INTRODUCTION TO APPLIED NUCLEAR PHYSICS

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This text was compiled on 04/15/2025

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CHAPTER OVERVIEW

1: Introduction to Nuclear Physics

1.1: Basic Concepts

In this chapter we review some notations and basic concepts in Nuclear Physics. The chapter is meant to setup a common language for the rest of the material we will cover as well as rising questions that we will answer later on.

Terminology

A given atom is specified by the number of

- neutrons: N
- protons: Z
- electrons: there are Z electron in neutral atoms

Atoms of the same *element* have same atomic number Z. They are not all equal, however. *Isotopes* of the same element have different # of neutrons N .

Isotopes are denoted by ${}^A_Z X_N$ or more often by

$$\boxed{{}^A_Z X}$$

where X is the chemical symbol and A = Z + N is the mass number. E.g.: ${}^{235}_{92}U$, ${}^{238}U$ [the Z number is redundant, thus it is often omitted].

When talking of different nuclei we can refer to them as

- Nuclide: atom/nucleus with a specific N and Z.
- Isobar: nuclides with same mass # A ($\neq$ Z, N).
- Isotone: nuclides with same N, $\neq$ Z.
- Isomer: same nuclide (but different energy state).

Units, dimensions and physical constants

Nuclear energies are measured in powers of the unit *Electronvolt*: $1\mathrm{eV} = 1.6 \times 10^{-19}$ J . The electronvolt corresponds to the kinetic energy gained by an electron accelerated through a potential difference of 1 volt. Nuclear energies are usually in the range of MeV (mega-electronvolt, or 10^6 eV).

Nuclear masses are measured in terms of the *atomic mass unit* : 1 amu or $1\mathrm{u} = 1.66 \times 10^{-27}$ kg . One amu is equivalent to 1/12 of the mass of a neutral ground-state atom of ^{12}C. Since electrons are much lighter than protons and neutrons (and protons and neutrons have similar mass), one nucleon has mass of about 1 amu.

Because of the mass-energy equivalence, we will often express masses in terms of energy units. To convert between energy (in MeV) and mass (in amu) the conversion factor is of course the speed of light square (since E = mc^2). In these units we have: $c^2 = 931.502\ \mathrm{MeV/u}$.

- Proton mass: 938.280MeV/c^2
- Neutron mass: 938.573MeV/c^2
- Electron mass: 0.511MeV/c^2

Note: you can find most of these values in Krane (and online!)

Scales of magnitude for typical lengths are femtometer (1 fm=10^{-15} m) also called Fermi (F) and Angstrom 1° A = 10^{-10} m (for atomic properties) while typical time scales span a very broad range.

Physical constants that we will encounter include the speed of light, c = 299, 792, 458 m s^{-1}, the electron charge, e = 1.602176487 × 10^{-19} C, the Planck constant h = 6.62606896 × 10^{-34} J s and $\hbar$, Avogadro's number N$_a$ = 6.02214179 × 1023 mol^{-1}, the permittivity of vacuum $\epsilon_0 = 8.854187817 \times 10^{-12}\ \mathrm{Fm}^{-1}$ (F=Faraday) and many others. A good reference (online) is NIST: http://physics.nist.gov/cuu/index.html

There you can also find a tool to convert energy in different units: http://physics.nist.gov/cuu/Constants/energy.html

Nuclear Radius

The radius of a nucleus is not well defined, since we cannot describe a nucleus as a rigid sphere with a given radius. However, we can still have a practical definition for the range at which the density of the nucleons inside a nucleus approximate our simple model of a sphere for many experimental situations (e.g. in scattering experiments). A simple formula that links the nucleus radius to the number of nucleons is the *empirical radius formula*:

$$\boxed{R = R_0 A^{1/3}}$$

1.2: Binding energy and Semi-empirical mass formula

Binding Energy

Two important nuclear properties that we want to study are the nuclear binding energy and the mass of nuclides. You could think that since we know the masses of the proton and the neutron, we could simply find the masses of all nuclides with the simple formula:

$$m_N \overset{?}{=} Zm_p + Nm_n. \tag{1.2.1}$$

However, it is seen experimentally that this is not the case. From special relativity theory, we know that to each mass corresponds some energy, $E = mc^2$. Then if we just sum up the masses of all the constituents of a nucleus we would have how much energy they represent. The mass of a nucleus is also related to its intrinsic energy. It thus makes sense that this is not only the sum of its constituent energies, since we expect that some other energy is spent to keep the nucleus together. If the energy were equal, then it wouldn't be favorable to have bound nuclei, and all the nuclei would be unstable, constantly changing from their bound state to a sum of protons and neutrons.

The binding energy of a nucleus is then given by the difference in mass energy between the nucleus and its constituents. For a nucleus ${}^A_Z X_N$ the binding energy B is given by

$$B = \left[Zm_p + Nm_n - m_N\left({}^A X\right)\right] c^2$$

However, we want to express this quantity in terms of experimentally accessible quantities. Thus we write the nuclear mass in terms of the atomic mass, that we can measure,

$$m_N\left({}^A X\right) c^2 = \left[m_A\left({}^A X\right) - Zm_e\right] c^2 + B_e \tag{1.2.2}$$

where $m_A\left({}^A X\right)$ is the *atomic* mass of the nucleus. We further neglect the electronic binding energy B_e by setting

$$m_N\left({}^A X\right) c^2 = \left[m_A\left({}^A X\right) - Zm_e\right] c^2. \tag{1.2.3}$$

We finally obtain the expression for the **nuclear binding energy**:

$$\boxed{B = \left\{Zm_p + Nm_n - \left[m_A\left({}^A X\right) - Zm_e\right]\right\} c^2}$$

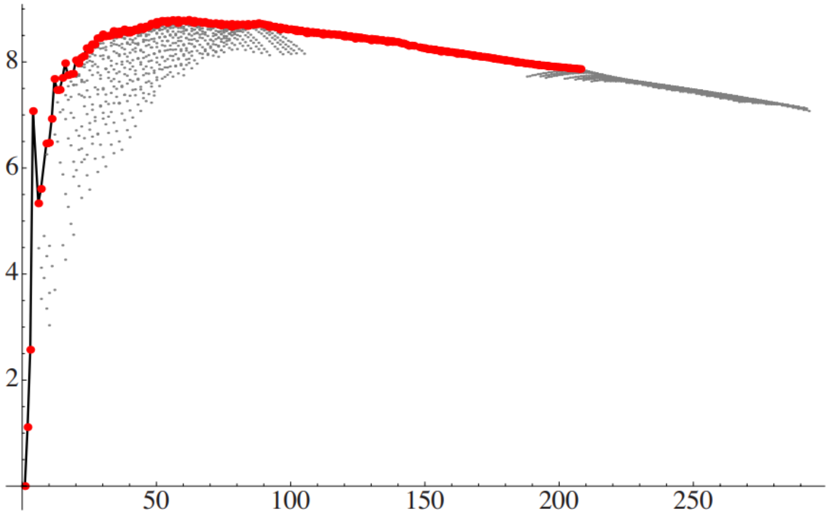


Figure 1.2.1: Binding energy per nucleon n (B/A in MeV vs. A) of stables nuclides (Red) and unstable nuclides (Gray). (CC BY-NC-ND; Paola Cappellaro)

Quantities of interest are also the neutron and proton separation energies:

$$\begin{aligned} S_n &= B\left({}^A_Z X_N\right) - B\left({}^{A-1}_Z X_{N-1}\right) \\ S_p &= B\left({}^A_Z X_N\right) - B\left({}^{A-1}_{Z-1} X_N\right) \end{aligned}$$

which are the analogous of the ionization energies in atomic physics, reflecting the energies of the *valence* nucleons. We will see that these energies show signatures of the shell structure of nuclei.

Semi-empirical mass formula

The binding energy is usually plotted as B/A or binding energy per nucleon. This illustrates that the binding energy is overall simply proportional to A, since B/A is mostly constant.

There are however corrections to this trend. The dependence of B/A on A (and Z) is captured by the ***semi-empirical mass formula***. This formula is based on first principle considerations (a model for the nuclear force) and on experimental evidence to find the exact parameters defining it. In this model, the so-called **liquid-drop** model, all nucleons are uniformly distributed inside a nucleus and are bound together by the nuclear force while the Coulomb interaction causes repulsion among protons. Characteristics of the nuclear force (its short range) and of the Coulomb interaction explain part of the semi-empirical mass formula. However, other (smaller) corrections have been introduced to take into account variations in the binding energy that emerge because of its quantum-mechanical nature (and that give rise to the **nuclear shell model**).

The semi-empirical mass formula (SEMF) is

$$M(Z,A)=Zm\left({}^{1}H\right)+Nm_n-B(Z,A)/c^2$$

where the binding energy B(Z, A) is given by the following formula:

$$\boxed{B(A,Z)=a_vA\ \ -a_sA^{2/3}-a_cZ(Z-1)A^{-1/3}-a_{sym}\frac{(A-2Z)^2}{A}+\delta a_pA^{-3/4}}$$

$$\nearrow\ \ \uparrow\ \ \uparrow\ \ \uparrow\ \ \nwarrow$$

$$\text{volume}\quad \text{surface}\quad \text{Coulomb}\quad \text{symmetry}\quad \text{pairing}$$

We will now study each term in the SEMF.

Volume term

The first term is the volume term a_VA that describes how the binding energy is mostly proportional to A. Why is that so?

Remember that the binding energy is a measure of the interaction among nucleons. Since nucleons are closely packed in the nucleus and the nuclear force has a very short range, each nucleon ends up interacting only with a few neighbors. This means that independently of the total number of nucleons, each one of them contribute in the same way. Thus the force is not proportional to $A(A-1)/2 \sim A^2$ (the total # of nucleons one nucleon can interact with) but it's simply proportional to A. The constant of proportionality is a fitting parameter that is found experimentally to be $a_v = 15.5\text{MeV}$.

This value is smaller than the binding energy of the nucleons to their neighbors as determined by the strength of the nuclear (strong) interaction. It is found (and we will study more later) that the energy binding one nucleon to the other nucleons is on the order of 50 MeV. The total binding energy is instead the difference between the interaction of a nucleon to its neighbor and the kinetic energy of the nucleon itself. As for electrons in an atom, the nucleons are fermions, thus they cannot all be in the same state with zero kinetic energy, but they will fill up all the kinetic energy levels according to Pauli's exclusion principle. This model, which takes into account the nuclear binding energy and the kinetic energy due to the filling of shells, indeed gives an accurate estimate for a_V.

Surface term

The surface term, $-a_sA^{2/3}$, also based on the strong force, is a correction to the volume term. We explained the volume term as arising from the fact that each nucleon interacts with a constant number of nucleons, independent of A. While this is valid for nucleons deep within the nucleus, those nucleons on the surface of the nucleus have fewer nearest neighbors. This term is similar to surface forces that arise for example in droplets of liquids, a mechanism that creates surface tension in liquids.

Since the volume force is proportional to $B_V \propto A$, we expect a surface force to be $\sim (B_V)^{2/3}$ (since the surface $S \sim V^{2/3}$). Also the term must be subtracted from the volume term and we expect the coefficient a_s to have a similar order of magnitude as a_V. In fact $a_s = 13 - 18\text{MeV}$.

Coulomb term

The third term $-a_c Z(Z-1)A^{-1/3}$ derives from the Coulomb interaction among protons, and of course is proportional to Z. This term is subtracted from the volume term since the Coulomb repulsion makes a nucleus containing many protons less favorable (more energetic).

To motivate the form of the term and estimate the coefficient a$_c$, the nucleus is modeled as a uniformly charged sphere. The potential energy of such a charge distribution is

$$E=\frac{1}{4\pi\epsilon_0}\frac{3}{5}\frac{Q^2}{R}$$

since from the uniform distribution inside the sphere we have the charge $q(r)=\frac{4}{3}\pi r^3\rho=Q\left(\frac{r}{R}\right)^3$ and the potential energy is then:

$$\begin{aligned} E &=\frac{1}{4\pi\epsilon_0}\int dq(\vec{r})\frac{q(\vec{r})}{|\vec{r}|}=\frac{1}{4\pi\epsilon_0}\int d^3\vec{r}\rho\frac{q(\vec{r})}{|\vec{r}|}=\frac{1}{4\pi\epsilon_0}\int_0^R dr4\pi r^2\rho\frac{q(r)}{r} \\ &=\frac{1}{4\pi\epsilon_0}\left(4\pi\int_0^R dr\frac{3Q}{4\pi R^3}r^2Q\left(\frac{r}{R}\right)^3\frac{1}{r}\right)=\frac{1}{4\pi\epsilon_0}\int_0^R dr\frac{3Q^2r^4}{R^6}=\frac{1}{4\pi\epsilon_0}\frac{3}{5}\frac{Q^2}{R}\end{aligned}$$

Using the empirical radius formula $R=R_0A^{1/3}$ and the total charge $Q^2=e^2Z(Z-1)$ (reflecting the fact that this term will appear only if Z > 1, i.e. if there are at least two protons) we have :

$$\frac{Q^2}{R}=\frac{e^2Z(Z-1)}{R_0A^{1/3}}$$

which gives the shape of the Coulomb term. Then the constant a$_c$ can be estimated from $a_c\approx\frac{3}{5}\frac{e^2}{4\pi\epsilon_0R_0}$, with R$_0$ = 1.25 fm, to be a$_c$ ≈ 0.691 MeV, not far from the experimental value.

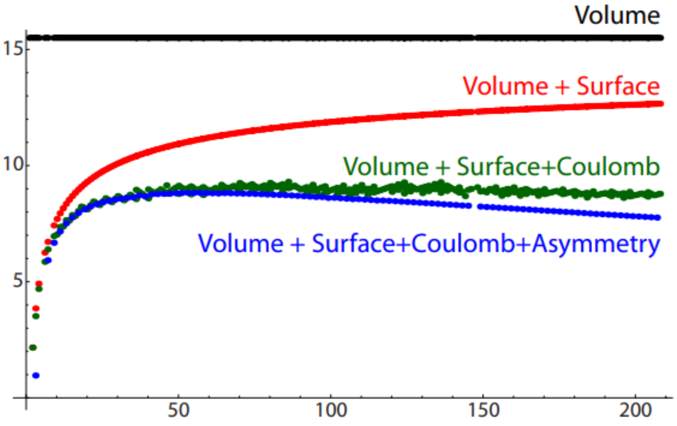


Figure 1.2.2: SEMF for stable nuclides. We plot B(Z, A)/A vs. A. The various term contributions are added one by one to arrive at the final formula. (CC BY-NC-ND; Paola Cappellaro)

Symmetry term

The Coulomb term seems to indicated that it would be favorable to have less protons in a nucleus and more neutrons. However, this is not the case and we have to invoke something beyond the liquid-drop model in order to explain the fact that we have roughly the same number of neutrons and protons in stable nuclei. There is thus a correction term in the SEMF which tries to take into account the symmetry in protons and neutrons. This correction (and the following one) can only be explained by a more complex model of the nucleus, the **shell model**, together with the quantum-mechanical *exclusion principle*, that we will study later in the class. If we were to add more neutrons, they will have to be more energetic, thus increasing the total energy of the nucleus. This increase more than off-set the Coulomb repulsion, so that it is more favorable to have an approximately equal number of protons and neutrons. The shape of the symmetry term is $\frac{(A-2Z)^2}{A}$. It can be more easily understood by considering the fact that this term goes to zero for A = 2Z and its effect is smaller for larger A (while for smaller nuclei the symmetry effect is more important). The coefficient is a$_{sym}$ = 23 MeV.

