internal spin and its angular momentum:

$$j = \left(l \pm \frac{1}{2} \right). \tag{20}$$

The energy states of the shell model are presented in **Table 4**, whereas the association between the magic numbers and these states is illustrated in **Figure 4**.

The model is never used to evaluate the mass of nuclei (the SEMF model is used for this purpose), but it is useful for classifying the energy levels of excited nuclei (denoted as $(^{N+Z}_{Z}\text{X})^{*}$) and for determining the magic numbers.

Table 4 Energy states in the shell model, where *g* is the degeneracy level of a state.

N	0	1	2	2	3	3	4	4	4
n	1	1	1	2	1	2	1	2	3
l	0	1	2	0	3	1	4	2	0
g	2	6	10	2	14	6	16	10	2
orbital	1s	1p	1d	2s	1f	2p	1g	2d	3s
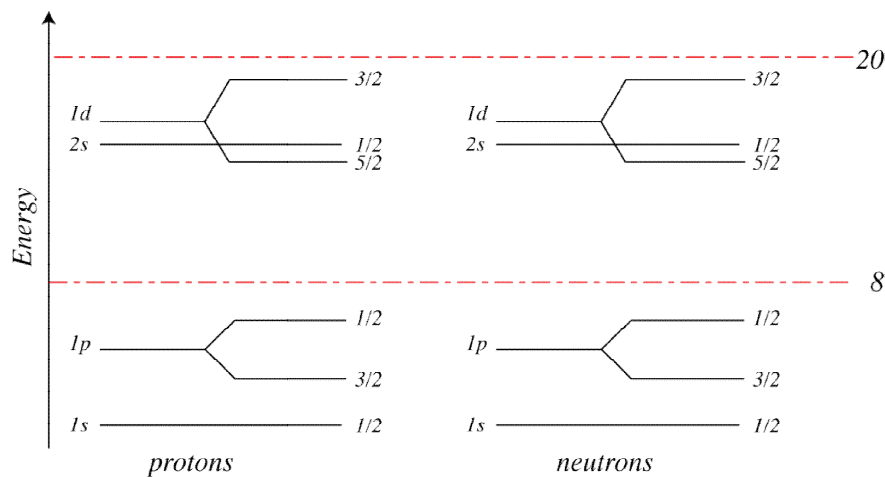
Figure 4 Shell model and magic numbers.

The second model that is often used is the collective model of the nucleus. Here, instead of looking at the motion of the individual nucleons, one considers the overall rotation and vibration movement of the nucleus. The justification for this model is that most nuclei take the shape of an ellipsoid (only nuclei that contain magic numbers of protons and neutrons are spherical). Distorted nuclei can then acquire rotational and vibrational motions, to which quantized energy levels can be associated. In classical mechanics, the energy of a rotating solid having a moment of inertia I and an angular momentum J is given by [Basdevant2005, Wong2004]:

$$E = \frac{J^2}{2I}, \tag{21}$$

In quantum mechanics, the angular momentum is quantized, with the energy levels being given by

$$E_J = \hbar^2 \frac{J(J+1)}{2I},$$ (22)

with $J = 0,1,2,\cdots$. For nucleus having an ellipsoid shape, only even values of J are allowed, and the energies satisfy the following relation:

$$E_2 = \frac{3}{10}E_4 = \frac{1}{17}E_6 = \frac{1}{12}E_8,$$ (23)

with

$$E_2 = \frac{15\hbar^2}{2MR^2},$$ (24)

where M and R are respectively the mass and radius of the nucleus. These energy levels are generally much smaller than those associated with the shell model.

2.6 Nuclear Fission and Fusion

Let us look back at **Figure 2**, where the average binding energy per nucleon is provided as a function of mass number. As mentioned previously, this curve indicates that the total binding of one heavy nuclide containing $A > 180$ nucleons, which is given by

$$E_A = AB(A),$$ (25)

is larger than that of two identical nuclides containing $A/2$ protons and neutrons:

$$2E_{A/2} = AB\left(\frac{A}{2}\right) > E_A.$$ (26)

In physical terms, this means that two lighter nuclides generally represent a lower energy state than a heavier nucleus. Accordingly, a spontaneous reaction where the heavy nuclide, H, breaks down into two smaller components (L_1 and L_2) is permitted from an energy-conservation point of view, with the energy released by the reaction given by $E_{L_1} + E_{L_2} - E_H$. This spontaneous reaction, called fission, has been observed experimentally for long-lived actinides such as ^{232}Th, ^{235}U, and ^{238}U, even though this is not their preferential decay mode (seven in 10^9 decays of ^{235}U follow this path). For example, the spontaneous fission reaction

$$^{235}_{92}U \Rightarrow 2\,^1_0n + \,^{133}_{50}Sn + \,^{100}_{42}Mo,$$ (27)
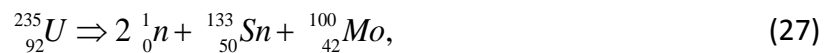
which releases 116 MeV, has been observed.

A second observation is that, even if a spontaneous fission reaction is very improbable, the fission process can be initiated externally by an absorption collision between a projectile and a heavy nuclide. For example, the neutron-induced reaction,

$$^1_0n + \,^{235}_{92}U \Rightarrow 3^1_0n + \,^{133}_{50}Sn + \,^{100}_{42}Mo,$$ (28)
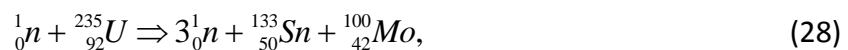
is possible even with very low-energy neutrons and produces the same amount of energy as the spontaneous fission reaction above. This reaction is facilitated by the fact that the main

interaction between the neutron and a nucleus is the attractive nuclear force. The fact that several neutrons are generally produced following such reactions finally leads to the concept of a controlled chain reaction, if sufficient neutrons are produced following a fission reaction to initiate another fission reaction. The conditions required to achieve and maintain such a chain reaction are discussed in Section 4.

Figure 2 also indicates that the nucleons inside very light nuclides are loosely bonded compared to intermediate-mass nuclei. Combining two such nuclides could therefore result in a nucleus that is more strongly bonded, again releasing energy. This process is called nuclear fusion. Examples of such exothermal fusion reactions are

$$_{1}^{2}H + _{1}^{3}H \Rightarrow _{0}^{1}n + _{2}^{4}He, \tag{29}$$

$$_{1}^{2}H + _{2}^{3}He \Rightarrow _{1}^{1}H + _{2}^{4}He, \tag{30}$$

which release respectively 17.6 and 18.3 MeV in the form of kinetic energy for the final fusion products. Producing such reactions is much more difficult than neutron-induced fission because the two initial nuclides have positive charges and must overcome the Coulomb force to come into close contact. This can be achieved by providing sufficient kinetic energy (plasma temperature) for a sufficient long time (confinement) to ensure that the energy released by fusion is greater than the energy required to reach these conditions (the break-even point). The two main technologies that are currently able to attain the conditions necessary for controlled nuclear fusion are based respectively on confinement by magnetic fields (Tokamak) and inertial confinement (fusion by laser).

3   Nuclear Reactions

From the nuclear chart (**Figure 1**), it is clear that only 266 nuclides are stable. This means that most of the bonded nuclei that can be created will decay. This raises two questions:

- How do they decay?
- How are they created?

Another observation is that if one succeeds in creating a nucleus (stable or not), it may not necessarily be in its fundamental (ground) energy state (see Section 2.5). These are the main questions to answer in the first part of this section. We start by discussing the decay process before continuing with a description of nuclear reactions. The second topic involves the interaction of particles with matter, with most of these particles being produced during the decay process.

3.1   Radioactivity and Nuclear Decay

Nuclear decay, the emission of radiation from an unstable nucleus or radioisotope, is a stochastic process controlled by the laws of statistics and physics. Therefore, it cannot take place unless several fundamental quantities are conserved [Basdevant2005, Smith2000]:

- total energy (including mass, which is a form of energy according to special relativity);
- linear momentum;
- angular momentum;
- electric charge;
- leptonic charge; and
- baryonic charge.

The latter two are required because of the intrinsic properties of quarks and leptons. For common nuclear reactions, these last two conservation relations can be translated to:

- conservation of electrons and neutrinos where the electron and the neutrino have a leptonic charge of +1 and the positron (anti-electron) and anti-neutrino have a leptonic charge of -1; and
- conservation of the total number of protons plus neutrons (mass number).

A decay process transforms, through emission of particles, a parent nucleus into a more stable daughter nucleus (a nucleus with a lower mass where the nucleons are more strongly bonded or equivalently have a lower mass). In fact, if one considers a nucleus at rest that decays according to the following reaction:

$$ {}^{A}_{Z}X \Rightarrow {}^{B}_{W}Y + \sum_{i=1}^{N} {}^{C_i}_{V_i}b, \tag{31} $$

then total energy conservation implies that

$$ m_{{}^{A}_{Z}X}c^2 = \left(m_{{}^{B}_{W}Y}c^2 + T_{{}^{B}_{W}Y} \right) + \sum_{i=1}^{N} \left(m_{{}^{C_i}_{V_i}b}c^2 + T_{{}^{C_i}_{V_i}b} \right), \tag{32} $$

where T is the kinetic energy of the different decay products. This reaction can take place spontaneously only if

$$ T_{{}^{B}_{W}Y} + \sum_{i=1}^{N} T_{{}^{C_i}_{V_i}b} = m_{{}^{A}_{Z}X}c^2 - m_{{}^{B}_{W}Y}c^2 - \sum_{i=1}^{N} m_{{}^{C_i}_{V_i}b}c^2 > 0, \tag{33} $$

$$ Z = W + \sum_{i=1}^{N} V_i, \tag{34} $$

$$ A = B + \sum_{i=1}^{N} C_i, \tag{35} $$

that is, when the energy balance is favourable (the last two equations are for mass number and charge conservation). For a nucleus in an excited state, the daughter nucleus will often be the same as the parent nucleus, but at a different energy level (ground or lower-lying excited state), the secondary particle being a photon (a γ-ray because the photon is produced following a nuclear reaction).

Nuclear decay is characterized by a constant λ defined according to [Smith2000, Nikjoo2012]:

$$ \lambda = \lim_{\Delta t \to 0} \frac{-\Delta N(t) / N(t)}{\Delta t}, \tag{36} $$

where $N(t)$ is the number of nuclei present at time t, $\Delta N(t)$ is the change (negative because of the decay process) in the number of nuclei after time Δt, and λ is known as the decay constant. This definition leads to the Bateman equation [Bell1982]:

$$ \frac{dN(t)}{dt} = -\lambda N(t) + S(t), \tag{37} $$

where $S(t)$ represents the net rate of production of nuclei (from the decay of other nuclei or from nuclear reactions). One can also define

$$A(t) = \lambda N(t),$$ (38)

the activity of a radionuclide that represents the number of decays per second taking place at time t. This activity is generally stated in Becquerels (Bq), where 1 Bq corresponds to one decay per second. For the case where $S(t) = 0$, the solution to the Bateman equation has the form

$$N(t_0 + \Delta t) = N(t_0)e^{-\lambda \Delta t},$$ (39)

where $N(t_0)$ is the number of nuclei at time t_0.

Two other concepts related to decay constants are also commonly used. The mean life, τ, defined as

$$\tau = \frac{1}{\lambda},$$ (40)

represents the average time required for the final number of nuclei to reach a value of $N(t_0)/e$:

$$N(t_0 + \tau) = \frac{N(t_0)}{e}.$$ (41)

Similarly, the half-life, $t_{1/2}$,

$$t_{1/2} = ln(2)\tau = \frac{ln(2)}{\lambda},$$ (42)

represents the average time required for the initial number of nuclei to decrease to a value of $N(t_0)/2$.

For some radionuclides, several decay reactions (decay channels) may be observed, each being characterized by a specific relative production yield Y_j such that

$$\sum_{j=1}^{J} Y_j = 1.$$ (43)

The decay constant associated with each channel is given by $\lambda_i = \lambda Y_i$. For example, potassium-40 ($^{40}_{19}K$), which has a mean life of 1.805×10^9 years, decays 89.28% of the time into calcium-40 ($Y_{^{40}_{20}Ca} = 0.8928$) and 10.72% of the time into argon-40 ($Y_{^{40}_{18}Ar} = 0.1072$).