Pairing term

The final term is linked to the physical evidence that like-nucleons tend to pair off. Then it means that the binding energy is greater ($\delta > 0$) if we have an even-even nucleus, where all the neutrons and all the protons are paired-off. If we have a nucleus with both an odd number of neutrons and of protons, it is thus favorable to convert one of the protons into a neutrons or vice-versa (of course, taking into account the other constraints above). Thus, with all other factor constant, we have to subtract ($\delta < 0$) a term from the binding energy for odd-odd configurations. Finally, for even-odd configurations we do not expect any influence from this pairing energy ($\delta = 0$). The pairing term is then

$$+\delta a_p A^{-3/4} = \begin{cases} +a_p A^{-3/4} \text{ even-even} \\ 0 \text{ even-odd} \\ -a_p A^{-3/4} \text{ odd-odd} \end{cases}$$

with $a_p \approx 34$MeV. [Sometimes the form $\propto A^{-1/2}$ is also found].

Line of Stability in the Chart of nuclides

By taking the first derivative wrt Z we can calculate the optimal Z such that the mass is minimum. We obtain:

$$\begin{aligned} Z_{\min} &= \frac{A}{2}\left(\frac{1+\frac{1}{4}A^{-1/3}\frac{a_c}{a_{sym}}}{1+\frac{1}{4}A^{2/3}\frac{a_c}{a_{sym}}}\right) \\ &\approx \frac{A}{2}\left(1+\frac{1}{4}A^{2/3}\frac{a_c}{a_{sym}}\right)^{-1} \\ &\approx \frac{A}{2}\left(1-\frac{1}{4}A^{2/3}\frac{a_c}{a_{sym}}\right) \end{aligned}$$

which gives $Z \approx \frac{A}{2}$ at small A, but has a correction for larger A such that $Z \approx 0.41A$ for heavy nuclei. [Note the approximation and series expansion is taken because $a_c \ll a_{sym}$]

If we plot Z/A vs. A the nuclides lie between 1/2 and 0.41. There is a line of stability, following the stable isotopes (red in Figure 1.2.4 and black in Figure 1.2.3). The isotopes are then variously labeled, for example here by their lifetime. Interactive information is available at www.nndc.bnl.gov/chart/.

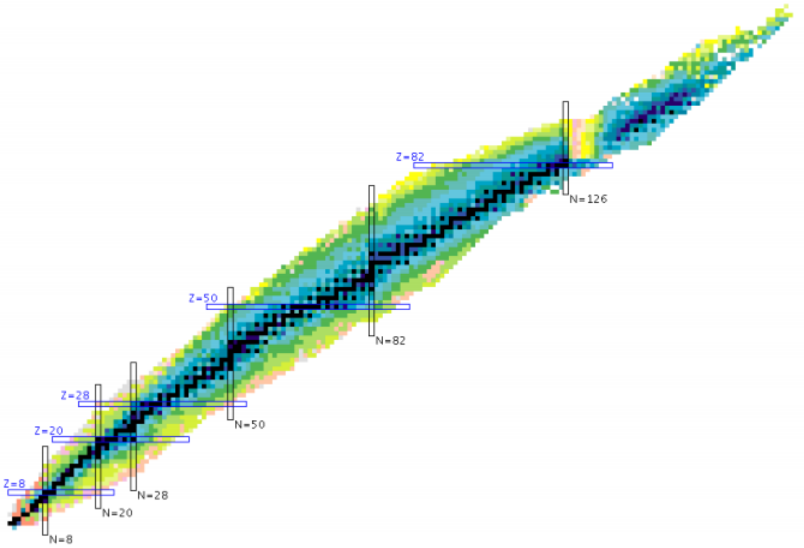


Figure 1.2.3: Chart of nuclides from www.nndc.bnl.gov/chart/ . Each nuclide is color-labeled by its half-life (black for stable nuclides) © Brookhaven National Laboratory. All rights reserved. This content is excluded from our Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.

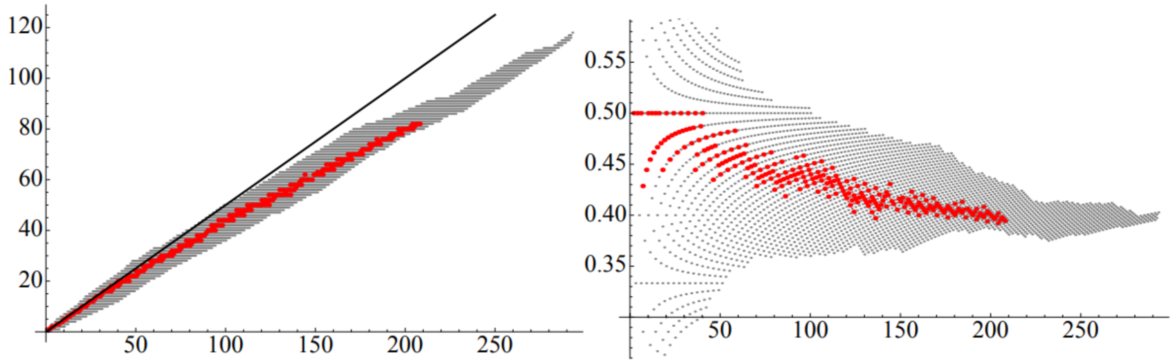


Figure 1.2.4: Nuclide chart (obtained with the software Mathematica). Left: Z vs. A, Right: Z/A vs. A. In red, stable nuclides. The black line represents Z = A/2. (CC BY-NC-ND; Paola Cappellaro)

1.3: Radioactive decay

Radioactive decay is the process in which an unstable nucleus spontaneously loses energy by emitting ionizing particles and radiation. This decay, or loss of energy, results in an atom of one type, called the **parent** nuclide, transforming to an atom of a different type, named the **daughter** nuclide.

The three principal modes of decay are called the alpha, beta and gamma decays. We will study their differences and exact mechanisms later in the class. However these decay modes share some common feature that we describe now. What these radioactive decays describe are fundamentally quantum processes, i.e. transitions among two quantum states. Thus, the radioactive decay is statistical in nature, and we can only describe the evolution of the expectation values of quantities of interest, for example the number of atoms that decay per unit time. If we observe a single unstable nucleus, we cannot know a priori when it will decay to its daughter nuclide. The time at which the decay happens is random, thus at each instant we can have the parent nuclide with some probability p and the daughter with probability 1 − p. This stochastic process can only be described in terms of the quantum mechanical evolution of the nucleus. However, if we look at an ensemble of nuclei, we can predict at each instant the average number of parent an daughter nuclides.

If we call the number of radioactive nuclei N, the number of decaying atoms per unit time is dN/dt. It is found that this rate is constant in time and it is proportional to the number of nuclei themselves:

$$\boxed{\frac{dN}{dt}=-\lambda N(t)}$$

The constant of proportionality λ is called the **decay constant**. We can also rewrite the above equation as

$$\lambda=-\frac{dN/dt}{N}$$

where the RHS is the probability per unit time for one atom to decay. The fact that this probability is a constant is a characteristic of all radioactive decay. It also leads to the *exponential law of radioactive decay*:

$$N(t)=N(0)e^{-\lambda t}$$

We can also define the **mean lifetime**

$$\boxed{\tau=1/\lambda}$$

and the **half-life**

$$\boxed{t_{1/2}=\ln(2)/\lambda}$$

which is the time it takes for half of the atoms to decay, and the **activity**

$$\mathcal{A}(t)=\lambda N(t)$$

Since $\mathcal{A}$ can also be obtained as $\left|\frac{dN}{dt}\right|$, the activity can be estimated from the number of decays ΔN during a small time δt such that $\delta t\ll t_{1/2}$.

A common situation occurs when the daughter nuclide is also radioactive. Then we have a chain of radioactive decays, each governed by their decay laws. For example, in a chain $N_1\rightarrow N_2\rightarrow N_3$, the decay of N_1 and N_2 is given by:

$$dN_1=-\lambda_1 N_1 dt,\quad dN_2=+\lambda_1 N_1 dt-\lambda_2 N_2 dt$$

Another common characteristic of radioactive decays is that they are a way for unstable nuclei to reach a more energetically favorable (hence stable) configuration. In α and β decays, a nucleus emits a α or β particle, trying to approach the most stable nuclide, while in the γ decay an excited state decays toward the ground state without changing nuclear species.

Alpha decay

If we go back to the binding energy per mass number plot (B/A vs. A) we see that there is a bump (a peak) for A ∼ 60 − 100. This means that there is a corresponding minimum (or energy optimum) around these numbers. Then the heavier nuclei will want to decay toward this lighter nuclides, by shedding some protons and neutrons. More specifically, the decrease in binding energy at high A is due to Coulomb repulsion. Coulomb repulsion grows in fact as Z^2, much faster than the nuclear force which is ∝ A.

This could be thought as a similar process to what happens in the fission process: from a parent nuclide, two daughter nuclides are created. In the α decay we have specifically:

$$ {}_{Z}^{A}X_{N} \longrightarrow {}_{Z-2}^{A-4}X'_{N-2} + \alpha $$

where α is the nucleus of He-4: ${}_{2}^{4}\mathrm{He}_{2}$.

The α decay should be competing with other processes, such as the fission into equal daughter nuclides, or into pairs including ^{12}C and ^{16}O that have larger B/A then α. However α decay is usually favored. In order to understand this, we start by looking at the energetic of the decay, but we will need to study the quantum origin of the decay to arrive at a full explanation.

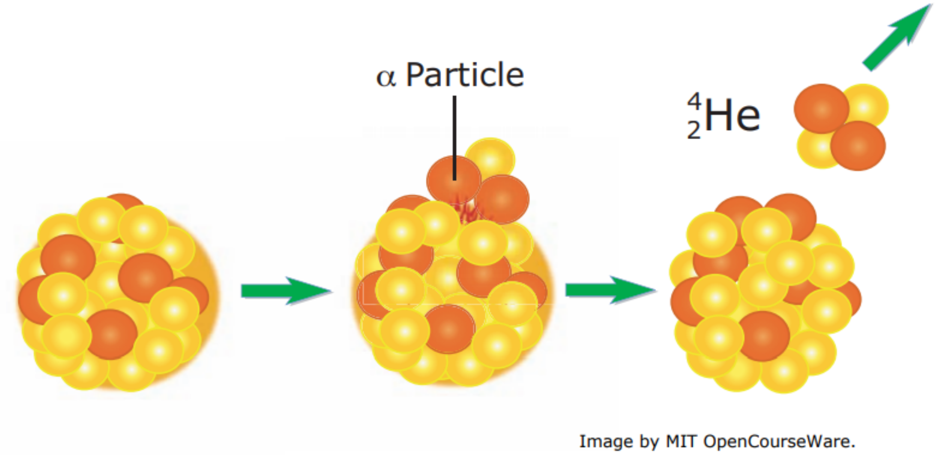


Figure 1.3.1: Alpha decay schematics. (CC BY-NC-ND; Paola Cappellaro)

Energetics

In analyzing a radioactive decay (or any nuclear reaction) an important quantity is Q, the net energy released in the decay: $Q = (m_X - m_{X'} - m_\alpha)c^2$. This is also equal to the total kinetic energy of the fragments, here $Q = T_{X'} + T_\alpha$ (here assuming that the parent nuclide is at rest).

When Q > 0 energy is released in the nuclear reaction, while for Q < 0 we need to provide energy to make the reaction happen. As in chemistry, we expect the first reaction to be a spontaneous reaction, while the second one does not happen in nature without intervention. (The first reaction is exo-energetic the second endo-energetic). Notice that it's no coincidence that it's called Q. In practice given some reagents and products, Q give the *quality* of the reaction, i.e. how energetically favorable, hence probable, it is. For example in the alpha-decay $\log\left(t_{1/2}\right) \propto \frac{1}{\sqrt{Q_\alpha}}$, which is the Geiger-Nuttall rule (1928).

The alpha particle carries away most of the kinetic energy (since it is much lighter) and by measuring this kinetic energy experimentally it is possible to know the masses of unstable nuclides. We can calculate Q using the SEMF. Then:

$$ Q_\alpha = B\left({}_{Z-2}^{A-4}X'_{N-2}\right) + B\left({}^4He\right) - B\left({}_{Z}^{A}X_{N}\right) = B(A-4, Z-2) - B(A, Z) + B\left({}^4He\right) $$

We can approximate the finite difference with the relevant gradient:

$$ \begin{aligned} Q_\alpha &= [B(A-4, Z-2) - B(A, Z-2)] + [B(A, Z-2) - B(A, Z)] + B\left({}^4He\right) \approx= -4\frac{\partial B}{\partial A} - 2\frac{\partial B}{\partial Z} + B\left({}^4He\right) \\ &= 28.3 - 4a_v + \frac{8}{3}a_s A^{-1/3} + 4a_c\left(1 - \frac{Z}{3A}\right)\left(\frac{Z}{A^{1/3}}\right) - 4a_{\text{sym}}\left(1 - \frac{2Z}{A} + 3a_p A^{-7/4}\right)^2 \end{aligned} $$

Since we are looking at heavy nuclei, we know that Z ≈ 0.41A (instead of Z ≈ A/2) and we obtain

$$ Q_\alpha \approx -36.68 + 44.9A^{-1/3} + 1.02A^{2/3}, $$

where the second term comes from the surface contribution and the last term is the Coulomb term (we neglect the pairing term, since a priori we do not know if a_p is zero or not).

Then, the Coulomb term, although small, makes Q increase at large A. We find that Q ≥ 0 for $A \gtrsim 150$, and it is Q ≈ 6MeV for A = 200. Although Q > 0, we find experimentally that α decay only arise for A ≥ 200.

Further, take for example Francium-200 $\left({}_{87}^{200}\mathrm{Fr}_{113}\right)$. If we calculate Q_α from the experimentally found mass differences we obtain $Q_\alpha \approx 7.6\mathrm{MeV}$ (the product is ^{196}At.) We can do the same calculation for the hypothetical decay into a ^{12}C and remaining fragment $\left({}_{81}^{188}\mathrm{Tl}_{107}\right)$:

$$Q_{^{12}C} = c^2\left[m\left({}_Z^A X_N\right) - m\left({}_{Z-6}^{A-12} X'_{N-6}\right) - m\left({}^{12}C\right)\right] \approx 28MeV$$

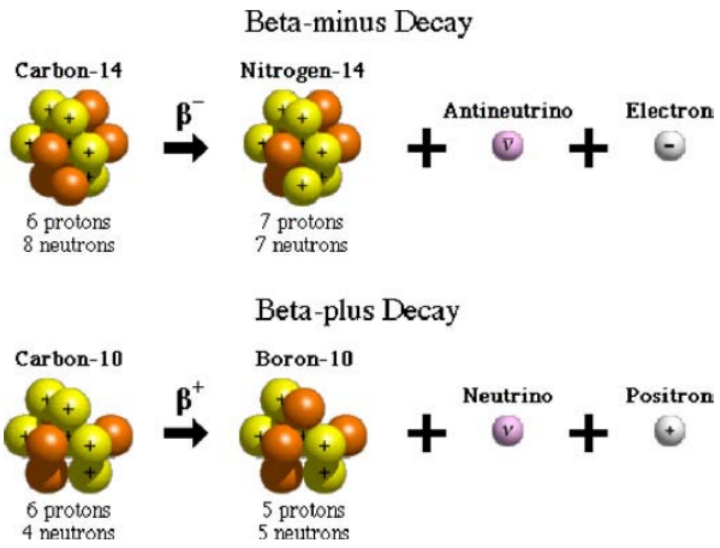
Thus this second reaction seems to be more energetic, hence more favorable than the alpha-decay, yet it does not occur (some decays involving C-12 have been observed, but their branching ratios are much smaller).