Note that the decay constant, λ, associated with a reaction can be evaluated using Fermi's second golden rule [Schiff1968]:

$$\lambda = \sum_f \int \frac{2\pi}{\hbar} \left| \langle f|H'|i \rangle \right|^2 \rho(f,\Xi)\,d\Xi,$$ (44)

where $|i\rangle$ is the wave function associated with the initial state, $\langle f|$ is the wave function associated with a final state, and H' is the interaction potential associated with the reaction. The integral is over phase space $d\Xi$, with the term $\rho(f, \Xi)$ being the density of state for the final wave function.

The most common decay reactions are the following:

γ-ray emission for an excited nucleus:
$$({}_{Z}^{A}X)^{*} \Rightarrow {}_{Z}^{A}X + \gamma. \tag{45}$$

Internal conversion for an excited nucleus:
$$({}_{Z}^{A}X)^{*} \Rightarrow [{}_{Z}^{A}X]^{+} + e_{-}. \tag{46}$$
This process corresponds to the direct ejection of an orbital electron leaving the nucleus in an ionized state ($[{}_{Z}^{A}X]^{+}$).

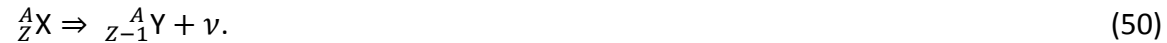β^{-} decay (weak interaction) for a nucleus containing too many neutrons:
$$_{Z}^{A}X \Rightarrow [{}_{Z+1}^{A}Y]^{+} + e_{-} + \bar{\nu}. \tag{47}$$

Neutron emission (nuclear interaction) for a nucleus having a very large neutron excess:
$$_{Z}^{A}X \Rightarrow {}^{A-1}_{Z}X + {}_{0}^{1}n. \tag{48}$$

β^{+} decay (weak interaction) for a nucleus containing too many protons:
$$_{Z}^{A}X \Rightarrow [{}_{Z-1}^{A}Y]^{-} + e_{+} + \nu. \tag{49}$$

Orbital electron capture (weak interaction) for a nucleus containing too many protons:
$$_{Z}^{A}X \Rightarrow {}_{Z-1}^{A}Y + \nu. \tag{50}$$

Proton emission (nuclear interaction) for a nucleus having a very large proton excess:
$$_{Z}^{A}X \Rightarrow [{}_{Z-1}^{A-1}Y]^{-} + {}_{1}^{1}p = {}_{Z-1}^{A-1}Y + H_{1}^{1}. \tag{51}$$
This process corresponds to the ejection of an atom of hydrogen.

α-emission for heavy nuclei (nuclear interaction):
$$_{Z}^{A}X \Rightarrow [{}_{Z-2}^{A-4}Y]^{2-} + {}_{2}^{4}\alpha = {}_{Z-2}^{A-4}Y + {}_{2}^{4}He. \tag{52}$$
This process corresponds to the ejection of an atom of helium.

Spontaneous fission for heavy nuclei (nuclear interaction):
$$_{Z}^{A}X \Rightarrow C\ {}_{0}^{1}n + {}_{Y}^{B}F + {}^{A-B-C}_{Z-Y}G. \tag{53}$$
This process corresponds to the fragmentation of a heavy nucleus into two or more smaller nuclei with the emission of several neutrons.
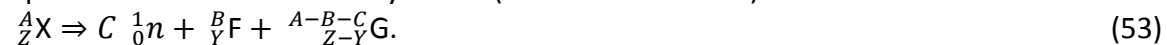
For heavy or very unstable nuclei (see, for example, **Figure 5** for uranium-238), several of these reactions must often take place before a stable isotope is reached.

The Janis software from OECD-NEA can be used to retrieve and process the decay chain for all isotopes [OECD-NEA2013].
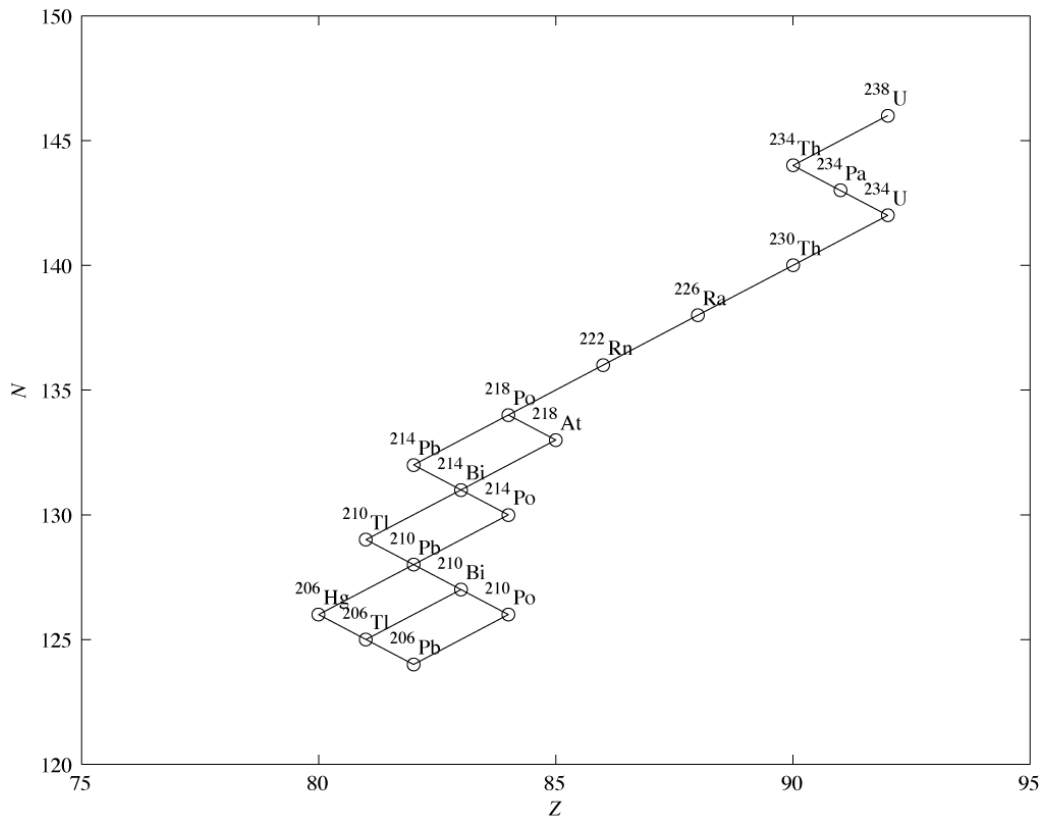
Figure 5 Decay chain for uranium-238 (fission excluded). The type of reaction (β or α-decay) can be identified by the changes in N and Z between the initial and final nuclides.

3.2   Nuclear Reactions

As we saw in the previous section, several types of particles are produced through decay of radioactive nuclides. These particles have kinetic energy, and as they travel through matter, they interact with orbital electrons and nuclei. A nuclear reaction takes place if these particles produce after a collision one or more nuclei that are different from the original nucleus (an excited state of the original nucleus or a new nucleus). Otherwise, the collision gives rise to a simple scattering reaction where kinetic energy is conserved.

For the case where charged particles are traveling through a material, scattering collisions with the orbital electrons or the nucleus are mainly observed (also called potential scattering). More rarely, the charged particles are captured by the nucleus to form a compound nucleus (a very short-lived, semi-bonded nucleus) that can decay through various channels.

Similarly, the electric and magnetic fields associated with the photons interact mostly with the nucleus or the orbital electrons. They can also initiate nuclear reactions after being absorbed in the nucleus. Finally, neutrons rarely interact with electrons because they are neutral particles and the electrons are not affected by the nuclear force (electromagnetic interaction with the quarks inside the nucleon, magnetic interactions with unpaired electrons, and weak interactions are still present). However, they can be scattered (nuclear potential scattering) or absorbed (nuclear reaction) by the nucleus. Again, this absorption can lead to the formation of a very unstable compound nucleus that will decay rapidly.

The main nuclear reactions of photons, electrons, neutrons, and charged heavy particles with nuclei are often the inverses of the decay reactions presented earlier:

γ − ray absorption:

$$\gamma + {}^A_Z X \Rightarrow \left({}^A_Z X \right)^*. \tag{54}$$

γ-ray scattering (elastic and inelastic):

$$\gamma + {}^A_Z X \Rightarrow \left({}^A_Z X \right)^* + \gamma^*. \tag{55}$$

electron capture:

$$e_- + {}^A_Z X \Rightarrow \left[{}^A_{Z-1} Y \right]^+ + v + \gamma. \tag{56}$$

positron capture:

$$e_+ + {}^A_Z X \Rightarrow \left[{}^A_{Z+1} Y \right]^- + \bar{v} + \gamma \tag{57}$$

proton capture:

$$p^1_1 + {}^A_Z X \Rightarrow \left[{}^{A+1}_{Z+1} Y \right]^- + \gamma. \tag{58}$$

α capture:

$$\alpha^4_2 + {}^A_Z X \Rightarrow \left[{}^{A+4}_{Z+2} Y \right]^{2-} + \gamma. \tag{59}$$

neutron capture:

$$ {}^1_0 n + {}^A_Z X \Rightarrow {}^{A+1}_Z X + \gamma. \tag{60}$$

neutron scattering (elastic and inelastic):

$$ {}^1_0 n + {}^A_Z X \Rightarrow \left({}^A_Z X \right)^* + {}^1_0 n + \gamma. \tag{61}$$

photon-induced fission:

$$\gamma + {}^A_Z X \Rightarrow C {}^1_0 n + {}^B_Y F + {}^{A-B-C}_{Z-Y} G + \gamma. \tag{62}$$

neutron-induced fission:

$$ {}^1_0 n + {}^A_Z X \Rightarrow C {}^1_0 n + {}^B_Y F + {}^{A+1-B-C}_{Z-Y} G + \gamma. \tag{63}$$

These reactions must obey the same conservation laws as those described earlier for the decay reaction. For most reactions (except elastic scattering), the final nucleus will be in a highly excited state and will decay rapidly by γ-ray emission (prompt photons).

The probability that any given reaction will take place between a nucleus and a particle is represented by the microscopic cross section σ. Much like the decay constant, the cross sections have a quantum mechanical interpretation and can be expressed in terms of the wave function $|i\rangle$ associated with the initial state (the product of the wave functions of the projectile and the nucleus), the wave function $\langle f|$ associated with the final state, and H', the interaction potential. The differential cross section is then given by Fermi's first golden rule, which can be written as:

$$\frac{d\sigma}{d\Xi} = \frac{2\pi V}{\hbar v_i} \left\langle \left| f | H' | i \right\rangle \right|^2 \rho(f), \tag{64}$$

where V is the volume of the system, v_i is the velocity of the projectile (assuming that the initial nucleus is at rest), and $\rho(f)$ is again the density of states in the phase space Ξ for final particles. The cross section, which is then the integration over the final phase space of the differential cross section, has units of surface. The most common unit used for the microscopic cross section is the barn (b), with $1\text{ b} = 10^{-24}\text{ cm}^2 = 10^{-28}\text{ m}^2$.

These cross sections are very difficult to evaluate explicitly because of the complexity of the wave functions (the wave function for a nucleus is the product of the wave functions of all the nucleons in the nucleus bonded by the nuclear potential) and the interaction potential. These are generally evaluated experimentally, and the results are stored in evaluated nuclear data files. A software package such as Janis can be used to retrieve and analyze these cross sections [OECD-NEA2013]. For computational reactor physics, the NJOY program is generally used to process the cross-section databases for neutron-induced reactions [MacFarlane2010].

3.3   Interactions of Charged Particles with Matter

As mentioned earlier, charged particles traveling through matter interact mainly with atomic electrons because they are much more numerous than nuclei (Z electrons for a nucleus with atomic number Z) and also because the wave functions associated with these electrons have a very large spatial extension (the size of an atom) compared to that associated with the nucleus.