Thus, looking only at the energetic of the decay does not explain some questions that surround the alpha decay:

- Why there's no ^{12}C-decay? (or to some of this tightly bound nuclides, e.g O-16 etc.)
- Why there's no spontaneous fission into equal daughters?
- Why there's alpha decay only for A ≥ 200?
- What is the explanation of Geiger-Nuttall rule? $\log t_{1/2} \propto \frac{1}{\sqrt{Q_\alpha}}$

Beta decay

The beta decay is a radioactive decay in which a proton in a nucleus is converted into a neutron (or vice-versa). Thus A is constant, but Z and N change by 1. In the process the nucleus emits a beta particle (either an electron or a positron) and quasi-massless particle, the **neutrino**



Courtesy of Thomas Jefferson National Accelerator Facility - Office of Science Education. Used with permission.

Figure 1.3.2: Beta decay schematics (CC BY-NC-ND; Paola Cappellaro)

There are 3 types of beta decay:

$$ {}_Z^A X_N \rightarrow {}_{Z+1}^{A} X'_{N-1} + e^- + \bar{\nu} $$

This is the β^- decay (or negative beta decay). The underlying reaction is:

$$ n \rightarrow p + e^- + \bar{\nu} $$

that corresponds to the conversion of a proton into a neutron with the emission of an electron and an anti-neutrino. There are two other types of reactions, the β^+ reaction,

$$ {}_Z^A X_N \rightarrow {}_{Z-1}^{A} X'_{N+1} + e^+ + \nu \quad \Longleftrightarrow \quad p \rightarrow n + e^+ + \nu $$

which sees the emission of a positron (the electron anti-particle) and a neutrino; and the electron capture:

$$ {}^{A}_{Z}X_N + e^- \rightarrow {}^{A}_{Z-1}X'_{N+1} + \nu \quad \Longleftrightarrow \quad p + e^- \rightarrow n + \nu $$

a process that competes with, or substitutes, the positron emission.

Recall the mass of nuclide as given by the semi-empirical mass formula. If we keep A fixed, the SEMF gives the binding energy as a function of Z. The only term that depends explicitly on Z is the Coulomb term. By inspection we see that B ∝ Z^2. Then from the SEMF we have that the masses of possible nuclides with the same mass number lie on a parabola. Nuclides lower in the parabola have smaller M and are thus more stable. In order to reach that minimum, unstable nuclides undergo a decay process to transform excess protons in neutrons (and vice-versa).

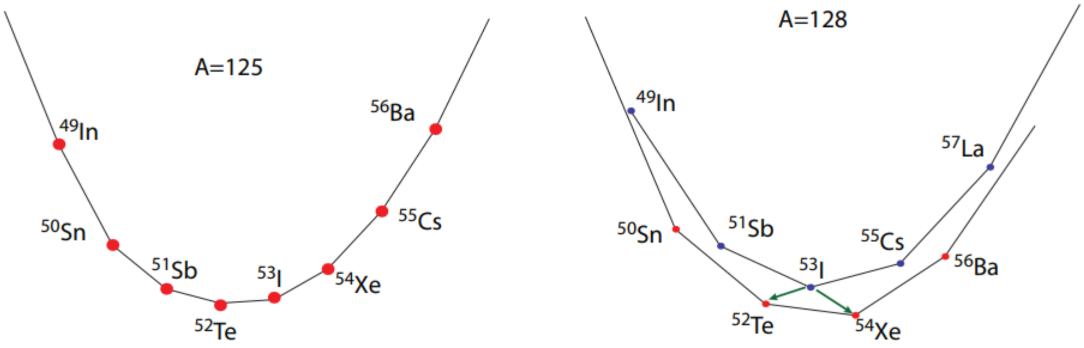


Figure 1.3.3: Nuclear Mass Chain for A=125, (left) and A=128 (right). (CC BY-NC-ND; Paola Cappellaro)

The beta decay is the radioactive decay process that can convert protons into neutrons (and vice-versa). We will study more in depth this mechanism, but here we want simply to point out how this process can be energetically favorable, and thus we can predict which transitions are likely to occur, based only on the SEMF.

For example, for A = 125 if Z < 52 we have a favorable n → p conversion (beta decay) while for Z > 52 we have p → n (or positron beta decay), so that the stable nuclide is Z = 52 (tellurium).

Conservation laws

As the neutrino is hard to detect, initially the beta decay seemed to violate energy conservation. Introducing an extra particle in the process allows one to respect conservation of energy.

The Q value of a beta decay is given by the usual formula:

$$ Q_{\beta^-} = \left[m_N \left({}^{A}X \right) - m_N \left({}^{A}_{Z+1}X' \right) - m_e \right] c^2 . $$

Using the atomic masses and neglecting the electron’s binding energies as usual we have

$$ Q_{\beta^-} = \left\{ \left[m_A \left({}^{A}X \right) - Zm_e \right] - \left[m_A \left({}^{A}_{Z+1}X' \right) - (Z+1)m_e \right] - m_e \right\} c^2 = \left[m_A \left({}^{A}X \right) - m_A \left({}^{A}_{Z+1}X' \right) \right] c^2 . $$

The kinetic energy (equal to the Q) is shared by the neutrino and the electron (we neglect any recoil of the massive nucleus). Then, the emerging electron (remember, the only particle that we can really observe) does not have a fixed energy, as it was for example for the gamma photon. But it will exhibit a spectrum of energy (or the number of electron at a given energy) as well as a distribution of momenta. We will see how we can reproduce these plots by analyzing the QM theory of beta decay.

Examples

$$ {}^{64}_{29}\mathrm{Cu} \begin{array}{l} \nearrow {}^{64}_{30}\mathrm{Zn} + e^- + \bar{\nu}, \quad Q_\beta = 0.57 \text{ MeV} \\ \searrow {}^{64}_{28}\mathrm{Ni} + e^+ + \nu, \quad Q_\beta = 0.66 \text{ MeV} \end{array} $$

The neutrino and beta particle ($\beta^\pm$) share the energy. Since the neutrinos are very difficult to detect (as we will see they are almost massless and interact very weakly with matter), the electrons/positrons are the particles detected in beta-decay and they present a characteristic energy spectrum (see Fig. 1.3.4).

The difference between the spectrum of the $\beta^\pm$ particles is due to the Coulomb repulsion or attraction from the nucleus.

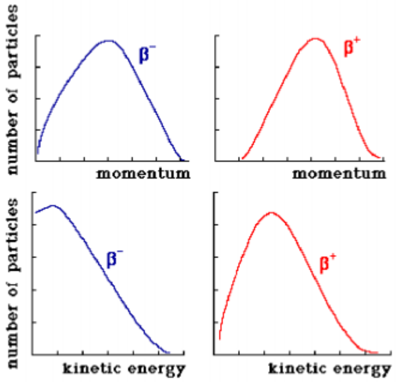


Figure 1.3.4: Beta decay spectra: Distribution of momentum (top plots) and kinetic energy (bottom) for β^- (left) and β^+ (right) decay.

Notice that the neutrinos also carry away angular momentum. They are spin-1/2 particles, with no charge (hence the name) and very small mass. For many years it was actually believed to have zero mass. However it has been confirmed that it does have a mass in 1998.

Other conserved quantities are:

- Momentum: The momentum is also shared between the electron and the neutrino. Thus the observed electron momentum ranges from zero to a maximum possible momentum transfer.
- Angular momentum (both the electron and the neutrino have spin 1/2)
- Parity? It turns out that parity is not conserved in this decay. This hints to the fact that the interaction responsible violates parity conservation (so it cannot be the same interactions we already studies, e.m. and strong interactions)
- Charge (thus the creation of a proton is for example always accompanied by the creation of an electron)
- Lepton number: we do not conserve the total number of particles (we create beta and neutrinos). However the number of massive, heavy particles (or baryons, composed of 3 quarks) is conserved. Also the lepton number is conserved. Leptons are fundamental particles (including the electron, muon and tau, as well as the three types of neutrinos associated with these 3). The lepton number is +1 for these particles and -1 for their antiparticles. Then an electron is always accompanied by the creation of an antineutrino, e.g., to conserve the lepton number (initially zero).

Although the energy involved in the decay can predict whether a beta decay will occur (Q > 0), and which type of beta decay does occur, the decay rate can be quite different even for similar Q-values. Consider for example ^{22}Na and ^{36}Cl. They both decay by β decay:

$$^{22}_{11}\mathrm{Na}_{11} \rightarrow ^{22}_{10}\mathrm{Ne}_{12} + \beta^+ + \nu, \quad Q = 0.22\mathrm{MeV}, \quad T_{\frac{1}{2}} = 2.6 \text{ years}$$

$$^{36}_{17}\mathrm{Cl}_{19} \rightarrow ^{36}_{18}\mathrm{Ar}_{18} + \beta^- + \bar{\nu} \quad Q = 0.25\mathrm{MeV}, \quad T_{\frac{1}{2}} = 3 \times 10^5 \text{ years}$$

Even if they have very close Q-values, there is a five order magnitude in the lifetime. Thus we need to look closer to the nuclear structure in order to understand these differences.

Gamma decay

In the gamma decay the nuclide is unchanged, but it goes from an excited to a lower energy state. These states are called isomeric states. Usually the reaction is written as:

$$^{A}_{Z}X^{*}_{N} \longrightarrow ^{A}_{Z}X_{N} + \gamma$$

where the star indicate an excited state. We will study that the gamma energy depends on the energy difference between these two states, but which decays can happen depend, once again, on the details of the nuclear structure and on quantum-mechanical selection rules associated with the nuclear angular momentum.

Spontaneous fission

Some nuclei can spontaneously undergo a fission, even outside the particular conditions found in a nuclear reactor. In the process a heavy nuclide splits into two lighter nuclei, of roughly the same mass.

Branching Ratios

Some nuclei only decay via a single process, but sometimes they can undergo many different radioactive processes, that compete one with the other. The relative intensities of the competing decays are called branching ratios.

Branching ratios are expressed as percentage or sometimes as partial half-lives. For example, if a nucleus can decay by beta decay (and other modes) with a branching ration b_β the partial half-life for the beta decay is $\lambda_\beta = b_\beta \lambda$.

CHAPTER OVERVIEW

2: Introduction to Quantum Mechanics

2.1: Laws of Quantum Mechanics

Every physical theory is formulated in terms of mathematical objects. It is thus necessary to establish a set of rules to map physical concepts and objects into mathematical objects that we use to represent them. Sometimes this mapping is evident, as in classical mechanics, while for other theories, such as quantum mechanics, the mathematical objects are not intuitive.

In the same way as classical mechanics is founded on Newton's laws or electrodynamics on the Maxwell-Boltzmann equations, quantum mechanics is also based on some fundamental laws, which are called the postulates or axioms of quantum mechanics.

We want in particular to develop a **mathematical model for the dynamics of closed quantum systems**[1]: therefore we are interested in defining

states – observables – measurements – evolution

Some subtleties will arise since we are trying to define measurement in a closed system, when the measuring person is instead outside the system itself. A more complete picture, that can explain some of the confusion arising from the measurement process, is possible, but we will not study it in this course.

We are interested in giving a description of physical phenomena and in particular in how they emerge during an experiment.

Note

[1] We define a *closed* system any system that is isolated, thus not exchanging any input or output and not interacting with any other system. An *open* system instead interacts e.g., with an external environment.

Experiments – A physical experiment can be divided into two steps: preparation and measurement. In classical mechanics (CM):

- the first step determines the possible outcomes of the experiment,
- while the measurement retrieves the value of the outcome.

In quantum mechanics (QM) the situation is slightly different:

- the first step (preparation) determines the *probabilities* of the various possible outcomes,
- the second step (measurement) retrieve the *value* of a particular outcome, in a statistic manner.

This separation of the experiment in two steps is reflected into the two types of operators that we find in QM.

- The first step corresponds to the concept of a **state** of the system,
- while the second step corresponds to **observables**.

In CM the state of a system is described by a set of properties. For example, if we consider a ball, we can define its state by giving its position, momentum, energy, angular momentum (if for example the ball is spinning), its temperature etc. We can then perform a measurement on this ball, for example measuring its position. This will give us one value for one possible observable (the position).

We can express this process in mathematical terms. The state of the system is defined by a set of values: $\{\vec{r}, \vec{p}, E, \vec{L}, T, \ldots\}$. All of these values (and there might be of course more that I haven't written down) are needed to fully describe the state of the ball. Performing a measurement of the position, will retrieve the values $\{r_x, r_y, r_z\} = \vec{r}$ (the same values that describe the state).

If we now consider a nucleus, we can as well give a description of its state. In quantum mechanics, a complete description of the state of a quantum object (or system) is given mathematically by the state vector $|\psi\rangle$ (or wavefunction $\psi(\vec{r})$) . The situation is however different than in classical mechanics.

The state vector is no longer a collection of values for different properties of the system. The state gives instead a complete description of the set of *probabilities* for all the physical properties (or observables). All the information is contained in the state, irrespectively on how I got the state, of its previous history.

On the other hand, the observables are all the physical properties that in principle can be measured, in the same way as it was in classical mechanics. Since however the state only gives probabilities for all observables, the result of measurement will be a statistical variable.

All of these considerations are made more formal in the axioms of quantum mechanics that also indicate the mathematical formalism to be used.

1. The properties of a quantum system are completely defined by specification of its state vector $|\psi\rangle$. The state vector is an element of a complex Hilbert space H called the space of states.
2. With every physical property $\mathcal{A}$ (energy, position, momentum, angular momentum, ...) there exists an associated linear, Hermitian operator A (usually called observable), which acts in the space of states H. The eigenvalues of the operator are the possible values of the physical properties.
3. (a) If $|\psi\rangle$ is the vector representing the state of a system and if $|\varphi\rangle$ represents another physical state, there exists a probability $p(|\psi\rangle, |\varphi\rangle)$ of finding $|\psi\rangle$ in state $|\varphi\rangle$, which is given by the squared modulus of the inner product on $\mathcal{H}: p(|\psi\rangle, |\varphi\rangle) = |\langle\psi \mid \varphi\rangle|^2$ (Born Rule).

   (b) If A is an observable with eigenvalues a_n and eigenvectors $|n\rangle$ [such that the eigenvalue equation is $A|n\rangle = a_n|n\rangle$], given a system in the state $|\psi\rangle$, the probability of obtaining a_n as the outcome of the measurement of A is $p(a_n) = |\langle n \mid \psi\rangle|^2$. After the measurement the system is left in the state projected on the subspace of the eigenvalue a_n (Wave function collapse).
4. The evolution of a closed system is unitary (reversible). The evolution is given by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = \mathcal{H}|\psi\rangle$$

where $\mathcal{H}$ is the Hamiltonian of the system (the energy operator) and $\hbar$ is the reduced Planck constant $h/2\pi$ (with h the Planck constant, allowing conversion from energy to frequency units).