Heavy particles, such as protons, α-particles, and ions, are scattered by the Coulomb potential produced by the electron, with the cross section given by the Mott scattering formula [Leroy2009, Bjorken1964]. As a result, a heavy particle loses a very small quantity of energy and momentum to secondary electrons and travels mainly in a straight line as it slows down. The secondary electrons, on the other hand, can gain enough energy to be knocked loose from the atom, leaving it in an ionized state.

For electrons and positrons traveling through matter, the problem is somewhat more complex. The cross section for electron-electron collisions is given by the Möeller scattering formula, while Bhabha scattering is used for positron-electron collisions [Leroy2009, Bjorken1964]. Positrons lose, on average, half their energy in collision with atomic electrons, and their trajectory is somewhat erratic. Positron-electron annihilation reactions can also take place, producing two γ-rays. Finally, the electrons and positrons that are accelerated in the strong electromagnetic field of a heavy nucleus lose some of their energy by γ-ray emission due to synchrotron radiation (also known as Bremsstrahlung) [Leroy2009, Bjorken1964].

One can approximate the energy loss of a particle of charge z and mass m inside a material of density ρ, atomic number Z, and atomic mass M using the continuous slowing-down approximation (CSDA), where one assumes that the particle is interacting constantly with an electron gas of density n given by

$$n = Z \frac{\rho}{M}\, \mathbb{N}_A.$$

(65)

The energy loss per unit distance traveled by the particle inside the material ($-dE/dx$), known as the stopping power, is then given by the Bethe-Block formula [Smith2000, Leroy2009]:

$$\left(-\frac{dE}{dx}\right)_{collision} = 4\pi n \frac{\left(z\alpha_e \hbar c\right)^2}{mv^2}\left(L(v) - F(v)\right),$$

(66)

where v is the speed of the particle and $L(v)$ the stopping number, which can be written as

$$L = ln\left(\frac{2mv^2}{I(1-(v/c)^2)}\right) - (v/c)^2,$$ (67)

where I is the mean excitation potential for the atomic electrons in this material. The correction term, $F(v)$, takes into account the fact that the atomic electrons are bonded as well as other quantum effects. For electrons, one must also consider the energy lost by synchrotron radiation, which is given approximately by [Leroy2009]:

$$\left(-\frac{dE}{dx}\right)_{radiation} \approx Zn\frac{\alpha_e^3\hbar^2}{m_e},$$ (68)

where m_e is the mass of the electron. Here, it is assumed that the kinetic energy of the electrons $T_e \ll m_e c^2$.

For heavy particles (protons, α-particles), nuclear slowing-down, $(-dE/dx)_{\text{nuclear}}$, becomes important when they reach a low energy.

The CSDA range R of a particle is defined as the distance (path of flight) that it must travel to lose all its kinetic energy. It is computed as

$$R = \int_0^T \frac{1}{\left(-\frac{dE}{dx}\right)_{total}} dE,$$ (69)

where T is the initial kinetic energy of the particle and

$$\left(-\frac{dE}{dx}\right)_{total} = \left(-\frac{dE}{dx}\right)_{collision} + \left(-\frac{dE}{dx}\right)_{radiation} + \left(-\frac{dE}{dx}\right)_{nuclear}.$$ (70)

These CSDA expressions are helpful to understand the general behaviour of particles slowing down in a material. However, for practical applications, tabulated values for $-dE/dx$ and R are more useful. This type of information for electrons, protons, and α-particles can be found on-line for various elements and different material compositions on the National Institute of Standard and Technology Web sites [Berger2013a]. The databases available are:

- ESTAR, for electrons;
- PSTAR, for protons;
- ASTAR, for α-particles.

For heavy particles, this site also provides information on nuclear stopping power. Also note that the stopping power and range are defined in a somewhat different way from the notation above. The following expressions are used instead:

$$-dE/dx(\text{MeV} \times \text{cm}^2/\text{g}) = -\frac{1}{\rho}dE/dx(\text{MeV}/\text{cm})$$ (71)

and

$$R(\text{g}/\text{cm}^2) = \rho R(\text{cm})$$ (72)

because these are the conventional units used in radiation shielding studies. Note that the number of electron/ion pairs produced per unit distance in a material is given approximately by

$$\frac{dn_{pairs}}{dx} = \frac{1}{W}\left(-\frac{dE}{dx}\right)_{total},$$ (73)

where W is the average energy required to ionize an atom in this material.

3.4 Interactions of Photons with Matter

The behaviour of photons as they travel in a material is somewhat different from that of charged particles, which lose their kinetic energy mainly by continuously interacting with electrons and nuclei, the Coulomb field being a long-range force. The photon is the quantum particle that carries the energy $E = h\nu$ and momentum $\vec{p} = \vec{n}h/\lambda$ of an electromagnetic field of frequency ν and wavelength $\lambda = c/\nu$ travelling in direction $\vec{n}$. Depending on its wavelength, the photon behaves as a wave (diffraction and interference for low-energy photons) or as a particle (photoelectric effect for high-energy photons) when it interacts with matter. Here, we will consider only the interactions with matter of the relatively high-energy photons ($E > 1$ keV) found in nuclear reactors. In this case, the photon behaves as a particle that is first absorbed by the atomic electrons or the nucleus. Following this absorption, secondary particles can be produced, including photons (scattering reactions), electrons and positrons (pair creation), and neutrons (photonuclear reaction).
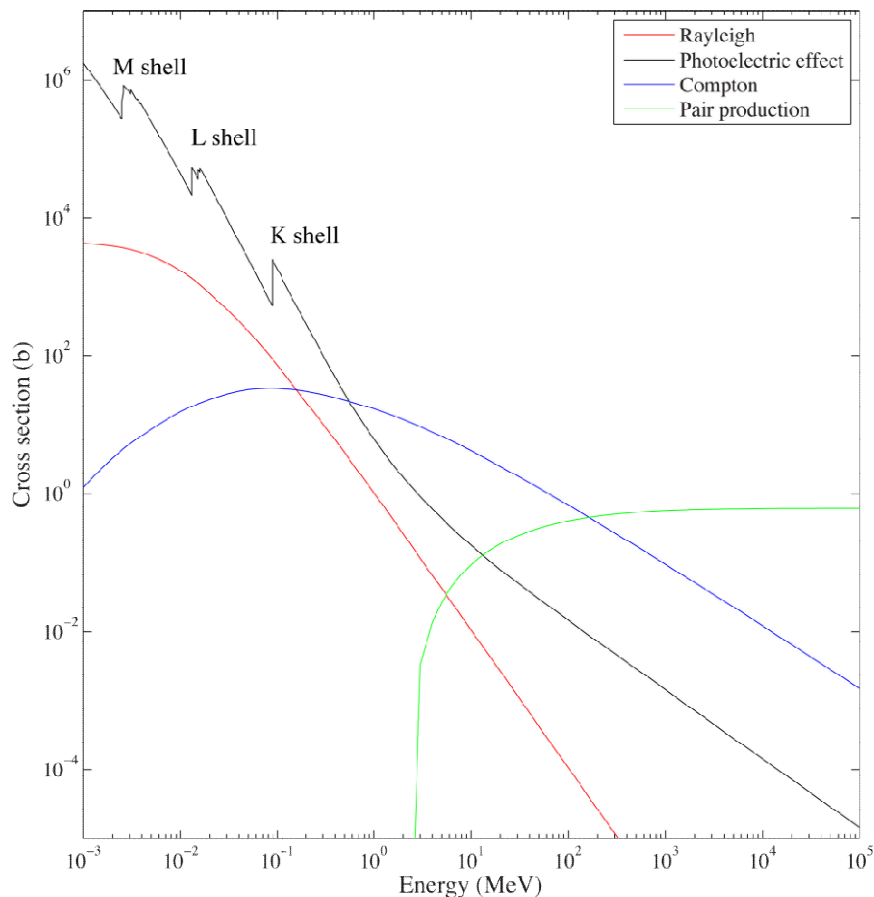
Figure 6 Microscopic cross section of the interaction of a high-energy photon with a lead atom.

The five main reactions taking place between high-energy photons and matter that are of interest in nuclear reactor-related studies are:

- Photoelectric effect;
- Rayleigh scattering;
- Compton scattering;
- Pair production; and
- Photonuclear reactions.

With each such reaction is associated a macroscopic cross section $\Sigma_{m,x}(E)$ representing the probability per unit distance travelled by a photon of energy E that an interaction of type x has taken place in material m. The macroscopic cross section takes into account the probabilities of interaction both between single photons and between particles and the fact that the material contains $N_{m,i}$ particles of type i per unit volume:

$$\Sigma_{m,x}(E) = \sum N_{m,i}\sigma_{i,x}(E), \tag{74}$$

where $\sigma_{i,x}(E)$ is the microscopic cross section of the interaction of a photon of energy E with a particle of type i through reaction x (see Section 3.2). The total microscopic photon cross section can be expressed as:

$$\sigma(E) = \sigma_{Photoelectric}(E) + \sigma_{Rayleigh}(E) + \sigma_{Compton}(E) + \sigma_{Pair\ production}(E) + \sigma_{Photonuclear}(E). \tag{75}$$

Examples of microscopic cross sections for the interaction of photons with a lead atom are presented in **Figure 6.**

Let us now describe in detail the five reactions contributing to $\sigma(E)$ and discuss their respective dependences on the energy of the incident photon.

3.4.1 Photoelectric effect

This effect is illustrated in **Figure 7**. A photon with an energy $E = h\nu$ that is greater than the binding energy W of atomic electrons around the nucleus is absorbed. Following this absorption, the electron becomes free, leaving behind an ion. The energy balance for this reaction is

$$T_e + T_N = E - W, \tag{76}$$

where T_e is the kinetic energy of the final electron and T_N that of the recoil nucleus (generally very small compared with T_e).
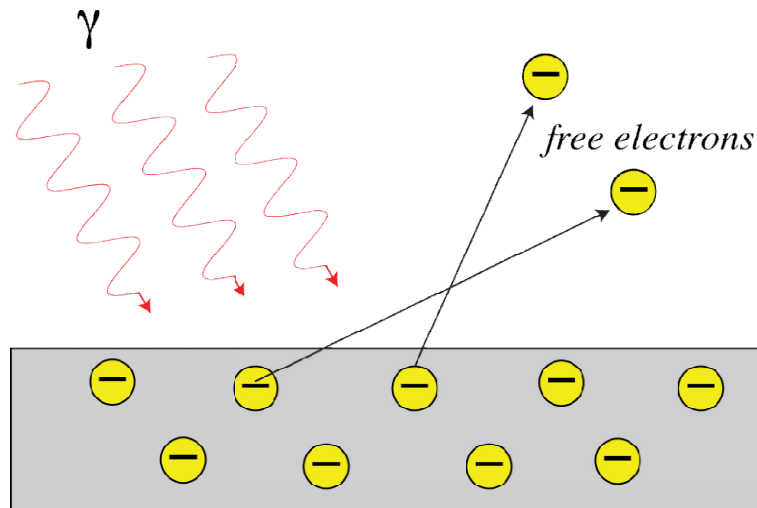
Figure 7 Photoelectric effect.

From quantum mechanics, the binding energy of electrons around a nucleus of charge Ze can be approximated using [Griffiths2005]:

$$W_n = \frac{13.61\, Z^2}{n^2}\, eV,\tag{77}$$

where $n = 1$ for K-shell electrons, 2 for L-shell electrons, and so on. Therefore, as the energy of the photon decreases, the electrons in the more tightly bonded shells (K, L, and M shells) are successively excluded, producing a large drop in the photoelectric cross section when the energy falls below W_n (see **Figure 6**). The evaluation of this cross section is therefore very difficult, and only approximate relations are available. For a K-shell electron, one can use [Leroy2009]:

$$\sigma_{Photoelectric,K}\left(E\right) \approx \frac{32\sqrt{2}\,\pi Z^5 \alpha_e^6 \left(m_e c^2\right)^{\frac{3}{2}}}{3\left(E\right)^{\frac{7}{2}}}\left(\hbar c\right)^2,\tag{78}$$

which is valid, within 2%, for photon with energies ranging from 100 keV to 200 MeV. The total photoelectric cross section (the sum over all energy shells) is given approximately by [Leroy2009]:

$$\sigma_{Photoelectric}\left(E\right) \approx \sigma_{Photoelectric,K}\left(E\right) \times \left(1 + 0.01481\left(\ln\left(Z\right)\right)^2 - 0.000788\left(\ln\left(Z\right)\right)^3\right).\tag{79}$$

Clearly, this cross section decreases rapidly with photon energy. It is dominant only for photons of energies less than a few tenths of an MeV.

Several processes can take place after this reaction. If the electron ejected from the atom was initially in the valence band, the ionized atom is in its ground state, and no further radiation emission is observed. When electrons coming from more tightly bonded energy levels are ejected, the ionized atom is left in an excited state. This excited ion can then decay to its ground state by two different means. First, an electron in a much higher energy state (i.e., a valence electron) can emit a photon and fill the vacant energy level. The electron can also come from a slightly higher energy level, leaving the ion in a less excited state that will further decay before reaching its ground state. When the photons emitted in these successive decays

are absorbed by less-bonded electrons, so-called soft Auger electrons are ejected from the atom, producing an Auger electron cascade.

3.4.2 Rayleigh scattering

This elastic scattering reaction takes place when a photon, after being absorbed by a bound atomic electron, is re-emitted with the same energy, but in a different direction, by the electron, returning the atom to its original state [Leroy2009, Jauch1976]. The cross section for this reaction is very difficult to evaluate because it depends strongly on the wave function of the bonded electrons surrounding the nucleus. It is generally written as an integral of the form

$$\sigma_{Rayleigh}\left(E\right) = \pi \left(\frac{\alpha_e \hbar c}{m_e c^2}\right)^2 \int_0^\pi \left(1+\cos^2\left(\theta\right)\right)\left[F\left(E,\theta,Z\right)\right]^2 \sin\left(\theta\right) d\theta, \tag{80}$$

where $F(E,\theta,Z)$ is the atomic form factor that represents the effect of the Z electrons surrounding the nucleus on the scattering of a photon at an angle θ with respect to the initial photon direction. Several theoretical expressions for $F(E,\theta,Z)$ are available in the literature for different values of Z and various energy ranges. For example, when the photon energy is greater than 100 keV, the main contributors to Rayleigh scattering are the electrons in the K-shell, and the relativistic Bethe-Levinger form factor is used [Hubbell1975]:

$$F\left(E,\theta,Z\right) = \frac{\sin(2\gamma \mathrm{atan}(Q))}{\gamma Q \left(1+Q^2\right)^\gamma}, \tag{81}$$

with

$$Q\left(E,\theta,Z\right) = \frac{2E\sin(\theta/2)}{\alpha_e Z m_e c^2}, \tag{82}$$

$$\gamma\left(Z\right) = \sqrt{1+\left(\alpha_e Z\right)^2}. \tag{83}$$

Because Rayleigh scattering is never the dominant photon reaction (see **Figure 6**) for the photon energy range considered in nuclear reactors, its contribution to the total cross section is often neglected.

3.4.3 Compton scattering

The Compton effect is the incoherent inelastic scattering of a photon by an electron that is weakly bonded to a nucleus (see **Figure 8**). Here, a photon with momentum $\vec{k}$ ($|\vec{k}| = h\nu/c = E/c$) is scattered at an angle θ with respect to its original direction, with the final momentum of the photon being $\vec{k}'$. The electron is then ejected with a kinetic energy T_e, obtained by conservation of momentum and energy:

$$T_e = E^2 \left(\frac{(1-\cos\theta)}{m_e c^2 + E(1-\cos\theta)}\right), \tag{84}$$

where the binding energy of the electron is assumed to be small compared to the photon energy, and the recoil energy carried by the nucleus is neglected. For a nearly free electron, the cross section for this reaction is given by the Klein-Nishina formula, which can be written as

$$\sigma_{Compton}(E) = \frac{\pi}{\varepsilon}\left(\frac{\alpha_e \hbar c}{m_e c^2}\right)^2 \left[ln(1+2\varepsilon)\left(1 - \frac{2(1+\varepsilon)}{\varepsilon^2}\right) + \frac{1}{2} + \frac{4}{\varepsilon} - \frac{1}{2(1+2\varepsilon)^2}\right],\qquad(85)$$

with $\varepsilon = E/(m_e c^2)$ This cross section decreases with energy, but much more slowly than for the photoelectric effect. It dominates the photoelectric reaction for energies above approximately 0.5 MeV.
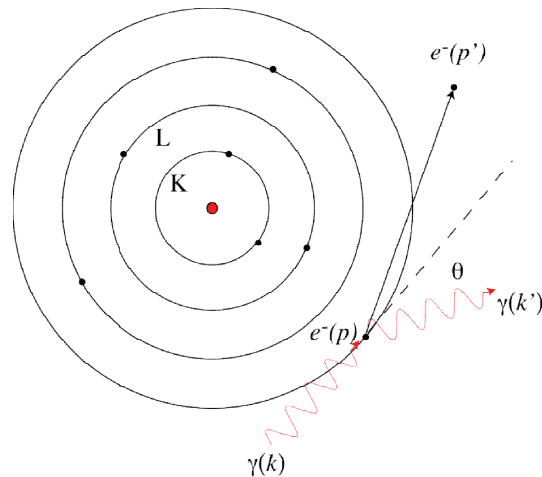
Figure 8 Compton effect.

3.4.4   Pair production

A photon with energy $E = h\nu > 2m_e c^2$ traveling through the Coulomb field of a nucleus of charge Z (or an electron) can be converted into an electron-positron pair. After the reaction, the nucleus carries a small part of the kinetic energy of the photon, with the bulk of the energy being transferred in the form of mass and kinetic energy to the pair. For photon energies in the range found in nuclear reactors, the cross section for this reaction is given approximately by [Leroy2009]:

$$\sigma_{Pair\ production}(E) \approx \alpha_e Z^2 \left(\frac{\alpha_e \hbar c}{m_e c^2}\right)^2 \left[\frac{28}{9}\ln(2\varepsilon) - \frac{218}{17} + \frac{129}{20\varepsilon}\right],\qquad(86)$$

with $\varepsilon = E/(m_e c^2)$. This cross section vanishes for $E < 1.02$ MeV and is larger than the Compton cross section above a few MeV.

3.4.5   Photonuclear reactions

Photonuclear reactions are the result of photons being absorbed by a nucleus to form an excited nucleus, which gets rid of its energy through different decay processes, namely the emission of a secondary photon, the ejection of one or more nucleons (protons and neutrons), the ejection of α-particles, or through a fission reaction. Photonuclear reactions occur only above a threshold, which lies between 7 and 9 MeV for heavy nuclides, but is considerably lower for very light isotopes (1.666 MeV and 2.226 MeV respectively for beryllium and deuterium). The absorption cross sections for these reactions (see **Figure 9**) are generally very difficult to evaluate, and only approximate expressions are available.
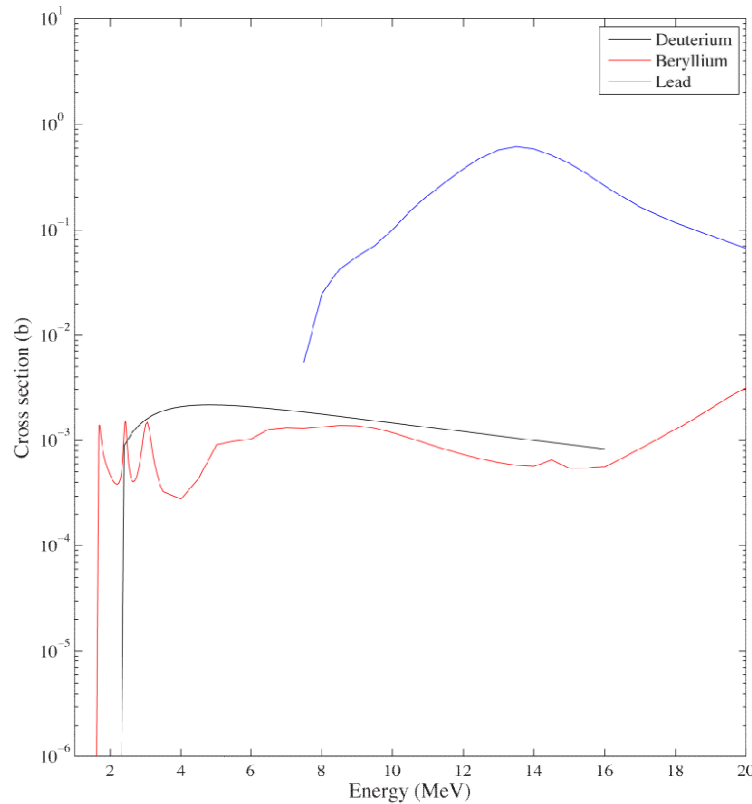
Figure 9 Photonuclear cross sections for deuterium, beryllium, and lead.

For deuterium, which is important to CANDU reactors because they use large amounts of heavy water, the expression [Leroy2009]

$$\sigma_{^2D,Photonuclear}(E) \approx C_{^2D} \frac{\left(\sqrt{E-2.226}\right)^3}{E^3} \tag{87}$$

is often used, where E, the photon energy, is given in MeV, $C_{^2D}$ varies between 0.061 and 0.0624, and $\sigma_D(E)$ is in barns. The end result of such a photonuclear reaction is a hydrogen atom and a fast neutron that can initiate a fission reaction (see Section 2.6).

Tabulated values for Rayleigh scattering (coherent scattering), photoelectric effect, Compton scattering (incoherent scattering), and pair production cross sections with different atoms or materials and for energies ranging from 1 keV to 100 GeV are available on-line on the Web site of the National Institute of Standards and Technology (NIST) [Berger2013b]. For photonuclear reactions, the energy-dependent cross sections for various isotopes can be obtained using the OECD-NEA Janis software [OECD-NEA2013].

For each reaction presented above, the photons first transfer all their energy to an electron or a nucleus following a collision. As a result, starting with $n(E, \vec{r}, \vec{\Omega})$ photons of energy E and direction $\vec{\Omega}$ incident at point $\vec{r}$ on a material of uniform macroscopic cross section $\Sigma(E)$, the number of initial photons $n(E, \vec{r} + s\vec{\Omega}, \vec{\Omega})$ still present after a distance s has been crossed is given by [Basdevant2005]:

$$n\left(E, \vec{r} + s\vec{\Omega}, \vec{\Omega}\right) = n\left(E, \vec{r}, \vec{\Omega}\right) e^{-\Sigma(E)s}. \tag{88}$$

The number of photons therefore decreases exponentially with distance. This behaviour is similar to what is observed when light is attenuated by passing through a material with a linear attenuation coefficient $\mu(E) = \Sigma(E)$. Secondary photons produced with energy E and direction $\vec{\Omega}$ following the absorption of photons of energy E' and direction $\vec{\Omega}'$ will also contribute to the total population of photons at point $\vec{r} + s\vec{\Omega}$. The equation that describes the photon population in a material, assuming a constant neutron incident population, is the static photon transport equation, which takes the form [Pomraning1991]:

$$\vec{\Omega}\cdot\vec{\nabla}\,n\left(E,\vec{\Omega},\vec{r}\right) = -\Sigma(E)n\left(E,\vec{\Omega},\vec{r}\right) + \int dE'\int d\vec{\Omega}'\,\Sigma_s\left(E' \to E,\vec{\Omega}' \to \vec{\Omega}\right)n\left(E',\vec{\Omega}',\vec{r}\right), \quad (89)$$

where $\Sigma_s\left(E' \to E, \vec{\Omega}' \to \vec{\Omega}\right)$ is the differential scattering cross section representing the probability that the absorption of a photon of energy E' and direction $\vec{\Omega}'$ produces a photon of energy E and direction $\vec{\Omega}$.