2.2: States, Observables and Eigenvalues

Definition: State vector

From the first postulate we see that the state of a quantum system is given by the state vector $|\psi(t)\rangle$ (or the **wavefunction** $\psi(\vec{x}, t)$). The state vector contains all possible information about the system. The state vector is a vector in the Hilbert space. A Hilbert space H is a complex vector space that possess an inner product.

An example of Hilbert space is the usual Euclidean space of geometric vectors. This is a particularly simple case since the space in this case is real. In general as we will see, Hilbert space vectors can be complex (that is, some of their components can be complex numbers). In the 3D Euclidean space we can define vectors, with a representation such as $\vec{v}=\{v_x, v_y, v_z\}$ or :

$$\vec{v}=\left[\begin{array}{c} v_x \\ v_y \\ v_z \end{array}\right]$$

This representation corresponds to choose a particular basis for the vector (in this case, the usual $\{x, y, z\}$ coordinates). We can also define the inner product between two vectors, $\vec{v}$ and $\vec{u}$ (which is just the usual scalar product):

$$\vec{v} \cdot \vec{u}=\left[\begin{array}{lll} v_x & v_y & v_z \end{array}\right] \cdot\left[\begin{array}{c} u_x \\ u_y \\ u_z \end{array}\right]=v_x u_x+v_y u_x+v_z u_z$$

Notice that we have taken the transpose of the vector $\vec{v}, \vec{v}^T$ in order to calculate the inner product. In general, in a Hilbert space, we can define the dual of any vector. The **Dirac notation** makes this more clear.

The notation $|\psi\rangle$ is called the Dirac notation and the symbol $|\cdot\rangle$ is called *ket*. This is useful in calculating inner products of state vectors using the *bra* $\langle\cdot|$ which is the dual of the ket), for example $\langle\varphi|$. An inner product is then written as $\langle\varphi \mid \psi\rangle$ (this is a *bracket*, hence the names).

We will often describe states by their wavefunction instead of state vector. The wavefunction is just a particular way of writing down the state vector, where we express the state vector in a *basis* linked to the position of a particle itself (this is called the position representation). This particular case is however the one we are mostly interested in this course. Mathematically, the wavefunction is a complex function of space and time. In the position representation (that is, the position basis) the state is expressed by the wavefunction via the inner product $\psi(x)=\langle x \mid \psi\rangle$.

The properties of Hilbert spaces, kets and bras and of the **wavefunction** can be expressed in a more rigorous mathematical way. In this course as said we are mostly interested in systems that are nicely described by the wavefunction. Thus we will just use this mathematical tool, without delving into the mathematical details. We will see some more properties of the wavefunction once we have defined observables and measurement.

Definition: Observable

All physical **observables** (defined by the prescription of experiment or measurement) are represented by a linear **operator** that operates in the Hilbert space H (a linear, complex, inner product vector space).

In mathematics, an operator is a type of function that acts on functions to produce other functions. Formally, an operator is a mapping between two function spaces[2] A : $g(I) \rightarrow f(I)$ that assigns to each function $g \in g(I)$ a function $f=A(g) \in f(I)$.

Examples of observables are what we already mentioned, e.g. position, momentum, energy, angular momentum. These operators are associated to classical variables. To distinguish them from their classical variable counterpart, we will thus put a *hat* on the operator name. For example, the position operators will be $\hat{x}, \hat{y}, \hat{z}$. The momentum operators $\hat{p}_x, \hat{p}_y, \hat{p}_z$ and the angular momentum operators $\hat{L}_x, \hat{L}_y, \hat{L}_z$. The energy operator is called Hamiltonian (this is also true in classical mechanics) and is usually denoted by the symbol $\mathcal{H}$.

There are also some operators that do not have a classical counterpart (remember that quantum-mechanics is more general than classical mechanics). This is the case of the spin operator, an observable that is associated to each particle (electron, nucleon, atom etc.). For example, the spin of an electron is usually denoted by S; this is also a vector variable (i.e. we can define \(S_{x}, S_{y}, S_{z})). I am omitting here the *hat* since there is no classical variable we can confuse the spin with. While the position, momentum etc. observable are continuous operator, the spin is a discrete operator.

The second postulate states that the possible values of the physical properties are given by the eigenvalues of the operators.

Note

[2] A function space $f(I)$ is a collection of functions satisfying certain properties.

Definition: Eigenvalues and eigenfunctions

Eigenvalues and eigenfunctions of an operator are defined as the solutions of the eigenvalue problem:

$$\boxed{A\left[u_n(\vec{x})\right]=a_n u_n(\vec{x})}$$

where n = 1, 2, . . . indexes the possible solutions. The a_n are the eigenvalues of A (they are scalars) and $u_n(\vec{x})$ are the eigenfunctions.

The eigenvalue problem consists in finding the functions such that when the operator A is applied to them, the result is the function itself multiplied by a scalar. (Notice that we indicate the action of an operator on a function by $A[f(\cdot)]$).

You should have seen the eigenvalue problem in linear algebra, where you studied eigenvectors and eigenvalues of matrices. Consider for example the spin operator for the electron S. The spin operator can be represented by the following matrices (this is called a matrix representation of the operator; it's not unique and depends on the basis chosen):

$$S_x=\frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad S_y=\frac{1}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad S_z=\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

We can calculate what are the eigenvalues and eigenvectors of this operators with some simple algebra. In class we considered the eigenvalue equations for S_x and S_z. The eigenvalue problem can be solved by setting the determinant of the matrix $S_\alpha - s1$ equal to zero. We find that the eigenvalues are $\pm\frac{1}{2}$ for both operators. The eigenvectors are different:

$$v_1^z=\begin{bmatrix}1\\0\end{bmatrix}, \quad v_2^z=\begin{bmatrix}0\\1\end{bmatrix}$$

$$v_1^x=\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}, \quad v_2^x=\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$$

We proved also that $v_1\cdot v_2=0$ (that is, the eigenvectors are orthogonal) and that they form a complete basis (we can write any other vector, describing the state of the electron spin, as a linear combination of either the eigenvectors of S_z or of S_x).

The eigenvalue problem can be solved in a similar way for continuous operators. Consider for example the differential operator, $\frac{d[\cdot]}{dx}$. The eigenvalue equation for this operator reads:

$$\frac{df(x)}{dx}=af(x)$$

where a is the eigenvalue and $f(x)$ is the eigenfunction.

Question

what is $f(x)$? What are all the possible eigenvalues (and their corresponding eigenfunctions)?

Examples

The eigenvalue equation for the operator is $x\frac{d[\cdot]}{dx}$ is:

$$x\frac{df(x)}{dx}=af(x)$$

which is solved by $f(x)=x^n$, a = n.

The ”standard” Gaussian function $\frac{1}{\sqrt{2\pi}}e^{-x^2/2}$ is the eigenfunction of the Fourier transform. The Fourier transform is an operation that transforms one complex-valued function of a real variable into another one (thus it is an operator):

$$\mathcal{F}_x : f(x) \rightarrow \tilde{f}(k), \quad \text{with} \quad \tilde{f}(k)=\mathcal{F}_x[f(x)](k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx$$

Notice that sometimes different normalizations are used. With this definition, we also find that the inverse Fourier transform is given by:

$$\mathcal{F}_k^{-1} : \tilde{f}(k) \rightarrow f(x), \quad f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \tilde{f}(k)e^{ikx}dk$$

Let’s now turn to quantum mechanical operators.

Definition: Position operator

The position operator for a single particle $\hat{\vec{x}}$ is simply given by the scalar $\vec{x}$. This means that the operator $\hat{\vec{x}}$ acting on the wavefunction $\psi(\vec{x})$ simply multiplies the wavefunction by $\vec{x}$. We can write

$$\boxed{\hat{\vec{x}}[\psi(\vec{x})]=\vec{x}\psi(\vec{x}).}$$

We can now consider the eigenvalue problem for the position operator. For example, for the x-component of $\vec{x}$ this is written as:

$$\hat{x}\left[u_n(x)\right]=x_n u_n(x) \rightarrow x u_n(x)=x_n u_n(x)$$

where we used the definition of the position operator. Here x_n is the eigenvalue and $u_n(x)$ the eigenfunction. The solution to this equation is not a proper function, but a distribution (a generalized function): the Dirac delta function: $u_n(x)=\delta\left(x-x_n\right)$

Definition: Dirac Delta function

Dirac Delta function $\delta\left(x-x_0\right)$ is equal to zero everywhere except at x_0 where it is infinite. The Dirac Delta function also has the property that $\int_{-\infty}^{\infty}\delta(x)dx=1$ and of course $x\delta\left(x-x_0\right)=x_0\delta\left(x-x_0\right)$ (which corresponds to the eigenvalue problem above). We also have:

$$\int dx\delta\left(x-x_0\right)f(x)=f\left(x_0\right)$$

That is, the integral of any function multiplied by the delta function gives back the function itself evaluated at the point x_0. [See any textbook (and recitations) for other properties.]

How many solutions are there to the eigenvalue problem defined above for the position operator? One per each possible position, that is an infinite number of solutions. Conversely, all possible positions are allowed values for the measurement of the position (a continuum of solutions in this case).

Definition: Momentum operator

The momentum operator is defined (in analogy with classical mechanics) as the generator of translations. This means that the momentum modifies the position of a particle from $\vec{x}$ to $\vec{x}+d\vec{x}$. It is possible to show that this definition gives the following form of the position operator (in the position representation, or position basis)

$$\boxed{\hat{p}_x=-i\hbar\frac{\partial}{\partial x}, \hat{p}_y=-i\hbar\frac{\partial}{\partial y}, \hat{p}_z=-i\hbar\frac{\partial}{\partial z}}$$

or in vector notation $\hat{\mathbf{p}}=-i\hbar\nabla$. Here $\hbar$ is the reduced Planck constant $h/2\pi$ (with h the Planck constant) with value

$$\hbar=1.054\times10^{-34}\text{ J s.}$$

Planck’s constant is introduced in order to make the values of quantum observables consistent with the corresponding classical values.

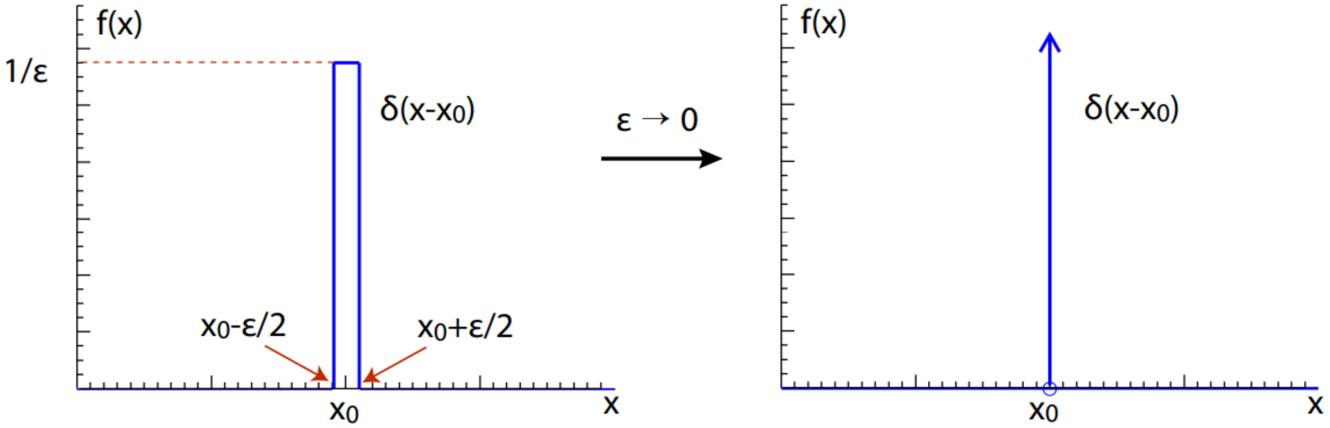


Figure 2.2.1: Schematics of Dirac’s delta function. Left: the rectangular function of base ϵ and height ϵ becomes the delta-function (right) in the limit of $\epsilon \rightarrow 0$. (CC BY-NC-ND; Paola Cappellaro)

We now study the momentum operator eigenvalue problem in 1D. The problem’s statement is

$$\hat{p}_x\left[u_n(x)\right]=p_n u_n(x) \rightarrow -i\hbar \frac{\partial u_n(x)}{\partial x}=p_n u_n(x)$$

This is a differential equation that we can solve quite easily. We set $k=p/\hbar$ and call k the wavenumber (for reasons clear in a moment). The differential equation is then

$$\frac{\partial u_n(x)}{\partial x}=i k_n u_n(x)$$

which has as solution the complex function:

$$u_n(x)=A e^{i k_n x}=A e^{i \frac{p_n}{\hbar} x}$$

The momentum eigenfunctions and eigenvalues are thus $u_n=A e^{i k_n x}$ and k_n.

Now remember the meaning of the eigenvalues. By the second postulate, the eigenvalues of an operator are the possible values that one can obtain in a measurement.

Obs. 1 There are no restrictions on the possible values obtained from a momentum measurements. All values $p=\hbar k$ are possible.

Obs. 2 The eigenfunction $u_n(x)$ corresponds to a wave traveling to the right with momentum $p_n=\hbar k_n$. This was also expressed by De Broglie when he postulated the existence of matter waves.

Louis de Broglie (1892-1987) was a French physicist. In his Ph.D thesis he postulated a relationship between the momentum of a particle and the wavelength of the wave associated with the particle (1922). In de Broglie’s equation a particle wavelength is the Planck’s constant divided by the particle momentum. We can see this behavior in the electron interferometer video[3]. For classical objects the momentum is very large (since the mass is large), then the wavelength is very small and the object loose its wave behavior. De Broglie equation was experimentally confirmed in 1927 when physicists Lester Germer and Clinton Davisson fired electrons at a crystalline nickel target and the resulting diffraction pattern was found to match the predicted values.

Note

[3] A. Tonomura, J. Endo, T. Matsuda, T. Kawasaki and H. Ezawa, Am. J. of Phys. 57, 117 (1989)

Properties of eigenfunctions

From these examples we can notice two properties of eigenfunctions which are valid for any operator:

1. The eigenfunctions of an operator are orthogonal functions. We will as well assume that they are normalized. Consider two eigenfunctions u_n, u_m of an operator A and the inner product defined by $\langle f \mid g\rangle=\int d^3 x f^*(\mathrm{x}) g(\mathrm{x})$. Then we have
$$\int d^3 x u_m^*(\mathrm{x}) u_n(\mathrm{x})=\delta_{n m}$$
2. The set of eigenfunctions forms a complete basis.
This means that any other function can be written in terms of the set of eigenfunctions $\{u_n(\mathrm{x})\}$ of an operator A:
$$f(\mathrm{x})=\sum_n c_n u_n(\mathrm{x}), \quad \text{with} \quad c_n=\int d^3 x u_n^*(\mathrm{x}) f(\mathrm{x})$$
[Note that the last equality is valid iif the eigenfunctions are normalized, which is exactly the reason for normalizing them].
If the eigenvalues are a continuous parameter, we have a continuum of eigenfunctions, and we will have to replace the sum over n with an integral.