3.5   Interactions of Neutrons with Matter

Neutron interaction with matter is the result of the nuclear force, although weak and electromagnetic interactions, the latter being the result of anomalous magnetic moment, are also possible. As a result, only neutron-nucleus interactions are generally considered, including

- elastic potential scattering with cross section $\sigma_{elastic}$;
- inelastic scattering with cross section $\sigma_{inelastic}$;
- neutron absorption with cross section $\sigma_{absorption}$; and
- spallation reactions, $\sigma_{spallation}$.

In the first three reactions, the neutron interacts with the nucleus as a whole. In spallation reactions, the neutrons interact directly with the nucleons in the nucleus. The latter reaction can take place only when the energy of the incident neutron $E_{n,i}$ is sufficiently high (threshold reactions with $E_{n,i} > 0.1$ MeV), and therefore $\sigma_{spallation}$ is either neglected, because it is too small, or simply included in the absorption cross section. The probability that the neutron interacts with a nucleus is then given by the total cross section, σ, where

$$\sigma(E_{n,i}) = \sigma_{absorption}\left(E_{n,i}\right) + \sigma_{scattering}\left(E_{n,i}\right), \quad (90)$$

$$\sigma_{scattering}\left(E_{n,i}\right) = \sigma_{elastic}\left(E_{n,i}\right) + \sigma_{inelastic}\left(E_{n,i}\right). \quad (91)$$

Elastic potential scattering is an interaction in which kinetic energy is conserved and the neutron does not penetrate the nucleus. As a result, the neutron is slowed down, transferring part of its energy to the nucleus. For a collision between a neutron with an initial kinetic energy $E_{n,i}$ and a nucleus of mass M_X at rest, the final neutron kinetic energy $E_{n,f}$ (momentum and energy conservation) will be given by [Bell1982]:

$$E_{n,f} = \frac{E_{n,i}}{(1+A)^2}\left(A^2 + 1 + 2A\cos\vartheta\right), \quad (92)$$

where $A = M_X/m_n$ and ϑ, the scattering angle for the final neutron in the of mass system, is related to the scattering angle in the laboratory system θ by

$$\cos\theta = \frac{A\cos\vartheta + 1}{\sqrt{\left(A^2 + 1 + 2A\cos\vartheta\right)}}. \tag{93}$$

On average, the neutron will lose an energy ΔE:

$$\Delta E = \frac{(1-\alpha)}{2} E_{n,i}, \tag{94}$$

$$\alpha = \frac{(A-1)^2}{(A+1)^2}, \tag{95}$$

after each collision. Because ΔE decreases as A increases, neutron slowing-down (also called moderation) is more efficient when scattering collisions with light rather than heavy nuclei are involved.

For low-energy neutrons, the potential scattering cross section in the centre of mass system is nearly constant and has the form [Bell1982]:
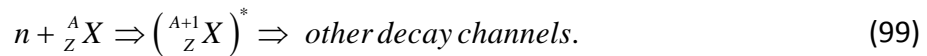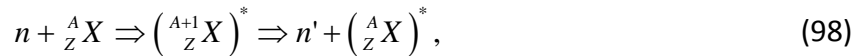
$$\sigma = 4\pi R^2, \tag{96}$$

where R is the nuclear radius for this material. At higher energy, one can use Fermi's golden rules to obtain an approximation for $\sigma(E)$ of the form

$$\sigma(E) = 4\pi \frac{\hbar^2 \sin^2 \delta}{2m_n E}, \tag{97}$$

where δ represents the phase shift of the neutron wave function in isotropic scattering.

Inelastic scattering and absorption reactions generally proceed by creation of a compound nucleus:

$$n + {}^{A}_{Z}X \Rightarrow \left({}^{A+1}_{Z}X\right)^* \Rightarrow n' + \left({}^{A}_{Z}X\right)^*, \tag{98}$$

$$n + {}^{A}_{Z}X \Rightarrow \left({}^{A+1}_{Z}X\right)^* \Rightarrow other\,decay\,channels. \tag{99}$$

The creation of the compound nucleus is a resonant reaction because the resulting weakly bonded nucleus can exist only if it corresponds to an excitation state of ${}^{A+1}_{Z}X$. The lifetime of this excited nucleus is generally very short ($\tau \approx 10^{-16}$ s), and with each decay channel k, including inelastic scattering, is associated a resonance width given by [Bell1982]:

$$\Gamma_k = \frac{\hbar}{\tau_k}, \tag{100}$$

with τ_k being the mean life for decay through this channel. The total resonance width for the creation of the excited nucleus Γ is then given by

$$\Gamma = \sum \Gamma_k. \tag{101}$$

For light nuclei, $\Gamma_{\text{inelastic}} \gg \Gamma_{\text{absorption}}$, and the inelastic scattering process dominates. For heavy nuclei, the reverse is true (absorption dominates). The resonance widths for inelastic scattering also increase with energy, the explicit dependence being

$$\Gamma_{inelastic}(E) = \Gamma_n(E) = \Gamma_0 \sqrt{E}, \tag{102}$$

where Γ_0 is a constant that depends on the nucleus considered.

The probability (cross section) for the creation of a compound nucleus with resonant energy E_0 is given by

$$\sigma_{_{Z}^{A+1}X}\left(E\right)=\left(2l+1\right)\frac{\pi\hbar^2}{2mE}\left(\frac{\Gamma_n\left(E\right)\Gamma}{\left(E-E_0\right)^2+\left(\frac{\Gamma}{2}\right)^2}\right),\tag{103}$$
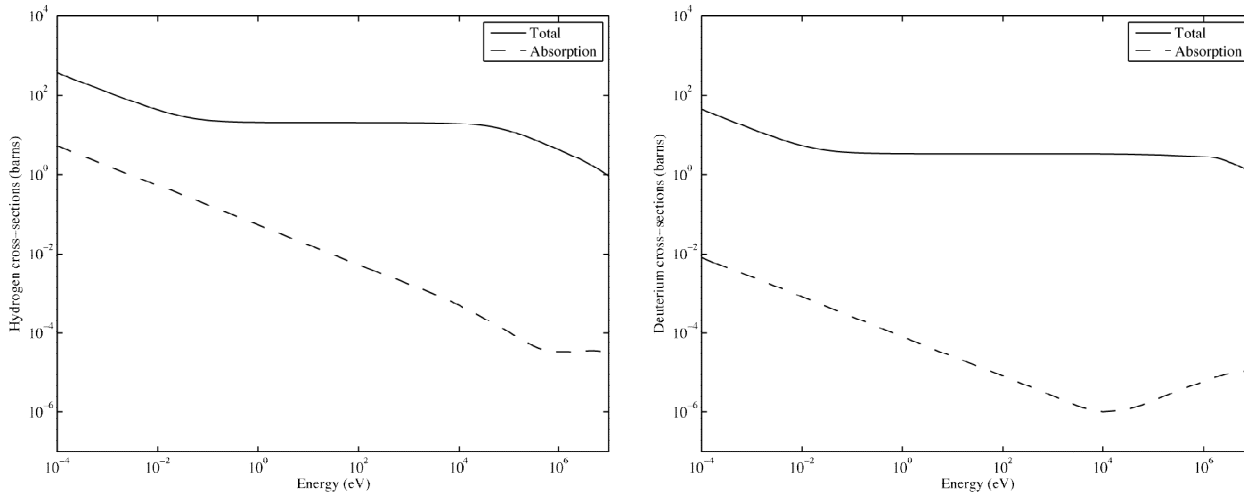
where l is the orbital-angular-momentum quantum number. For a nucleus that decays through channel k, the cross section is

$$\sigma_k\left(E\right)=\sigma_{_{Z}^{A+1}X}\left(E\right)\frac{\Gamma_k}{\Gamma}.\tag{104}$$

Note that at low energy ($E \ll E_0$), $\Gamma_n = \Gamma_0\sqrt{E}$,

$$\sigma_k\left(E\right)\approx\left(2l+1\right)\frac{\pi\hbar^2\Gamma_0\Gamma_k}{2m\sqrt{E}}=\frac{\sigma_0}{v},\tag{105}$$

and the cross section is a function of $1/v$, with v being the incoming neutron velocity.

Figure 10 Cross sections for hydrogen (left) and deuterium (right) as functions of energy.

Examples of cross sections for light (hydrogen and deuterium) and heavy nuclei ($^{235}_{92}$U and $^{238}_{92}$U) are presented in **Figure 10** and **Figure 11**. For light nuclides, the scattering process clearly dominates. One can also observe that the total cross section of hydrogen is about ten times larger than that of deuterium (better scattering nucleus for neutron moderation). With absorption representing 10% of the total cross section of hydrogen, one out of ten collisions will lead to neutron capture. For deuterium, the ratio of neutron absorptions to collisions is closer to 1%, making this isotope a better neutron moderator overall. For heavy nuclides, the absorption reaction is the most prevalent and exhibits a very large number of resonances. At very high energy, these resonances do not disappear, but are so closely packed that they produce a nearly continuous cross section.
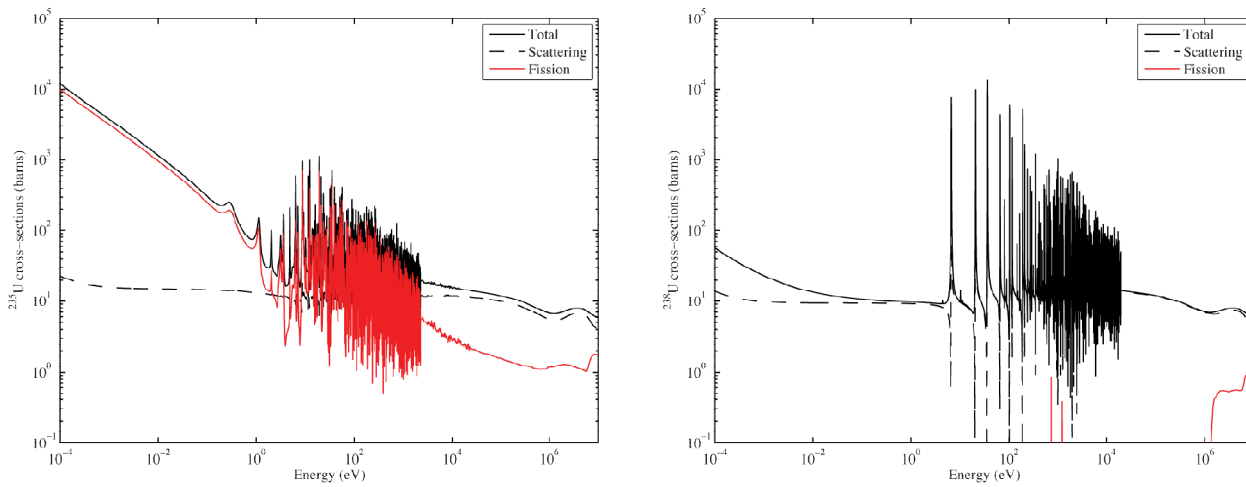
Figure 11 Cross sections for $^{235}_{92}\text{U}$ (left) and $^{238}_{92}\text{U}$ (right) as functions of energy.

The derivations above are valid only if one assumes that the nucleus is at rest. This is clearly not the case for material having temperatures $T > 0$, because atoms acquire an average kinetic energy that is proportional to the temperature of their medium. The resulting effect on the cross sections can be taken into account for a material at temperature T using [Bell1982]:

$$\sigma_k\left(E,T\right) = \frac{1}{\sqrt{2mE}} \int \left|\vec{v}_n - \vec{v}_X\right| \sigma_k\left(\left|\vec{v}_n - \vec{v}_X\right|\right) p\left(E_X\right) dE_X, \tag{106}$$

where $\vec{v}_n$ and $\vec{v}_X$ are the velocity of the neutron and the nucleus respectively. Here, $p(E_X)dE_X$ is the Maxwell-Boltzmann distribution, which represents the probability of finding a nucleus with energy E in the range $E_X < E < E_X + dE_X$ due to thermal motion:

$$p\left(E_X\right) dE_X = \frac{2\pi}{\left(\pi k_B T\right)^{3/2}} \sqrt{E_X} e^{-E_X/(k_B T)} dE_X, \tag{107}$$

where k_B is the Boltzmann constant. This thermal motion of nuclei has no impact on cross sections exhibiting $1/v$ behaviour (i.e., absorption cross sections of hydrogen at low energy). At low neutron energies, the scattering cross section for light nuclides also exhibits $1/v$ behaviour and is not affected by this transformation, although the energy distribution of the final neutrons resulting from these collisions will be such that they end up in thermal equilibrium with the nuclides in the medium [Bell1982].

The thermal motion of atoms also changes the form of resonant cross sections by reducing the height of the resonance while increasing its width (see **Figure 12**). This widening of the resonance is known as the Doppler effect.
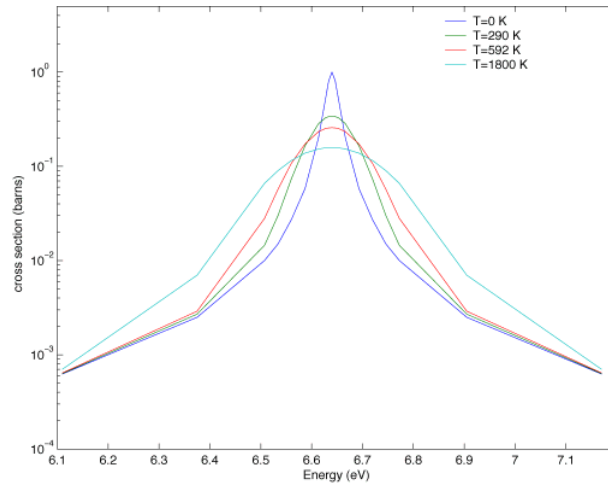
Figure 12 Effect of temperature on U^{238} absorption cross section around the 6.64-eV resonance.

The neutron-nucleus interaction cross sections are very complex and in most cases are evaluated using a combination of theory and experiment. They are generally tabulated in evaluated nuclear data files that can be read by nuclear calculation software (NJOY, for example) [MacFarlane2010]. They can also be extracted on-line from nuclear databases or off-line using the Janis software [KAERI2013, Livermore2013, OECD-NEA2013].

Once the energy-dependent cross sections are known, one can easily evaluate the number of reactions of type x per second (the reaction rate $R_{m,x}(v)$) taking place inside a region of volume V containing N_m nuclei per cm^3 of a material m (cross section $\sigma_{m,x}(v)$) with a population of $n(v)$ neutrons per cm^3 having a velocity $v = \sqrt{2E_n/m}$:

$$R_{m,x}\left(v\right) = V\frac{N_m\sigma_{m,x}\left(v\right)n\left(v\right)}{v} = V\Sigma_{m,x}\left(v\right)\phi\left(v\right),$$
(108)

where $\phi(v) = n(v)/v$ is the neutron flux and $\Sigma_{m,x}(v) = N_m\,\sigma_{m,x}(v)$ the macroscopic cross section for a reaction of type x in this material.

4   Fission and Nuclear Chain Reaction

The concept of controlled energy production in a nuclear reactor is based on three fundamental ideas that were discussed in Sections 2.6, 3.1, and 3.2, namely:

* energy is released if a heavy nucleus is fragmented into lighter nuclei, the fragmentation process being called nuclear fission;
* the spontaneous nuclear fission process, which has a very low yield for several heavy nuclei, generates neutrons in addition to the light nuclei as end products;
* the nuclear fission process can be initiated by neutrons and photons.

Accordingly, a neutron of kinetic energy T_n travelling through a medium containing heavy nuclei at rest could initiate a fission reaction:

$$_o^1 n + {}_Z^A X \Rightarrow C\,_o^1 n + {}_Y^B F + {}_{Z-Y}^{A-B-C+1} G.$$
(109)
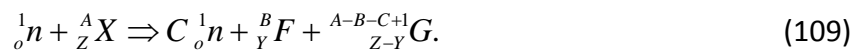
The kinetic energy T_R released by this reaction is then

$$T_R = T_n + (1-C)m_n c^2 + m_{_Z^A X}c^2 - m_{_Y^B F}c^2 - m_{_{Z-Y}^{A-B-C+1}G}c^2,$$
(110)

with part of the energy carried by the neutrons and the lighter nuclei. These lighter nuclei rapidly lose their energy in matter (see Section 3.3), thereby producing heat that is removed by the coolant and transformed to electricity.

Not all the neutrons produced after this reaction initiate a fission reaction. A number of them are absorbed by material without producing a fission reaction. Others simply leave the system (with or without collisions). Provided that on average a single neutron per fission reaction can initiate a new fission, a controlled exothermal chain reaction can be established. Establishing such a chain reaction looks relatively simple; however, this is far from the case, as shown in the following subsections.

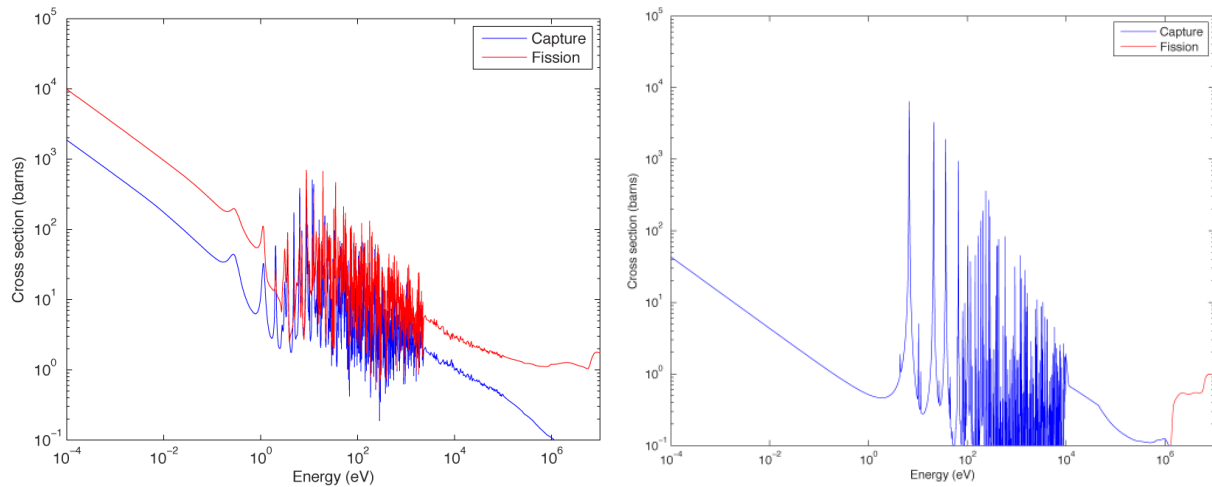## 4.1 Fission Cross Sections

The probability of fission is given by the value of the fission cross sections associated with a nucleus and depends on the energy of the neutron that initiates the reaction. All isotopes with atomic number $Z > 90$ are fissionable (have a non-zero probability of undergoing fission following the capture of a neutron). **Table 5** compares the average energy, U, required to initiate a fission reaction in different nuclei with the energy, Q, available in the compound nucleus after a neutron with a vanishing kinetic energy has been captured. For nuclei containing an even number of protons and an odd number of neutrons, $Q > U$. Such isotopes are called fissile isotopes because the internal energy of the compound nucleus resulting from neutron capture is sufficient to surmount the potential barrier for fission even when the incident neutrons are very slow ($T_n \approx 0$). For isotopes with $Q < U$, the fission barrier can be overcome only using neutrons with relatively high kinetic energy. Fission for these nuclei is a threshold reaction.

Table 5 Comparison of the energy, *U*, required for a fission reaction in a compound nucleus with the energy, *Q*, available after a neutron collision with different isotopes.

Isotope	Q(MeV)	U(MeV)
$^{232}_{90}$Th	5.1	5.9
$^{233}_{92}$U	6.6	5.5
$^{235}_{92}$U	6.4	5.8
$^{238}_{92}$U	4.9	5.9
$^{239}_{94}$Pu	6.4	5.5

As shown in **Figure 13**, the energy dependence of the fission cross sections for $^{235}_{92}$U and $^{238}_{92}$U reflects the behaviour described above. The probability that a neutron of energy $E_n < 1.0$ MeV will collide with $^{238}_{92}$U and result in a fission reaction is very low. For $^{235}_{92}$U, there is no lower limit on the neutron energy, and the fission probability increases as the energy of the neutron decreases. The neutron capture cross section (neutron absorption followed by photon emission) for $^{238}_{92}$U dominates at low energy, while for $^{235}_{92}$U, it remains relatively small compared to the fission cross section (approximately 10%) over the full energy range. As a result, most neutron absorption in $^{235}_{92}$U will lead to fission followed by production of new neutrons (neutrons are regenerated). For $^{238}_{92}$U, a collision with a neutron having energy below

the fission threshold will lead to a net neutron loss. As a result, the natural uranium fuels used in CANDU reactors (0.72 atomic% of $^{235}_{92}\text{U}$) will be much less reactive (prone to fission) than the enriched fuels (enrichment factors ϵ ranging from 2.5 to 5 atomic% of $^{235}_{92}\text{U}$) used in light water reactors (LWR).

Figure 13 Capture and fission cross sections of $^{235}_{92}\text{U}$ (left) and $^{238}_{92}\text{U}$ (right) as functions of energy.

4.2   Fission Products and the Fission Process

The fission process generally produces two light nuclei, called fission products, although three or more nuclei can also be generated. The relative rate of production of a given nuclide I, called the fission yield, is denoted by Y_I and satisfies

$$\sum_I Y_I = 2, \tag{111}$$

assuming that only two nuclei are produced by each fission reaction. As one can see in **Figure 14**, where the fission yields of all the nuclei resulting from the fission of $^{235}_{92}\text{U}$ are plotted as a function of their mass number, the fission process favours the production of relatively light nuclides ($90 < A{<}105$) combined with heavier isotopes ($130 < A{<}145$).
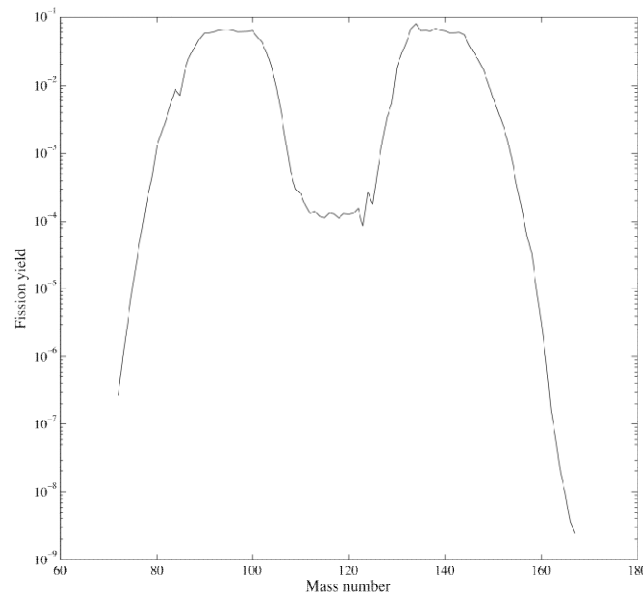
Figure 14 Relative fission yield for $^{235}_{92}\mathrm{U}$ as a function of mass number.

The average number υ of neutrons emitted by the fission process (see **Table 6**) is relatively small compared to the neutron excess $N - Z > 40$ required for heavy isotopes to exist. The value of υ for a given reaction depends on the nature of the fissile nuclides, the fission products released, and the energy of the neutrons. Most fission products are therefore very neutron-rich and unstable. They will reach stability through two main processes: β^- decay and neutron emission. All the transformations that take place within 10^{-14}s of the fission reaction are generally included in the so-called prompt contribution (prompt neutrons, prompt electrons, and prompt photons). Particles produced on a longer time scale (from milliseconds to minutes) due to decay of isotopes with longer mean lifetimes are called delayed.

Table 6 Average numbers of neutrons produced by the fission of common heavy nuclides.