Consider the two examples we saw. From the property of the Dirac Delta function we know that we can write any function as:

$$f(x)=\int d x^{\prime} \delta\left(x^{\prime}-x\right) f\left(x^{\prime}\right)$$

We can interpret this equation as to say that any function can be written in terms of the position eigenfunction $\delta\left(x^{\prime}-x\right)$ (notice that we are in the continuous case mentioned before, since the x-eigenvalue is a continuous function). In this case the coefficient c_n becomes also a continuous function

$$c_n \rightarrow c\left(x_n\right)=\int d x \delta\left(x-x_n\right) f(x)=f\left(x_n\right) .$$

This is not surprising as we are already expressing everything in the position basis.

If we want instead to express the function $f(x)$ using the basis given by the momentum operator eigenfunctions we have: (consider 1D case)

$$f(x)=\int d k u_k(x) c(k)=\int d k e^{i k x} c(k)$$

where again we need an integral since there is a continuum of possible eigenvalues. The coefficient $c(k)$ can be calculated from

$$c(k)=\int d x u_k^*(x) f(x)=\int d x e^{-i k x} f(x)$$

We then have that $c(k)$ is just the Fourier transform of the function $f(x)$ (up to a multiplier).

The Fourier transform is an operation that transforms one complex-valued function of a real variable into another:

$$\mathcal{F}_x: f(x) \rightarrow \tilde{f}(k), \quad \text{with} \quad \tilde{f}(k)=\mathcal{F}_x[f(x)](k)=\frac{1}{\sqrt{2 \pi}} \int_{-\infty}^{\infty} f(x) e^{-i k x} d x$$

Notice that sometimes different normalizations are used. With this definition, we also find that the inverse Fourier transform is given by:

$$\mathcal{F}_k^{-1}: \tilde{f}(k) \rightarrow f(x), \quad f(x)=\frac{1}{\sqrt{2 \pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{i k x} d k$$

Review of linear Algebra

This is a very concise review of concepts in linear algebra, reintroducing some of the ideas we saw in the previous paragraphs in a slightly more formal way.

Vectors and vector spaces

Quantum mechanics is a linear theory, thus it is well described by vectors and vector spaces. Vectors are mathematical objects (distinct from scalars) that can be added one to another and multiplied by a scalar. In QM we denote vectors by the Dirac notation:

$|\psi\rangle, |\varphi\rangle, \ldots$. Then, these have the properties:

- If $|\psi_1\rangle$ and $|\psi_2\rangle$ are vectors, then $|\psi_3\rangle = |\psi_1\rangle + |\psi_2\rangle$ is also a vector.
- Given a scalar s, $|\psi_4\rangle = s\,|\psi_1\rangle$ is also a vector.

A vector space is a collection of vectors. For example, for vectors of finite dimensions, we can define a vector space of dimensions N over the complex numbers as the collection of all complex-valued N-dimensional vectors.

✓ Example A.1

A familiar example of vectors and vector space are the Euclidean vectors and the real 3D space.

✓ Example A.2

Another example of a vector space is the space of polynomials of order n. Its elements, the polynomials $P_n = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$ can be proved to be vectors since they can be summed to obtain another polynomial and multiplied by a scalar. The dimension of this vector space is n + 1.

✓ Example A.3

In general, functions can be considered vectors of a vector space with infinite dimension (of course, if we restrict the set of functions that belong to a given space, we must ensure that this is still a well-defined vector space. For example, the collection of all function $f(x)$ bounded by $3[f(x) < 3, \forall x]$ is not a well defined vector-space, since $sf(x)$ (with s a scalar > 1) is not a vector in the space.

Inner product

We denote by $\langle\psi \mid \varphi\rangle$ the scalar product between the two vectors $|\psi\rangle$ and $|\varphi\rangle$. The inner product or scalar product is a mapping from two vectors to a complex scalar, with the following properties:

- It is linear in the second argument: $\langle\psi \mid a_1\varphi_1 + a_2\varphi_2\rangle = a_1\langle\psi \mid \varphi_1\rangle + a_2\langle\psi \mid \varphi_2\rangle$.
- It has the property of complex conjugation: $\langle\psi \mid \varphi\rangle = \langle\varphi \mid \psi\rangle^*$.
- It is positive-definite: $\langle\psi \mid \psi\rangle = 0 \Leftrightarrow |\psi\rangle = 0$.

✓ Example B.1

For Euclidean vectors the inner product is the usual scalar product $\vec{v}_1 \cdot \vec{v}_2 = |\vec{v}_1|\,|\vec{v}_2| \cos\vartheta$.

✓ Example B.2

For functions, the inner product is defined as:

$$\langle f \mid g\rangle = \int_{-\infty}^{\infty} f(x)^* g(x) dx$$

Linearly independent vectors (and functions)

We can define linear combinations of vectors as $|\psi\rangle = a_1|\varphi_1\rangle + a_2|\varphi_2\rangle + \ldots$. If a vector cannot be expressed as a linear superposition of a set of vectors, than it is said to be linearly independent from these vectors. In mathematical terms, if

$$|\xi\rangle \neq \sum_i a_i |\varphi_i\rangle, \quad \forall a_i$$

then $|\xi\rangle$ is linearly independent of the vectors $\{|\varphi_i\rangle\}$.

Basis

A basis is a linearly independent set of vectors that spans the space. The number of vectors in the basis is the vector space dimension. Any other vector can be expressed as a linear combination of the basis vectors. The basis is not unique, and we will usually choose an orthonormal basis.

Example D.1

For the Polynomial vector space, a basis are the monomials $\left\{x^{k}\right\}, k=0, \ldots, n$. For Euclidean vectors the vectors along the 3 coordinate axes form a basis.

We have seen in class that eigenvectors of operators form a basis.

Unitary and Hermitian operators

An important class of operators are self adjoint or Hermitian operators, as observables are described by them. We need first to define the adjoint of an operator A. This is denoted A† and it is defined by the relation:

$$\left\langle\left(A^{\dagger} \psi\right) \mid \varphi\right\rangle=\langle\phi \mid(A \psi)\rangle \quad \forall\{|\psi\rangle,|\varphi\rangle\}$$

This condition can also be written (by using the second property of the inner product) as:

$$\left\langle\psi\left|A^{\dagger}\right| \varphi\right\rangle=\langle\varphi|A| \psi\rangle^{*}$$

If the operator is represented by a matrix, the adjoint of an operator is the conjugate transpose of that operator: $A_{k, j}^{\dagger}=\left\langle k\left|A^{\dagger}\right| j\right\rangle=\langle j|A| k\rangle^{*}=A_{j, k}^{*}$.

Definition: Self-adjoint

A self adjoint operator is an operator such that A† = A, or more precisely

$$\langle\psi|A| \varphi\rangle=\langle\varphi|A| \psi\rangle^{*}$$

For matrix operators, $A_{k i}=A_{i k}^{*}$.

An important properties of Hermitian operators is that their eigenvalues are always real (even if the operators are defined on the complex numbers). Then, all the observables must be represented by hermitian operators, since we want their eigenvalues to be real, as the eigenvalues are nothing else than possible outcomes of experiments (and we wouldn't want the position of a particle, for example, to be a complex number).

Then, for example, the Hamiltonian of any system is an hermitian operator. For a particle in a potential, it's easy to check that the operator is real, thus it is also hermitian.

Definition: Unitary operators

U are such that their inverse is equal to their adjoint: $U^{-1}=U^{\dagger}$, or

$$U U^{\dagger}=U^{\dagger} U=1.$$

We will see that the evolution of a system is given by a unitary operator, which implies that the evolution is time-reversible.

2.3: Measurement and Probability

From the second postulate we have seen that the possible outcomes of a measurement are the eigenvalues of the operator corresponding to the measured observable. The question of which one of the eigenvalue we will obtain is still open. This question is resolved by the third postulate, which gives a recipe on how to predict which outcome will be observed. However, this mathematical recipe does not tell us (in general) with absolute certainty which one of the eigenvalue will be the outcome. It only provides us with the probability of obtaining each eigenvalue.

In postulate 3.b we consider an observable $\mathcal{A}$ and a system in the state $|\psi\rangle$. The eigenvalue equation for the operator A (corresponding to $\mathcal{A}$) can be expressed as

$$A|n\rangle = a_n|n\rangle$$

where a_n are the eigenvalues and $|n\rangle$ the eigenvectors . The postulate states that the probability of obtaining a_n as the outcome of the measurement of A is $p\left(a_n\right) = |\langle n \mid \psi\rangle|^2$.

We want to re-express the postulate in terms of the wavefunction $\psi(\vec{x})$. To do so, we need to define the inner product in the Hilbert space of the wavefunctions. Given two wave functions $\psi(\vec{x})$ and $\varphi(\vec{x})$, the inner product $\langle\varphi \mid \psi\rangle$ is given by:

$$\langle\varphi \mid \psi\rangle = \int d^3\vec{x}\varphi(x)^*\psi(x)$$

(where ∗ indicates the complex conjugate).

We first rewrite the eigenvalue problem for the operator A in terms of the eigenfunctions $u_n(\vec{x})$ and the associated eigenvalues a_n:

$$A\left[u_n(\vec{x})\right] = a_n u_n(\vec{x})$$

Then, we have seen that any function can be expressed in terms of the eigenfunctions $u_n(\vec{x})$. We can as well express the wavefunction in terms of these eigenfunctions:

$$\psi(\vec{x}) = \sum_n c_n u_n(\vec{x}), \text{ with } c_n = \int d^3\vec{x} u_n^*(\vec{x})\psi(\vec{x})$$

Finally, according to postulate 3.b the probability of obtaining the outcome a_n if the system is in the state $\psi(\vec{x})$ is given by the inner product :

$$\boxed{p\left(a_n\right) = \left|\int d^3\vec{x} u_n^*(\vec{x})\psi(\vec{x})\right|^2 = \left|c_n\right|^2}$$

where the last equality follows from the orthogonality of the eigenfunctions $\int d^3\vec{x} u_n^*(\vec{x}) u_m(\vec{x}) = 0$, for $m \neq n$. Since $\left|c_n\right|^2 = p\left(a_n\right)$ is a probability, the coefficients c_n of the wavefunction expansion are called *probability amplitude*s. We now confirm that the wavefunction contain all information about the state of the system, since given the wavefunction we can calculate all the probabilities of each outcome for each possible observable with the following procedure:

1. Find the eigenfunctions of the observable’s operator. E.g., given an operator O, we will calculate its eigenfunctions $w_n(x)$, such that $O\left[w_n(x)\right] = o_n w_n(x)$.
2. Find the probability amplitude of the wavefunction with respect to the eigenfunction of the desired eigenvalue outcome. E.g., if the outcome is o_m, such that $O\left[w_m(x)\right] = o_m w_m(x)$ we will calculate $c_m = \int d^3\vec{x} w_m^*(\vec{x})\psi(\vec{x})$.
3. The probability of obtaining the given eigenvalue in the measurement is the probability amplitude modulus square. E.g. $p\left(o_m\right) = \left|c_m\right|^2$.

Wavefunction collapse

The third postulate states also that after the measurement the system is left in the eigenstate corresponding to the eigenvalue found (more generally, if more than one eigenstate is associated to the same eigenvalue, the state is projected on the subspace of the eigenvalue a_n, that is, the subspace spanned by all the eigenstates associated with a_n).

This is the **wavefunction collapse**, a concept that is usually quite puzzling in quantum mechanics. We can make this statement at least a bit less puzzling by taking into account the following two considerations.

The wavefunction collapse is puzzling because it predicts an instantaneous evolution of the system from its pre-measurement state $\psi(x)$ to its post-measurement state $u_n(x)$ (when we measure a_n). This type of evolution is very different than the usual evolution predicted by the fourth postulate (that we will see in a later lecture). However, this weird behavior arises from considering the measurement apparatus (and hence the measurement) as a classical system, outside the realm of quantum mechanics. Although this view gives most of the time a correct answer – and thus we will use it in this class – it is a quite imprecise description. More rigorous descriptions of the measurement process, invoking for example **decoherence**[4], can give a better picture of what actually happens (e.g. the wave-function collapse can take a finite time and be measured experimentally in some cases).

More pragmatically, the wavefunction collapse is needed in order to make experiment consistent. What the collapse entails is that if I make a measurement and I obtain as an outcome the eigenvalue a_n, I can check that result again, by repeating the measurement just after the first one (with no time for any change in the system between the two measurement). If I could not make this second check, I could never be able to be confident that I got the correct answer the first time (e.g. my detector could be wrong) and so I could never gain any knowledge at all on my system.

Obs.: I want to clarify the meaning of “subspace of the eigenvalue a_n”. If there is a set of eigenstates associated with the eigenvalue a_n, $|n_j\rangle$, then the state $|\psi\rangle$ is projected onto a superposition of these eigenstates $|\psi\rangle \rightarrow |n\rangle = \sum_j c_j |n_j\rangle$.

Note

4 Decoherence is the phenomenon by which an *open* quantum system, interacting with the environment, undergoes an irreversible evolution that often leaves it in a state best described by the rules of classical mechanics.

Position measurement

We have already calculated the eigenvalues and eigenfunctions of the position operator. The eigenfunctions were $u_n(x) = \delta\left(x - x_n\right)$ with eigenvalues x_n. We also calculated the expansion of a function in terms of the position eigenfunctions. Repeating the calculation for the wavefunction we find:

$$c\left(x_n\right) = \int dx \delta\left(x - x_n\right)\psi(x) = \psi\left(x_n\right),$$

from which we obtain that the probability of finding a particle in the position x_n is given by:

$$p\left(x_n\right) = \left|\psi\left(x_n\right)\right|^2$$

More generally, since x is continuous, we can drop the subscript n, as any value of x is an eigenvalue. Then, generalizing to the 3D case, we can say that the probability of finding a particle described by the wavefunction $\psi(\vec{x})$ at the position $\vec{x}$ is given by the modulus square of the wavefunction itself:

$$\boxed{p(\vec{x}) = |\psi(\vec{x})|^2}$$

We can also say that the wavefunction is the probability amplitude for the position measurement. More precisely, we should say that the probability of finding a particle between x and $x + dx$ is $p(x)dx = |\psi(x)|^2 dx$ while $|\psi(x)|^2$ is a **probability density** (per unit length). In 3D, $|\psi(\vec{x})|^2$ is the probability density per unit volume and the probability is given by $|\psi(\vec{x})|^2 d^3x$.

Given this interpretation of the wavefunction, it becomes natural to require that the wavefunction be normalized. We require that integrating the probability of a particular position over all possible position we obtain 1 (i.e. certainty, the particle **has** to be somewhere!). Then

$$\int d^3\vec{x} p(\vec{x}) = 1 \quad \rightarrow \quad \int d^3\vec{x} |\psi(\vec{x})|^2 = 1$$

From being a very abstract notion, the wavefunction has thus assumed a very physical meaning. We can still say that the wavefunction describes the state of a system and contains all the information about this system. In addition, and more concretely, the absolute value of the wavefunction tells us where it is more probable to find the system.