Isotope	$\upsilon(E_n<1$ eV)	$\upsilon(E_n>1$ MeV)
$^{232}_{90}\mathrm{Th}$	0	2.2
$^{233}_{92}\mathrm{U}$	2.50	2.6
$^{235}_{92}\mathrm{U}$	2.43	2.6
$^{238}_{92}\mathrm{U}$	0	2.6
$^{239}_{94}\mathrm{Pu}$	2.89	3.1

The fission reaction (see Section 2.6) also releases a large amount of kinetic energy (on the order of 200 MeV) that is distributed between fission products, neutrons, γ-rays, etc. (see **Table 7**). Clearly, the fission products carry most of the energy, and because of their very short range in matter, this energy heats the nuclear fuel. Similarly, the charged electrons (β^- particles) also lose most of their energy in the fuel. The highly penetrating γ-rays will end up depositing their energy in the reactor structures, while the weakly interacting neutrinos will generally be lost to the environment. Finally, for LWR and CANDU reactors, only a very small

part of the neutron energy will be transferred to the fuel in the form of heat, with most of it being lost to the environment (mostly through slowing-down in the moderator).

Table 7 Distribution of kinetic energy among the particles produced by a fission reaction.

Particles	Kinetic energy (MeV)
Fission products	168
Prompt γ-rays	7
Delayed γ-rays	7
Electrons	8
Neutrinos	12
Neutrons	7
Total	207

Note that the data presented in **Table 7** represent average values, meaning that the neutrons produced in the fission process have an energy distribution. The probability that a neutron of energy E_n is produced in the fission process, which is known as the fission spectrum, $\chi(E_n)$, is often approximated by the Watt relationship [Watt1952]:

$$\chi\left(E_n\right) = Ce^{-aE_n}\sinh\left(\sqrt{bE_n}\right), \tag{112}$$

where a and b are constants associated with the isotope undergoing fission and depend weakly on the incident neutron energy. The normalization factor C is defined so that

$$\int_0^\infty \chi\left(E_n\right)dE_n = 1 \tag{113}$$

and has the value

$$C = \frac{2a^{2/3}e^{-b/4a}}{\sqrt{\pi b}}. \tag{114}$$

This fission spectrum for $^{235}_{92}\text{U}$ is illustrated in **Figure 15**. Clearly, most of the neutrons are released with energies greater than 1 MeV and can initiate fission reactions with fissionable material. However, the fission cross section for this energy range is relatively low (see **Figure 13**), and fissions at such energies are highly improbable. Nevertheless, a controlled chain reaction that relies mainly on fast fission can be achieved in so-called "fast neutron reactors", where $^{239}_{94}\text{Pu}$ is often used because of its large fission cross section for high-energy neutrons. The alternative to fast neutron reactors is moderated reactors, in which the fast neutrons are slowed down to energies where the fission cross section is significantly larger (below 1 eV). This is the concept used in "thermal neutron reactors", which are discussed in the next section.

Now, let us look at the properties of fission products. These nuclides have intermediate masses and vanishing fission cross sections. However, they can have very large neutron-capture cross sections and thereby can have a considerable negative impact on the neutron population in the fuel where they are produced. For this reason, they are often called neutron poisons. Examples of poisons that have a large impact on nuclear-reactor operation are $^{135}_{54}$Xe ($\sigma_a = 3.1 \times 10^6$ b) and $^{149}_{62}$Sm ($\sigma_a = 6.1 \times 10^4$ b). A second observation is that most of these nuclides are unstable and decay naturally through one of the reactions described in Section 3.1. These reactions produce both particles, including delayed neutrons, and energy that is often deposited in the fuel. These delayed neutrons play an important role in the control of nuclear reactors, as will be explained in Chapter 5. Moreover, energy will still be produced in the fuel for a long time after the controlled fission reaction has been stopped, due to the decay of fission products. This is the main source of the heat produced in neutron-irradiated nuclear fuels (some energy is also produced through photonuclear fission). This residual heat is removed from shut-down reactors and irradiated fuel pools by continuously circulating the coolant.
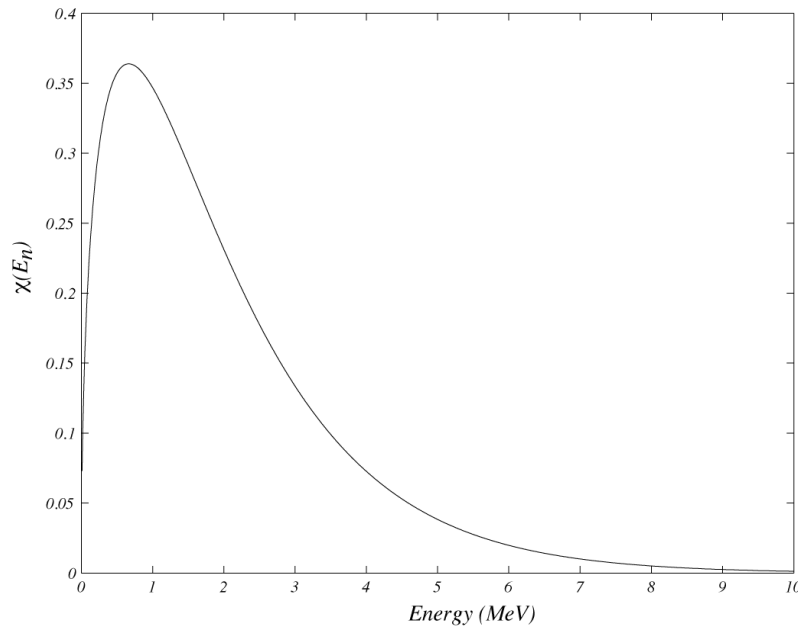
Figure 15 Fission spectrum for $^{235}_{92}$U.

Finally, we must address the problem of the changes in the composition of a material exposed to a neutron flux. In Section 3.1, we introduced the Bateman equation, which takes the form [Smith2000, Nikjoo2012, Magill2005]:

$$\frac{dN_I(t)}{dt} = -\lambda_I N_I(t) - L_I(t) + P_I(t), \tag{115}$$

where $N_I(t)$ is the concentration of isotope I in the material and the net source $S(t)$ is now divided into a production $P_I(t)$ and a loss $L_I(t)$ term. The loss term, from sources other than decay, is the result of a neutron being absorbed (captured) by isotope I:

$$L_I(t) = N_I(t) \int_0^\infty \sigma_{I,absorption}(E)\phi(E)dE, \tag{116}$$

where $\phi(E)$ is the neutron flux. The production term has two contributions: decay from other nuclei, and transformation of a different nucleus into I following a neutron-induced nuclear reaction:

$$P_I(t) = \sum_J Y_{J,I}^d \lambda_J N_J(t) + \sum_J \sum_x Y_{J,I}^x N_J(t) \int_0^\infty \sigma_{J,x}(E)\phi(E)dE, \qquad (117)$$

where $Y_{J,I}^d$ is the yield for the production of isotope I from the decay of isotope J, while $Y_{J,I}^x$ is the isotope I production yield from a reaction of type x (fission, capture, etc.) between a neutron and isotope J.

4.3   Nuclear Chain Reaction and Nuclear Fission Reactors

The previous sections have introduced all the concepts required to design a conceptual nuclear fission reactor:

- The nuclear fuel contains heavy isotopes that are broken into lighter nuclides (fission products) following a neutron-induced fission reaction. Such a reaction also generates energy and secondary neutrons that can be used to maintain a chain reaction.
- Most of the energy released as a result of the fission process is carried away by the fission products and deposited in the fuel because of the short range of these nuclei.
- The secondary neutrons produced in the fission process are fast neutrons.
- These neutrons can lose their energy through scattering collisions with the various materials present in our conceptual reactor. Neutron slowing-down by collisions with light isotopes is more efficient than by collision with heavy isotopes (see Section 3.5).
- This energy deposition increases the temperature of the fuel, which must then be cooled to make use of the heat and avoid damage to the reactor. For a power reactor, this heat is collected in a coolant (generally gas or liquids circulating around the fuel) and used to generate electricity.

Now let us look at the fuel and coolant materials that are the most readily available.

Three heavy fissionable isotopes are present in nature: $^{232}_{90}\text{Th}$, $^{238}_{92}\text{U}$, and $^{235}_{92}\text{U}$. Of these, only $^{235}_{92}\text{U}$ is fissile by neutrons of all energies. Because the density of thorium is 11,000 kg/m^3 and it has a microscopic fission cross section of 0.1 barn for 1 MeV neutrons, the mean free path of a neutron for fission in this material is 3.5 m. The mean free path for neutron capture in thorium is very similar in magnitude. Therefore, nearly half the 2.2 neutrons emitted by fission in thorium will be lost to unproductive capture. For $^{238}_{92}\text{U}$, which represents 99.27% of all the atoms found in natural uranium (density of 18,000 kg/m^3), the odds are slightly better, with mean free paths for fission and capture respectively of 50 and 300 cm and fewer neutrons emitted per fission are lost to capture.

The main advantage of $^{235}_{92}\text{U}$, even though it represents only 0.72% of natural uranium composition, is that its fission cross section is quite high (1000 barns at 0.01 eV), giving a mean free path for fission of 2 cm. The capture cross section of $^{235}_{92}\text{U}$ at this energy is also six times smaller than the fission cross section. It is possible to decrease the mean free path for fission with $^{235}_{92}\text{U}$ by increasing its relative concentration in uranium-based fuel (fuel enrichment). The ratio of capture to fission in uranium-enriched fuels remains small even if the fuel contains a large amount of $^{238}_{92}\text{U}$ (capture cross section less than 1 barn).

The heat produced in the fuel can then easily be extracted by conventional means (by circulating a fluid such as water). The main problem is to slow down the secondary fission neutrons to low energies (< 1 eV) while ensuring that few are lost by capture inside other materials or by leaving the reactor. A neutron slowing-down material, the moderator, must therefore be introduced into the reactor to serve this purpose.

Table 8 Maximum values of the elastic scattering and absorption cross sections for ^1_1H, ^2_1D, and $^{12}_6\text{C}$ in the energy range 0.1 eV < E <0.1 MeV.

Isotope	$\sigma_{\text{scattering}}$ (b)	$\sigma_{\text{absorption}}$ (b)
^1_1H	18	0.17
^2_1D	3.4	0.00025
$^{12}_6\text{C}$	4.6	0.0016

For this moderator, two questions are of prime importance: what should be its composition, and where should it be located? The first question is easily answered by combining the kinetics of the neutron-nucleus collision and a survey of the scattering and absorption cross sections of the most promising candidates. In Section 3.5, we concluded that the slowing-down efficiency of a nucleus increases as its mass number decreases, which points to the use of light nuclides as moderators. The most promising candidates are the isotopes of hydrogen and carbon that are readily available in water and graphite. **Table 8** provides the maximum values of the elastic scattering and absorption cross sections for ^1_1H, ^2_1D, and $^{12}_6\text{C}$ in the energy range $0.1\,\text{eV} < E < 0.1\,\text{MeV}$. As one can see, ^1_1H is the best moderator if one does not take into account its absorption cross section. However, up to one in ten collisions of a neutron with ^1_1H could lead to absorption (for 1eV neutrons). On the other hand, even if the number of collisions required to slow down neutrons using ^2_1D and $^{12}_6\text{C}$ is significantly higher (the distance the neutron will travel between collisions is longer), less than 0.007% of the collisions with ^2_1D and 0.03% of the collisions with $^{12}_6\text{C}$ (1 eV neutron) lead to capture. Accordingly, if one wants to build a core that is compact, a ^1_1H-based moderator is a requirement (light water, for example in LWR); otherwise the best candidate is a moderator that contains large concentrations of ^2_1D (heavy water in CANDU).

Now let us try to answer the question of the spatial distribution of this moderator. Two very different options can be considered: a homogeneous mixture of fuel and moderator, and small isolated fuel elements placed strategically in the moderator. Again, the answer to this question can be inferred from **Figure 13**. The neutrons in a homogeneous mixture of fuel and moderator materials have a large chance of colliding with fuel isotopes as they are slowing down. This means that neutrons with energies in the "resonance" range ($4\,\text{eV} < E < 10\,\text{keV}$) will be in direct contact with fuel nuclides. Because their capture cross sections at resonance energies increase, often by several orders of magnitude with respect to the background value, neutron capture will have a detrimental effect on the number of neutrons that can reach energies below 1 eV. On the other hand, by separating different fuel elements by a sufficient amount of moderating materials to ensure that a maximum number of neutrons escape the resonance energy range, one decreases neutron loss by capture and increases the probability of fission.

These are the general physics considerations that led to current reactor designs, including the pressurized water (PWR) and CANDU reactors. In the next section, we conclude this chapter by introducing the neutron transport equation, which provides a means to evaluate numerically the neutron population in the reactor and to determine whether a given reactor concept can lead to a sustained chain reaction. This equation also provides the neutron flux that is required to follow the evolution of the fuel and the fission products in the reactor using the Bateman equation.

4.4　Reactor Physics and the Transport Equation

When designing a nuclear power reactor, physicists have two main objectives:

- controlling the nuclear chain reaction;
- extracting the energy produced inside the fuel to avoid damage to the core and to use this energy to produce electricity.

Because most of the energy produced in a nuclear reactor is the result of the fission process, the power produced in the core can be expressed by:

$$P(t) = \int_V d^3r \int_0^\infty dE \sum_J \kappa_J \Sigma_{f,J}(\vec{r},t,E) \int_{4\pi} \phi(\vec{r},t,E,\vec{\Omega}) d^2\Omega, \tag{118}$$

where V is the reactor volume, $\phi(\vec{r},t,E,\vec{\Omega})$ is the flux of neutrons with energy E and direction $\vec{\Omega}$ at a point $\vec{r}$ in space and a time t, and $\Sigma_{f,J}(\vec{r},t,E)$ is the macroscopic fission cross section for isotope J given by

$$\Sigma_{f,J}(\vec{r},t,E) = N_J(\vec{r},t)\sigma_{f,J}(E), \tag{119}$$

where $N_J(\vec{r},t)$ is the time-dependent concentration of J, the solution of the flux-dependent Bateman equations (see Section 4.2). Finally, κ_J represents the average energy produced by the fission of isotope J, which we assume to be energy-independent.

Now let us consider the flux, which is a measure of the neutron population in the reactor (Section 3.5). For a given time interval dt, the change of the neutron population $dn(\vec{r},t,E,\vec{\Omega}) = d\phi(\vec{r},t,E,\vec{\Omega})/v$ due to loss of neutrons by collisions is [Bell1982, Duderstadt1979, Hébert2009, Lewis1993]:

$$L_C(\vec{r},t,E,\vec{\Omega})dt = -\Sigma(\vec{r},t,E)\phi(\vec{r},t,E,\vec{\Omega})dt, \tag{120}$$

where Σ is the total cross section and $L_C(\vec{r},t,E,\vec{\Omega})$ the rate of collision per unit volume of neutrons with energy E and direction $\vec{\Omega}$ at point $\vec{r}$ and time t. This term includes both absorbed and scattered neutrons. Some neutrons will be lost to migration when the net flow of neutrons reaching a region in space of volume d^3r is different from that leaving this same region. This rate of neutron loss due to migration is given by

$$L_M(\vec{r},t,E,\vec{\Omega})dt = -\vec{\Omega}\cdot\vec{\nabla}\phi(\vec{r},t,E,\vec{\Omega})dt, \tag{121}$$

meaning that neutrons, which can be considered to form a gas, tend to move towards regions of low neutron population (the kinetic theory of gas). Neutron with energy E and direction $\vec{\Omega}$ can also be produced in this region of space due to scattering of neutrons with different directions and energies:

$$S_S\left(\vec{r},t,E,\vec{\Omega}\right)dt = \int\limits_0^\infty dE' \int\limits_{4\pi} d^2\Omega' \, \Sigma_s\left(\vec{r},t,E' \to E, \vec{\Omega}' \to \vec{\Omega}\right)\phi\left(\vec{r},t,E',\vec{\Omega}'\right)dt, \qquad (122)$$

where $\Sigma_s(\vec{r},t,E' \to E, \overrightarrow{\Omega}' \to \overrightarrow{\Omega})$ is the probability (also known as the double differential scattering cross section) that a neutron of energy E' moving in direction $\overrightarrow{\Omega}'$ is scattered in direction $\overrightarrow{\Omega}$ with energy E. For the case where fission takes place, the neutron production rate is

$$S_F\left(\vec{r},t,E,\vec{\Omega}\right)dt = \sum_j \chi_j(E)\int\limits_0^\infty dE' \; \nu_j \Sigma_{f,J}(\vec{r},t,E')\int\limits_{4\pi} d^2\Omega' \phi(\vec{r},t,E',\vec{\Omega}')dt, \qquad (123)$$

where $\chi_j(E)$ is the fission spectrum and ν_j the average number of neutrons produced by fission of isotope J. Neutron productions from other sources $S_E\left(\vec{r},t,E,\vec{\Omega}\right)$ can also be added to the balance, for example, sources for other types of nuclear reactions (photonuclear fission and photoneutron production in $_1^2D$) or flux-independent contributions from the decay of radioactive isotopes.

The global neutron population will then satisfy the following balance equation:

$$\frac{1}{v}\frac{d\phi\left(\vec{r},t,E,\vec{\Omega}\right)}{dt} = L_C\left(\vec{r},t,E,\vec{\Omega}\right) + L_M\left(\vec{r},t,E,\vec{\Omega}\right) + S_S\left(\vec{r},t,E,\vec{\Omega}\right) + S_F\left(\vec{r},t,E,\vec{\Omega}\right) + S_E\left(\vec{r},t,E,\vec{\Omega}\right),(124)$$

which is known as the Boltzmann transport equation. If one assumes that the cross sections are nearly constant over time (the change in the composition of the materials in the reactor varies substantially only over long time periods) and that the core is at static equilibrium (the flux remains constant), one obtains the following time-independent neutron transport equation [Lewis1993]:

$$\vec{\Omega}\cdot\vec{\nabla}\phi\left(\vec{r},E,\vec{\Omega}\right) + \Sigma(\vec{r},E)\phi\left(\vec{r},E,\vec{\Omega}\right) =$$

$$\int\limits_0^\infty dE' \int\limits_{4\pi} d^2\Omega' \, \Sigma_s\left(\vec{r},E' \to E, \vec{\Omega}' \to \vec{\Omega}\right)\phi\left(\vec{r},E',\vec{\Omega}'\right) + \frac{1}{k}\sum_j \chi_j(E)\int\limits_0^\infty dE' \; \nu_j \Sigma_{f,J}\left(\vec{r},E'\right)\int\limits_{4\pi} d^2\Omega' \phi\left(\vec{r},E',\vec{\Omega}'\right),$$

$$(125)$$

where k is known as the multiplication factor. It is inserted in the transport equation to modify the fission rate in such a way as to reach this static equilibrium. When $k = 1$, equilibrium is achieved, and the reactor is critical. For $k < 1$, the reactor is sub-critical, and neutron generation is insufficient to compensate for losses, whereas for $k > 1$, the reactor is super-critical, and neutron production exceeds losses.

For reactor calculations, where fission reactions take place only inside the core, boundary conditions of the form

$$\phi\left(\vec{r}_B,E,\vec{\Omega}\right) = 0 \;\; \text{for} \; \vec{\Omega}\cdot\vec{N} < 0 \qquad (126)$$

are generally imposed on the transport equation. Here, the point $\vec{r}_B$ is on the outer boundary of the reactor, with $\vec{N}$ being a unit vector normal to this boundary and directed outwards. This condition simply means that no neutrons will enter the reactor from the outside.

The static transport equation is an eigenvalue equation, with k being the inverse of the eigenvalue. Therefore, the neutron flux is the eigenvector for this equation and is only defined

to within a normalization constant. Therefore, if $\phi\left(\vec{r}, E, \vec{\Omega}\right)$ is a solution, so is $a\phi\left(\vec{r}, E, \vec{\Omega}\right)$, with a an arbitrary constant. For reactor calculations, the normalization constant is directly related to the power produced in the core.

Solving the transport problem is not trivial, even for very simple cases (static, one velocity neutrons in one dimension). In Chapters 4 (static) and 5 (time-dependent), approximation to and simplification of the transport equation commonly used in reactor simulations will be discussed. One should then be able to extract, from the solutions of the resulting simplified equations, information useful for the design, operation, and control of nuclear reactors.

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6 Summary of Relationship to Other Chapters

This chapter explains the structure of the nucleus and introduces the various interactions of charged particles, photons, and neutrons with matter. It also defines the basic quantities and concepts needed to study the fission chain reaction and to approach the analysis of reactors. The Bateman equations are presented and used in other chapters to evaluate the rate of evolution of fuel composition. The Boltzmann transport equation, which provides a way to evaluate the neutron population in a nuclear reactor, is also introduced. This is the fundamental equation from which the neutron diffusion equation used in Chapters 4 and 5 is derived.

Chapter 4 starts with the static transport equation to derive the time-independent neutron-diffusion equation for the analysis of steady-state (time-independent) neutron distributions either in the presence of external sources or in fission reactors. It also discusses the evolution of the fuel composition in an operating reactor based on the coupled solution of the transport and Bateman equations using a quasi-static approximation.

Chapter 5 covers the time-dependent neutron-diffusion equations and studies the phenomena of fast-neutron kinetics, fission-product poisoning, reactivity coefficients, etc., in reactors.

Chapter 12 deals with radioprotection and uses the concept defined in the present chapter for the interactions of charged particles, photons, and neutrons with matter with the goal of reducing the damage to living tissues.

Chapter 19 examines the behaviour of fuel after irradiation in a nuclear reactor, particularly its composition and the residual energy that it produces.

7   Problems

1. Evaluate the intensity of the electromagnetic force acting between two protons in an atom of helium.
2. Determine the atomic mass of natural chlorine if it is composed of 75.77 %atomic $^{35}_{17}Cl$ and 24.23 %atomic $^{37}_{17}Cl$.
3. What is the atomic concentration of $^{235}_{92}U$ in a sample of uranium oxide (UO_2) of density ρ=10.4 g /cm^3 enriched at a level of 3.5 %weight?
4. Using the semi-empirical mass formula, evaluate the atomic mass of ^{56}Fe and compare with the exact value.
5. What is the ground state energy level of a neutron in the Saxon-Wood potential for $^{238}_{92}U$?
6. Complete the following nuclear reactions and determine the net energy in MeV released by these reactions:
   a) $^{2}_{1}H + ^{3}_{1}H = ^{A}_{Z}X + ^{1}_{0}n$
   b) $^{1}_{0}n + ^{241}_{96}Cm = ^{A}_{Z}X + ^{90}_{36}Kr + 3^{1}_{0}n$
7. What is the activity of one gram of potassium-40?
8. Assuming that the activity of a sample of water due to tritium is 100 Bq, determine the mass of tritium in this sample. What will be the activity of this sample after three years?
9. Using the information available on the ESTAR web site, plot the CSDA range in cm for an electron in dry air at sea level as a function of its energy for 100 keV <E < 10 MeV.
10. Draw the deuterium cross section for photonuclear reactions as a function of energy in the range 2.23 MeV < E < 10MeV (here assume $C_{2_D} = 0.062$). Compare with the deuterium cross section for neutron radiative capture at 300 K in the same energy range.
11. How many collisions are required on average to slow down a neutron to half its speed (1/4 of its energy) through elastic collisions with deuterium nuclei?
12. Evaluate the potential scattering cross section for oxygen and hydrogen at low energy.
13. A CANDU bundle contains 19.5 kg of natural uranium (enrichment of 0.711 %weight). Compute the fission rate in a bundle due to $^{235}_{92}U$ if it is exposed to a flux of 10^{14} neutrons/cm^2/s of energy E=0.01 eV.
14. Show that the mean free path of 1 MeV neutrons in thorium is 3.5 m.

8   Acknowledgments

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