Momentum measurement

We calculated the eigenvalues and eigenfunctions of the momentum operator to be

$$p=\hbar k \quad \text{and} \quad u_k(x)=\Upsilon e^{ikx}$$

(Notice that we could have labeled the wave-numbers as k_n —and the momentum p_n— to have the eigenvalue equation: $\hat{p}u_n=p_n u_n$, but we omitted the subscript n since momentum is a continuous variable; then we also simply label the eigenfunctions by k instead of n).

As usual, we would like the eigenfunctions to be normalized. However notice that $\int u_k^*(x)u_k(x)dx=\int|\Upsilon|^2dx=\infty$, so we cannot fix Υ such that the result is normalized as usual. For convention we set $\Upsilon=-\frac{1}{\sqrt{2\pi}}:u_k(x)=-\frac{1}{\sqrt{2\pi}}e^{ikx}$ (we are considering the 1D case). Now we can calculate the probability amplitude for the momentum measurement, by calculating the coefficients of the expansion of the wavefunction in terms of the momentum eigenfunctions basis. Here we rename the coefficients $c(k)$ of the expansion $\varphi(k)$. This is given by:

$$c(k)\equiv\varphi(k)=\int u_k(x)^*\psi(x)\rightarrow\varphi(k)=\frac{1}{\sqrt{2\pi}}\int e^{-ikx}\psi(x)$$

Notice that this last equation is simply stating that the probability amplitude for the momentum measurement is the Fourier transform of the wavefunction, $\varphi(k)=\mathcal{F}[\psi(x)]$. Then

$$p(k\rightarrow k+dk)=|\varphi(k)|^2dk$$

is the probability of finding that the particle has a momentum between $\hbar k$ and $\hbar(k+dk)$ when measuring the momentum.

Flux of particles

The choice of the coefficient Υ implies that:

$$\int u_k^*(x)u_{k'}(x)dx=\delta\left(k-k'\right)$$

which is not the usual normalization for the wavefunction.

Why is it not possible to normalize the momentum eigenstates?

We saw that for the wavefunction, the normalization was related to its interpretation as the probability amplitude for the position. If a wavefunction is in a momentum eigenstate $\psi(x)=u_k(x)$, then we cannot really talk about a particle, but rather the system is better described by a wave. In fact, the probability of finding the system at any position x is constant and equal to Υ. Thus the coefficient Υ can be better linked to a flux of particles rather than a particle density.

We can set $v|\psi|^2=\Gamma$ where $v=\frac{p}{m}=\frac{\hbar k}{m}$ is the velocity and Γ correspond to a flux of particle, as described by the plane wave e^{ikx}. Then $\frac{\hbar k}{m}|\Upsilon|^2=\Gamma$ fixes the value of Υ to $\Upsilon=\sqrt{\frac{m\Gamma}{\hbar k}}$.

Expectation values

We have just seen that the outcome of a measurement is a random quantity (although it is of course limited to a given set of values –the eigenvalues– from which we can choose from). In order to know more about the state of a system we need then to repeat the measurement several times, in order to build a statistics of the observable.

For example, we could be interested in knowing what is the average of the measurements of a particular observable. This quantity is usually called in QM the **expectation value** of an observable.

How do we usually calculate the average of a given quantity? Consider for example the average number obtained by throwing a dice. In an experiment, I would have to repeatedly throw the dice, record the number that comes out (say n_i) and then calculate the sum: $\langle n\rangle=\frac{1}{N}\sum_{i=1}^N n_i$. Equivalently, I could count the number of times t_n that each number n appears and calculate the average number from the frequencies $\nu_n=t_n/N:\langle n\rangle=\sum_{n=1}^6\nu_n n$. In the limit of N → ∞, the frequencies ν_n approach the probabilities $\nu_n\rightarrow p_n$. Then for the dice we have $p_n=1/6(\forall n)$ and the average is just calculates from the sum $\frac{1}{6}(1+2+\ldots 6)=3.5$.

The procedure for calculating the average (or expectation value) of a quantity is very general. We have for discrete and continuous probability distribution functions respectively

$$\langle x\rangle=\sum_i p_i x_i \qquad \langle x\rangle=\int dx p(x) x$$

In QM we just need to replace the probability p by its value as given by the third postulate. For example, the expectation value of the position can be expressed in terms of the probability density function given by the modulus square of the wavefunction:

$$\boxed{\langle x\rangle=\int_{-\infty}^{\infty} x|\psi(x, t)|^2 dx}$$

How can we in practice obtain this expectation value? (that is, by performing real experiments). If we make a first measurement on a single particle and then repeat the measurement over and over again this is not what we measure. In fact, in that case we know (from the postulates) that after the first measurement we expect always to get the same result. In fact, these repeated successive measurement are only a way to check that yes, we got the first answer correct. (otherwise we could never be certain of anything, since we would not even know that our experimental apparatus works).

Instead what we can do is adopt one of two strategies. Either we can repeat the same *experiment* (not measurement) many times on the same system. This implies first preparing the system in a given state with a reproducible procedure and then performing a measurement. The second option is to make the experiment on a set (an *ensemble*) of identical systems. In order to obtain the exact expectation value we would need an infinite number (of repetitions or systems), however a large enough sample is usually practically enough.

Obs.: Notice that we can rewrite the expression above for the expectation value of the position as

$$\langle x\rangle=\int_{-\infty}^{\infty} \psi(x, t)^* x \psi(x, t) dx=\int_{-\infty}^{\infty} \psi(x, t)^* \hat{x}[\psi(x, t)] dx$$

This last form is a more general one that is valid for any operator.

Definition: Expectation value

The expectation value of an observable $\hat{\mathcal{O}}$ is

$$\boxed{\langle\hat{\mathcal{O}}\rangle=\langle\psi|\hat{\mathcal{O}}| \psi\rangle=\int_{-\infty}^{\infty} \psi(x, t)^* \hat{\mathcal{O}}[\psi(x, t)] dx}$$

where we first used the Dirac notation to express the expectation value, which is an even more general expression.

Example

The expectation value for the momentum operator is given by:

$$\int_{-\infty}^{\infty} \psi(x, t)^* \hat{p}[\psi(x, t)] dx=\int_{-\infty}^{\infty} \psi(x, t)^*\left(-i \hbar \frac{\partial \psi(x, t)}{\partial x}\right) dx$$

2.4: Energy Eigenvalue Problem

The energy operator is called **Hamiltonian**. The first postulate stated that the time dependence of the wavefunction is dictated by the Schrödinger equation:

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t}=\mathcal{H}\psi(\vec{x},t)$$

If we assume that $\psi(\vec{x},t)$ is the product of a time-dependent part T(t) and a time-independent one $\varphi(\vec{x})$, we can attempt to solve the equation by separation of variables. From $\psi(\vec{x},t)=T(t)\varphi(\vec{x})$, we can rewrite the Schrödinger equation (using the fact that $\mathcal{H}$ does not change T(t)):

$$i\hbar\frac{\partial T(t)\varphi(\vec{x})}{\partial t}=\mathcal{H}[T(t)\varphi(\vec{x},t)] \quad \rightarrow \quad \varphi(\vec{x})\cdot i\hbar\frac{\partial T(t)}{\partial t}=T(t)\cdot\mathcal{H}[\varphi(\vec{x},t)]$$

and we rearrange terms based on their dependence on t or $\vec{x}$

$$\frac{1}{T(t)}i\hbar\frac{\partial T(t)}{\partial t}=\frac{1}{\varphi(\vec{x})}\mathcal{H}[\varphi(\vec{x},t)]$$

Each side has to be equal to a constant, in order for the equality to hold. Then the time-independent wavefunction obeys the time-independent Schrödinger equation:

$$\boxed{\mathcal{H}\varphi(\vec{x})=E\varphi(\vec{x})}$$

where E is identified as the energy of the system. If the wavefunction is given by just its time-independent part, $\psi(\vec{x},t)=\varphi(\vec{x})$, the state is *stationary*. Thus, the time-independent Schrödinger equation allows us to find stationary states of the system, given a certain Hamiltonian.

Notice that the time-independent Schrödinger equation is nothing else than the eigenvalue equation for the Hamiltonian operator. It is thus particularly interesting to study eigenvalues and eigenfunctions of this operator (which, as said, correspond to the energies and stationary states of the system)[5].

In general, the wavefunction describing the state of a quantum system is not.

The energy of a particle has contributions from the kinetic energy as well as the potential energy:

$$E=\frac{1}{2m}\left(p_x^2+p_y^2+p_z^2\right)+V(x,y,z)$$

In quantum mechanics we can find the equivalent operator by substituting the quantum operators for the position and momentum in the above expression:

$$\mathcal{H}=\frac{1}{2m}\left(\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2\right)+V(\hat{x},\hat{y},\hat{z})$$

or more explicitly:

$$\mathcal{H}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x,y,z)$$

and in a compact form

$$\boxed{\mathcal{H}=-\frac{\hbar^2}{2m}\nabla^2+V(x,y,z)}$$

(Notice that V (x, y, z) is just a multiplicative operator, in the same way as the position is).

Note

5 I want to clarify the distinction between eigenfunctions and wavefunctions. In this class we are interested in both. The eigenfunctions are related to a given operator, and they are the solutions to the eigenvalue equation for that operator. They are

> important since they form a basis and they allow us to calculate the probability of obtaining a given measurement outcome. The wavefunction describes the state of the quantum system. In general, it is not an eigenfunction. However, *if* we are considering a *stationary* state, the wavefunction that represents it must be an eigenfunction of the Hamiltonian (energy) operator. Thus in that particular case only (which is a quite common case!) the wavefunction is also an eigenfunction.

Free particle

In 1D, for a free particle there is no potential energy, but only kinetic energy that we can rewrite as:

$$\mathcal{H}=\frac{1}{2m}p^2=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

The eigenvalue problem $\mathcal{H}w_n(x)=E_nw_n(x)$ is then the differential equation

$$\mathcal{H}w_n(x)=E_nw_n(x)\rightarrow-\frac{\hbar^2}{2m}\frac{\partial^2 w_n(x)}{\partial x^2}=E_nw_n(x)$$

we rewrite it as:

$$\frac{\partial^2 w_n(x)}{\partial x^2}+\frac{2mE_n}{\hbar^2}w_n=0\rightarrow\frac{\partial^2 w_n(x)}{\partial x^2}+k_n^2w_n=0$$

where we used the identity

$$\boxed{\frac{\hbar^2k_n^2}{2m}=E_n}$$

between the kinetic energy eigenvalue E_n and the wavenumber k_n (and the momentum $p_n=\hbar k_n$).

For a free particle there is no restriction on the possible energies, E_n can be any positive number. The solution to the eigenvalue problem is then the eigenfunction:

$$w_n(x)=A\sin(k_nx)+B\cos(k_nx)=A'e^{ik_nx}+B'e^{-ik_nx}$$

We see that there are two independent functions for each eigenvalue E_n. Also there are two distinct momentum eigenvalues $\pm k_n$ for each energy eigenvalue, which correspond to two different directions of propagation of the wave function $e^{\pm ik_nx}$.

2.5: Operators, Commutators and Uncertainty Principle

Commutator

Definition: Commutator

The Commutator of two operators A, B is the operator C = [A, B] such that C = AB − BA.

Example 2.5.1

If the operators A and B are scalar operators (such as the position operators) then AB = BA and the commutator is always zero.

Example 2.5.2

If the operators A and B are matrices, then in general $AB \neq BA$. Consider for example:

$$A=\frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad B=\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Then

$$AB=\frac{1}{2}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}, \quad BA=\frac{1}{2}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$$

Then [A, B] = 2AB.

Example 2.5.3

A is Turn to your right. B is Take 3 steps to your left.

Question

Do these two operators commute?

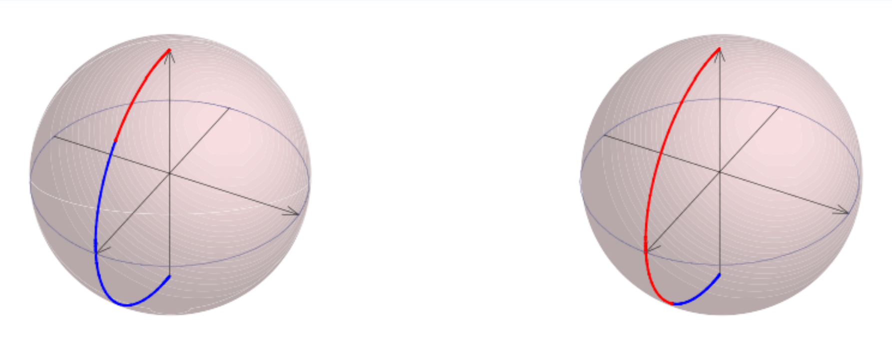


Figure 2.5.1: Two rotations A, B along the x-axis. Left: we apply AB (first the 3π/4 rotation), right we apply BA. Since the two operators commute, the result is the same. (CC BY-NC-ND; Paola Cappellaro)

Example 2.5.4

Let A and B be two rotations. First assume that A is a π/4 rotation around the x direction and B a 3π/4 rotation in the same direction. Now assume that the vector to be rotated is initially around z. Then, if we apply AB (that means, first a 3π/4 rotation around x and then a π/4 rotation), the vector ends up in the negative z direction. The same happen if we apply BA (first A and then B).

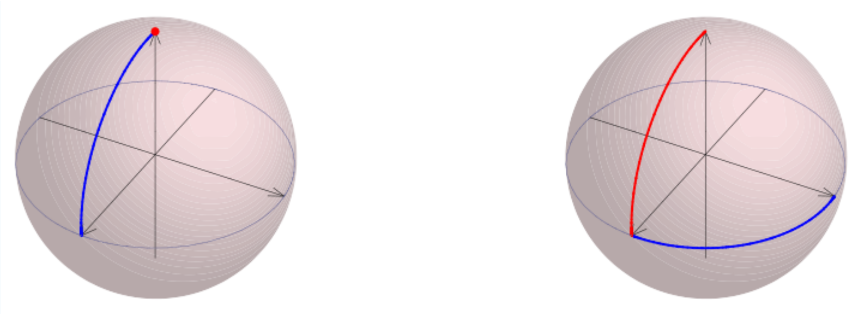


Figure 2.5.2: Two rotations A, B along the x- and z-axis. Left: we apply AB (first the $\pi/2$ rotation along z), right: we apply BA. Since the two operators do not commute, the result is not the same. (CC BY-NC-ND; Paola Cappellaro)

Now assume that A is a $\pi/2$ rotation around the x direction and B around the z direction. When we apply AB, the vector ends up (from the z direction) along the y-axis (since the first rotation does not do anything to it), if instead we apply BA the vector is aligned along the x direction. In this case the two rotations along different axes do not commute.

These examples show that commutators are not specific of quantum mechanics but can be found in everyday life. We now want an example for QM operators.

The most famous commutation relationship is between the position and momentum operators. Consider first the 1D case. We want to know what is $[\hat{x}, \hat{p}_x]$ (I'll omit the subscript on the momentum). We said this is an operator, so in order to know what it is, we apply it to a function (a wavefunction). Let's call this operator $C_{xp}, C_{xp} = [\hat{x}, \hat{p}_x]$.

$$[\hat{x}, \hat{p}]\psi(x) = C_{xp}[\psi(x)] = \hat{x}[\hat{p}[\psi(x)]] - \hat{p}[\hat{x}[\psi(x)]] = -i\hbar\left(x\frac{d}{dx} - \frac{d}{dx}x\right)\psi(x)$$

$$-i\hbar\left(x\frac{d\psi(x)}{dx} - \frac{d}{dx}(x\psi(x))\right) = -i\hbar\left(x\frac{d\psi(x)}{dx} - \psi(x) - x\frac{d\psi(x)}{dx}\right) = i\hbar\psi(x)$$

From $[\hat{x}, \hat{p}]\psi(x) = i\hbar\psi(x)$ which is valid for all $\psi(x)$ we can write

$$\boxed{[\hat{x}, \hat{p}] = i\hbar}$$

Considering now the 3D case, we write the position components as $\{r_x, r_y r_z\}$. Then we have the commutator relationships:

$$\boxed{[\hat{r}_a, \hat{p}_b] = i\hbar\delta_{a,b}}$$

that is, vector components in different directions commute (the commutator is zero).

Properties of commutators

- Any operator commutes with scalars $[A, a] = 0$
- [A, BC] = [A, B]C + B[A, C] and [AB, C] = A[B, C] + [A, C]B
- Any operator commutes with itself [A, A] = 0, with any power of itself [A, A^n] = 0 and with any function of itself $[A, f(A)] = 0$ (from previous property and with power expansion of any function).

From these properties, we have that the Hamiltonian of the free particle commutes with the momentum: $[p, \mathcal{H}] = 0$ since for the free particle $\mathcal{H} = p^2/2m$. Also, $[x, p^2] = [x, p]p + p[x, p] = 2i\hbar p$.

We now prove an important theorem that will have consequences on how we can describe states of a systems, by measuring different observables, as well as how much information we can extract about the expectation values of different observables.

Theorem 2.5.1

If A and B commute, then they have a set of non-trivial common eigenfunctions.

Proof

Let φ_a be an eigenfunction of A with eigenvalue a:

$$A\varphi_a = a\varphi_a$$

Then

$$BA\varphi_a = aB\varphi_a$$

But since [A, B] = 0 we have BA = AB. Let’s substitute in the LHS:

$$A\left(B\varphi_a\right) = a\left(B\varphi_a\right)$$

This means that $(B\varphi_a)$ is also an eigenfunction of A with the same eigenvalue a. If φ_a is the only linearly independent eigenfunction of A for the eigenvalue a, then $B\varphi_a$ is equal to φ_a at most up to a multiplicative constant: $B\varphi_a \propto \varphi_a$.

That is, we can write

$$B\varphi_a = b_a\varphi_a$$

But this equation is nothing else than an eigenvalue equation for B. Then φ_a is also an eigenfunction of B with eigenvalue b_a. We thus proved that φ_a is a common eigenfunction for the two operators A and B. □

✓ Example 2.5.5

We have just seen that the momentum operator commutes with the Hamiltonian of a free particle. Then the two operators should share common eigenfunctions.

This is indeed the case, as we can verify. Consider the eigenfunctions for the momentum operator:

$$\hat{p}\left[\psi_k\right] = \hbar k\psi_k \quad \rightarrow \quad -i\hbar\frac{d\psi_k}{dx} = \hbar k\psi_k \quad \rightarrow \quad \psi_k = Ae^{-ikx}$$

What is the Hamiltonian applied to ψ_k?

$$\mathcal{H}\left[\psi_k\right] = -\frac{\hbar^2}{2m}\frac{d^2\left(Ae^{-ikx}\right)}{dx^2} = \frac{\hbar^2 k^2}{2m}Ae^{-ikx} = E_k\psi_k$$

thus we found that ψ_k is also a solution of the eigenvalue equation for the Hamiltonian, which is to say that it is also an eigenfunction for the Hamiltonian.

Commuting observables

Degeneracy

In the proof of the theorem about commuting observables and common eigenfunctions we took a special case, in which we assume that the eigenvalue a was *non-degenerate*. That is, we stated that φ_a was the only linearly independent eigenfunction of A for the eigenvalue a (functions such as $4\varphi_a, \alpha\varphi_a$ don’t count, since they are not linearly independent from φ_a).

Definition: Degeneracy

In general, an eigenvalue is degenerate if there is more than one eigenfunction that has the same eigenvalue. The degeneracy of an eigenvalue is the number of eigenfunctions that share that eigenvalue.

For example a is n-degenerate if there are n eigenfunction $\left\{\varphi_j^a\right\}, j = 1, 2, \ldots, n$, such that $A\varphi_j^a = a\varphi_j^a$.

What happens if we relax the assumption that the eigenvalue a is not degenerate in the theorem above? Consider for example that there are two eigenfunctions associated with the same eigenvalue:

$$A\varphi_1^a = a\varphi_1^a \quad \text{and} \quad A\varphi_2^a = a\varphi_2^a$$

then any linear combination $\varphi^a = c_1\varphi_1^a + c_2\varphi_2^a$ is also an eigenfunction with the same eigenvalue (there’s an infinity of such eigenfunctions). From the equality $A\left(B\varphi^a\right) = a\left(B\varphi^a\right)$ we can still state that $(B\varphi^a)$ is an eigenfunction of A but we don’t know which one. Most generally, there exist $\tilde{c}_1$ and $\tilde{c}_2$ such that

$$B\varphi_1^a = \tilde{c}_1\varphi_1^a + \tilde{c}_2\varphi_2^a$$

but in general $B\varphi_1^a \not\propto \varphi_1^a$, or φ_1^a is not an eigenfunction of B too.

Example 2.5.6

Consider again the energy eigenfunctions of the free particle. To each energy $E = \frac{\hbar^2 k^2}{2m}$ are associated two linearly-independent eigenfunctions (the eigenvalue is doubly degenerate). We can choose for example $\varphi_E = e^{ikx}$ and $\varphi_E = e^{-ikx}$. Notice that these are also eigenfunctions of the momentum operator (with eigenvalues ±k). If we had chosen instead as the eigenfunctions cos(kx) and sin(kx) these are not eigenfunctions of $\hat{p}$.

Theorem 2.5.2

In general, it is always possible to choose a set of (linearly independent) eigenfunctions of A for the eigenvalue a such that they are also eigenfunctions of B.

For the momentum/Hamiltonian for example we have to choose the exponential functions instead of the trigonometric functions. Also, if the eigenvalue of A is degenerate, it is possible to label its corresponding eigenfunctions by the eigenvalue of B, thus lifting the degeneracy. For example, there are two eigenfunctions associated with the energy E: $\varphi_E = e^{\pm ikx}$. We can distinguish between them by labeling them with their momentum eigenvalue $\pm k$: $\varphi_{E,+k} = e^{ikx}$ and $\varphi_{E,-k} = e^{-ikx}$.

Proof

Assume now we have an eigenvalue a with an n-fold degeneracy such that there exists n independent eigenfunctions φ_k^a, k = 1, . . . , n. Any linear combination of these functions is also an eigenfunction $\tilde{\varphi}^a = \sum_{k=1}^n \tilde{c}_k \varphi_k^a$. For any of these eigenfunctions (let's take the h^{th} one) we can write:

$$B\left[A\left[\varphi_h^a\right]\right] = A\left[B\left[\varphi_h^a\right]\right] = aB\left[\varphi_h^a\right]$$

so that $\bar{\varphi}_h^a = B\left[\varphi_h^a\right]$ is an eigenfunction of A with eigenvalue a. Then this function can be written in terms of the $\left\{\varphi_k^a\right\}$:

$$B\left[\varphi_h^a\right] = \bar{\varphi}_h^a = \sum_k \bar{c}_{h,k} \varphi_k^a$$

This notation makes it clear that $\bar{c}_{h,k}$ is a tensor (an n × n matrix) operating a transformation from a set of eigenfunctions of A (chosen arbitrarily) to another set of eigenfunctions. We can write an eigenvalue equation also for this tensor,

$$\bar{c} v^j = b^j v^j \quad \rightarrow \quad \sum_h \bar{c}_{h,k} v_h^j = b^j v^j$$

where the eigenvectors v^j are vectors of length n.

If we now define the functions $\psi_j^a = \sum_h v_h^j \varphi_h^a$, we have that ψ_j^a are of course eigenfunctions of A with eigenvalue a. Also

$$B\left[\psi_j^a\right] = \sum_h v_h^j B\left[\varphi_h^a\right] = \sum_h v_h^j \sum_{k=1}^n \bar{c}_{h,k} \varphi_k^a$$

$$= \sum_k \varphi_k^a \sum_h \bar{c}_{h,k} v_h^j = \sum_k \varphi_k^a b^j v_k^j = b^j \sum_k v_k^j \varphi_k^a = b^j \psi_j^a$$

We have thus proved that ψ_j^a are eigenfunctions of B with eigenvalues b^j. The ψ_j^a are simultaneous eigenfunctions of both A and B.

Consider the set of functions $\left\{\psi_j^a\right\}$. From the point of view of A they are not distinguishable, they all have the same eigenvalue so they are degenerate. Taking into account a second operator B, we can lift their degeneracy by labeling them with the index j corresponding to the eigenvalue of B (b^j).

Example 2.5.7

Assume that we choose $\varphi_1 = \sin(kx)$ and $\varphi_2 = \cos(kx)$ as the degenerate eigenfunctions of $\mathcal{H}$ with the same eigenvalue $E_k = \frac{\hbar^2 k^2}{2m}$. We now want to find with this method the common eigenfunctions of $\hat{p}$. We first need to find the matrix $\bar{c}$ (here a 2×2 matrix), by applying $\hat{p}$ to the eigenfunctions.

$$\hat{p}\varphi_1 = -i\hbar \frac{d\varphi_1}{dx} = i\hbar k \cos(kx) = -i\hbar k \varphi_2$$

and $\hat{p}\varphi_2 = i\hbar k \varphi_1$. Then the matrix $\bar{c}$ is:

$$\bar{c} = \begin{pmatrix} 0 & i\hbar k \\ -i\hbar k & 0 \end{pmatrix}$$

with eigenvalues , and eigenvectors (not normalized)

$$v^1 = \begin{bmatrix} -i \\ 1 \end{bmatrix}, \quad v^2 = \begin{bmatrix} i \\ 1 \end{bmatrix}$$

We then write the ψ eigenfunctions:

$$\psi^1 = v_1^1 \varphi_1 + v_2^1 \varphi_2 = -i\sin(kx) + \cos(kx) \propto e^{-ikx}, \quad \psi^2 = v_1^2 \varphi_1 + v_2^2 \varphi_2 = i\sin(kx) + \cos(kx) \propto e^{ikx}$$

Complete set of commuting observables

We have seen that if an eigenvalue is degenerate, more than one eigenfunction is associated with it. Then, if we measure the observable A obtaining a we still do not know what the state of the system after the measurement is. If we take another observable B that commutes with A we can measure it and obtain b. We have thus acquired some extra information about the state, since we know that it is now in a common eigenstate of both A and B with the eigenvalues a and b. Still, this could be not enough to fully define the state, if there is more than one state φ_{ab}. We can then look for another observable C, that commutes with both A and B and so on, until we find a set of observables such that upon measuring them and obtaining the eigenvalues a, b, c, d, . . . the function $\varphi_{abcd...}$ is uniquely defined. Then the set of operators {A, B, C, D, . . . } is called a complete set of commuting observables. The eigenvalues a, b, c, d, . . . that specify the state are called *good quantum numbers* and the state is written in Dirac notation as $|abcd\dots\rangle$.

Obs. The set of commuting observable is not unique.

Uncertainty principle

Uncertainty for waves

The uncertainty principle, which you probably already heard of, is not found just in QM. Consider for example the propagation of a wave. If you shake a rope rhythmically, you generate a stationary wave, which is not localized (where is the wave??) but it has a well defined wavelength (and thus a momentum).

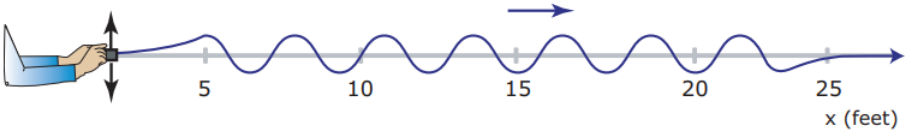


Image by MIT OpenCourseWare.

Figure 2.5.3: A wave with a well defined wavelength but no well-defined position (CC BY-NC-ND; Paola Cappellaro)

If instead you give a sudden jerk, you create a well localized wavepacket. Now however the wavelength is not well defined (since we have a superposition of waves with many wavelengths). The position and wavelength cannot thus be well defined at the same time. In QM we express this fact with an inequality involving position and momentum $p = \frac{2\pi\hbar}{\lambda}$. Then we have $\sigma_x \sigma_p \geq \frac{\hbar}{2}$. We are now going to express these ideas in a more rigorous way.

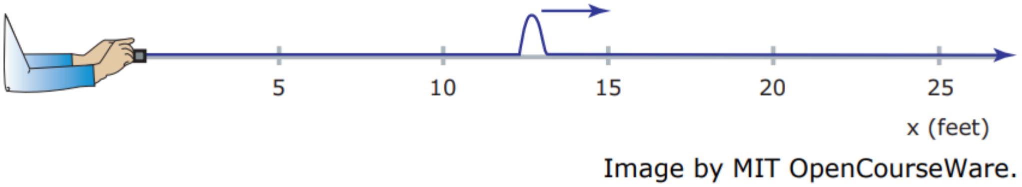


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Figure 2.5.4: A wave packet with a well defined position but no well-defined wavelength. (From Griffith) (CC BY-NC-ND; Paola Cappellaro)

Repeated measurements

Recall that the third postulate states that after a measurement the wavefunction *collapses* to the eigenfunction of the eigenvalue observed.

Let us assume that I make two measurements of the same operator A one after the other (no evolution, or time to modify the system in between measurements). In the first measurement I obtain the outcome a_k (an eigenvalue of A). Then for QM to be consistent, it must hold that the second measurement also gives me the same answer a_k. How is this possible? We know that if the system is in the state $\psi=\sum_k c_k\varphi_k$, with φ_k the eigenfunction corresponding to the eigenvalue a_k (assume no degeneracy for simplicity), the probability of obtaining a_k is $|c_k|^2$. If I want to impose that $|c_k|^2=1$, I must set the wavefunction after the measurement to be $\psi=\varphi_k$ (as all the other $c_h, h\neq k$ are zero). This is the so-called *collapse of the wavefunction*. It is not a mysterious accident, but it is a prescription that ensures that QM (and experimental outcomes) are consistent (thus it's included in one of the postulates).

Now consider the case in which we make two successive measurements of two different operators, A and B. First we measure A and obtain a_k. We now know that the state of the system after the measurement must be φ_k. We now have two possibilities.

If [A, B] = 0 (the two operator commute, and again for simplicity we assume no degeneracy) then φ_k is also an eigenfunction of B. Then, when we measure B we obtain the outcome b_k with certainty. There is no uncertainty in the measurement. If I measure A again, I would still obtain a_k. If I inverted the order of the measurements, I would have obtained the same kind of results (the first measurement outcome is always unknown, unless the system is already in an eigenstate of the operators).

This is not so surprising if we consider the classical point of view, where measurements are not probabilistic in nature.

The second scenario is if $[A, B]\neq 0$. Then, φ_k is not an eigenfunction of B but instead can be written in terms of eigenfunctions of B, $\varphi_k=\sum_h c_h^k\psi_h$ (where ψ_h are eigenfunctions of B with eigenvalue b_h). A measurement of B does not have a certain outcome. We would obtain b_h with probability $|c_h^k|^2$.

There is then an intrinsic uncertainty in the successive measurement of two non-commuting observables. Also, the results of successive measurements of A, B and A again, are different if I change the order B, A and B.

It means that if I try to know with certainty the outcome of the first observable (e.g. by preparing it in an eigenfunction) I have an uncertainty in the other observable. We saw that this uncertainty is linked to the commutator of the two observables. This statement can be made more precise.

Theorem 2.5.3

Define C = [A, B] and ΔA and ΔB the uncertainty in the measurement outcomes of A and B: $\Delta A^2=\left\langle A^2\right\rangle-\langle A\rangle^2$, where $\langle\hat{O}\rangle$ is the expectation value of the operator $\hat{O}$ (that is, the average over the possible outcomes, for a given state: $\langle\hat{O}\rangle=\langle\psi|\hat{O}|\psi\rangle=\sum_k O_k|c_k|^2$).

Then:

$$\boxed{\Delta A\Delta B\geq\frac{1}{2}|\langle C\rangle|}$$

This is **Heisenberg Uncertainty Principle**.

✓ Example 2.5.8

The most important example is the uncertainty relation between position and momentum. We know that these two operators do not commute and their commutator is $[\hat{x}, \hat{p}]=i\hbar$. Then

$$\boxed{\Delta\hat{x}\Delta\hat{p} \geq \frac{\hbar}{2}}$$

CHAPTER OVERVIEW

3: Radioactive Decay I

Thumbnail: Alpha particle decay of a nucleus. (Public Domain; Inductiveload via Wikipedia)

3.1: Review - Energy Eigenvalue Problem

The time-independent wavefunction obeys the time-independent Schrödinger equation:

$$\boxed{\mathcal{H}\varphi(\vec{x}) = E\varphi(\vec{x})}$$

where E is identified as the energy of the system. If the wavefunction is given by just its time-independent part, $\psi(\vec{x}, t) = \varphi(\vec{x})$, the state is *stationary*. Thus, the time-independent Schrödinger equation allows us to find stationary states of the system, given a certain Hamiltonian.

Notice that the time-independent Schrödinger equation is nothing else than the eigenvalue equation for the Hamiltonian operator.

The energy of a particle has contributions from the kinetic energy as well as the potential energy:

$$\mathcal{H} = \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right) + V(\hat{x}, \hat{y}, \hat{z})$$

or more explicitly:

$$\mathcal{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z)$$

which can be written in a compact form as

$$\boxed{\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x, y, z)}$$

(Notice that V (x, y, z) is just a multiplicative operator, in the same way as the position is).

In 1D, for a free particle there is no potential energy, but only kinetic energy that we can rewrite as:

$$\mathcal{H} = \frac{1}{2m}p^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

The eigenvalue problem $\mathcal{H}w_n(x) = E_n w_n(x)$ is then the differential equation

$$\mathcal{H}w_n(x) = E_n w_n(x) \rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2 w_n(x)}{\partial x^2} = E_n w_n(x)$$

For a free particle there is no restriction on the possible energies, E_n can be any positive number. The solution to the eigenvalue problem is then the eigenfunction:

$$w_n(x) = A\sin(k_n x) + B\cos(k_n x) = A' e^{i k_n x} + B' e^{-i k_n x}$$

which represents two waves traveling in opposite directions.

We see that there are two independent functions for each eigenvalue E_n. Also there are two distinct momentum eigenvalues $\pm k_n$ for each energy eigenvalue, which correspond to two different directions of propagation of the wave function $e^{\pm i k_n x}$.

3.2: Unbound Problems in Quantum Mechanics

We will then solve the time-independent Schrödinger equation in some interesting 1D cases that relate to scattering problems.

Infinite Barrier

We first consider a potential as in Figure $3.2.1$. We consider two cases:

- Case A. The system (a particle) has a total energy larger than the potential barrier $E > V_H$.
- Case B. The energy is smaller than the potential barrier, $E < V_H$.

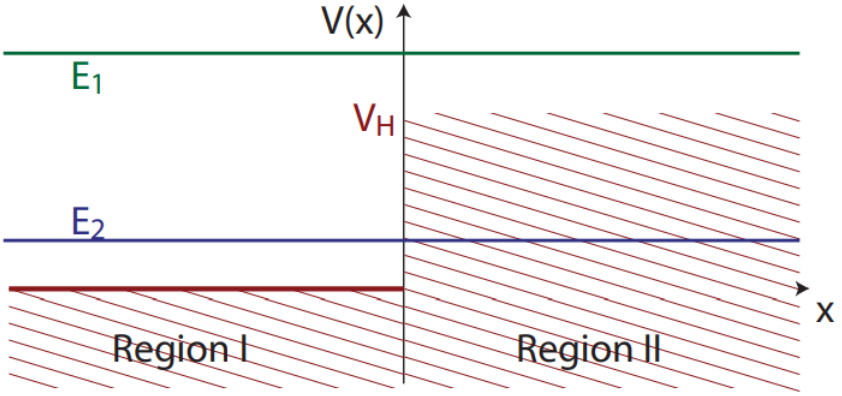


Figure $3.2.1$: Potential function and total energy of the particle. (CC BY-NC-ND; Paola Cappellaro)

Let's first consider the classical problem. The system is a rigid ball with total energy E given by the sum of the kinetic and potential energy. If we keep the total energy fixed, the kinetic energies are different in the two regions:

$$T_I = E \quad T_{II} = E - V_H$$

If E > V_H, the kinetic energy in region two is $T_{II} = \frac{p^2}{2m} = E - V_H$, yielding simply a reduced velocity for the particle. If E < V_H instead, we would obtain a negative T_{II} kinetic energy. This is not an allowed solution, but it means that the particle cannot travel into Region II and it's instead confined in Region I: The particle bounces off the potential barrier.

In quantum mechanics we need to solve the Schrödinger equation in order to find the wavefunction describing the particle at any position. The time-independent Schrödinger equation is

$$\mathcal{H}\psi(x) = -\frac{\hbar^2 d^2}{2m dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \rightarrow \begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \text{ in Region I} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (E - V_H)\,\psi(x) \text{ in Region II} \end{cases}$$

The two cases differ because in Region II the energy difference $\Delta E = E - V_H$ is either positive or negative.

Positive energy

Let's first consider the case in which $\Delta E = E - V_H > 0$. In both regions the particle behaves as a free particle with energy E_I = E and E_{II} = E − V_H. We have already seen the solutions to such differential equation. These are:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_{II}(x) = Ce^{ik'x} + De^{-ik'x}$$

where $\frac{\hbar^2 k^2}{2m} = E$ and $\frac{\hbar^2 k'^2}{2m} = E - V_H$.

We already interpreted the function e^{ikx} as a wave traveling from left to right and e^{-ikx} as a wave traveling from right to left. We then consider a case similar to the classical case, in which a ball was sent toward a barrier. Then the particle is initially described as a wave traveling from left to right in Region I. At the potential barrier the particle can either be reflected, giving rise to a wave traveling from right to left in Region I, or be transmitted, yielding a wave traveling from left to right in Region II. This solution is described by the equations above if we set D = 0, implying that there is no wave originating from the far right.

Since the wavefunction should describe a physical situation, we want it to be a continuous function and with continuous derivative. Thus we have to match the solution values and their derivatives at the boundary x = 0. This will give equations for the coefficients, allowing us to find the exact solution of the Schrödinger equation. This is a *boundary conditions* problem.

From

$$\psi_I(0)=\psi_{II}(0) \quad \text{and} \quad \psi_I'(0)=\psi_{II}'(0)$$

and D = 0 we obtain the conditions:

$$A+B=C, \quad ik(A-B)=ik'C$$

with solutions

$$B=\frac{k-k'}{k+k'}A, \quad C=\frac{2k}{k+k'}A$$

We can further find A by interpreting the wavefunction in terms of a flux of particles. We thus fix the incoming wave flux to be Γ which sets $|A|=\sqrt{\frac{m\Gamma}{\hbar k}}$ (we can consider A to be a real, positive number for simplicity). Then we have:

$$B=\frac{k-k'}{k+k'}\sqrt{\frac{m\Gamma}{\hbar k}}, \quad C=\frac{2k}{k+k'}\sqrt{\frac{m\Gamma}{\hbar k}}$$

We can also verify the following identity

$$k|A|^2=k|B|^2+k'|C|^2$$

which follows from:

$$\begin{aligned} k|B|^2+k'|C|^2 &= \frac{|A|^2}{(k+k')^2}\left[k(k-k')^2+k'(2k)^2\right] \\ &= k|A|^2\frac{(k-k')^2+4k'k}{(k+k')^2} \end{aligned}$$

Let us multiply it by $\hbar/m=$:

$$\frac{\hbar k}{m}|A|^2=\frac{\hbar k}{m}|B|^2+\frac{\hbar k'}{m}|C|^2$$

Recall the interpretation of $\psi(x)=Ae^{ikx}$ as a wave giving a flux of particles $|\psi(x)|^2v=|A|^2\frac{\hbar k}{m}$. This relationship similarly holds for the flux in region II as well as for the reflected flux. Then we can interpret the equality above as an equality of particle flux:

The incoming flux $\Gamma=\frac{\hbar k}{m}|A|^2$ is equal to the sum of the reflected $\Gamma_R=\frac{\hbar k}{m}|B|^2$ and transmitted $\Gamma_T=\frac{\hbar k}{m}|C|^2$ fluxes. The particle flux is conserved. We can then define the reflection and transmission coefficients as:

$$\Gamma=\Gamma_R+\Gamma_T=R\Gamma+T\Gamma$$

where

$$\begin{aligned} R &= \frac{k|B|^2}{k|A|^2} \\ &= \left(\frac{k-k'}{k+k'}\right)^2, \\ T &= \frac{k'|C|^2}{k|A|^2} \\ &= \left(\frac{2k}{k+k'}\right)^2\frac{k'}{k} \end{aligned}$$

It’s then easy to see that $T+R=1$ and we can interpret the reflection and transmission coefficients as the reflection and transmission probability, respectively.

In line with the probabilistic nature of quantum mechanics, we see that the solution of the Schrödinger equation does not give us a precise location for the particle. Instead it describes the probability of finding the particle at any point in space. Given the wavefunction found above we can then calculate various quantity of interest, such as the probability of the particle having a given momentum, position and energy.

Negative Energy

Now we turn to the case where E < V_H, so that $\Delta E<0.$. In the classical case we saw that this implied the impossibility for the ball to be in region II. In quantum mechanics we cannot simply guess a solution based on our intuition, but we need again to solve the Schrödinger equation. The only difference is that now in region II we have $\frac{\hbar^2 k''2}{2m}=E-V_H<0$.

As quantum mechanics is defined in a complex space, this does not pose any problem (we can have negative kinetic energies even if the total energy is positive) and we can solve for k'' simply finding an imaginary number $k''=i\kappa$, $\kappa=\sqrt{\frac{2m}{\hbar^2}(V_H-E)}$ (with κ real).

The solutions to the eigenvalue problem are similar to what already seen:

$$\psi_I(x)=Ae^{ikx}+Be^{-ikx}$$

$$\psi_{II}(x)=Ce^{ik''x}=Ce^{-\kappa x},$$

where we took D = 0 as before.

Quantum mechanics allows the particle to enter the classical forbidden region, but the wavefunction becomes a vanishing exponential function. This means that even if the particle can indeed enter the forbidden region, it cannot go very far, the probability of finding the particle far away from the potential barrier (given by $P(x>0)=|\psi_{II}(x)|^2=|C|^2e^{-2\kappa x}$ becomes smaller and smaller.

Again we match the function and its derivatives at the boundary to find the coefficients:

$$\psi_I(0)=\psi_{II}(0)\rightarrow A+B=C$$

$$\psi_I'(0)=\psi_{II}'(0)\rightarrow ik(A-B)=-\kappa C$$

with solutions

$$B=\frac{k-i\kappa}{k+i\kappa}A,\quad C=\frac{2k}{k+i\kappa}A$$

The situation in terms of flux is instead quite different. We now have the equality: $k|B|^2=k|A|^2$:

$$k|B|^2=k\left|\frac{k-i\kappa}{k+i\kappa}\right|^2=k\frac{k^2+\kappa^2}{k^2+\kappa^2}=k$$

In terms of flux, we can write this relationship as $\Gamma=\Gamma_R$, which implies R = 1 and T = 0. Thus we have no transmission, just perfect reflection, although there is a penetration of the probability in the forbidden region. This can be called an **evanescent transmitted wave**.

Finite barrier

We now consider a different potential which creates a finite barrier of height V_H between x = 0 and L. As depicted in Figure 3.2.2 this potential divides the space in 3 regions. Again we consider two cases, where the total energy of the particle is greater or smaller than V_H. Classically, we consider a ball initially in Region I. Then in the case where

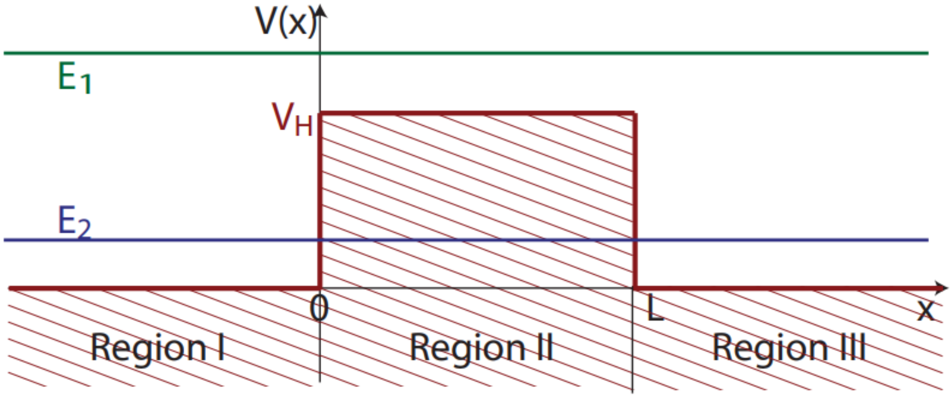


Figure 3.2.2: Finite barrier potential (CC BY-NC-ND; Paola Cappellaro)

E > V_H the ball can travel everywhere, in all the three regions, while for E < V_H it is going to be confined in Region I, and we have perfect reflection. We will consider now the quantum mechanical case.

Positive kinetic energy

First we consider the case where $\Delta E=E-V_H>0$. The kinetic energies in the three regions are

$$\begin{array}{ccc}\text{Region I} & \text{Region II} & \text{Region III}\\ T=\frac{\hbar^2k^2}{2m}=E & T=\frac{\hbar^2k'^2}{2m}=E-V_H & T=\frac{\hbar^2k^2}{2m}=E\end{array}$$

And the wavefunction is

$$\begin{array}{ccc}\text{Region I} & \text{Region II} & \text{Region III}\\ Ae^{ikx}+Be^{-ikx} & Ce^{ik'x}+De^{-ik'x} & Ee^{ikx}\end{array}$$

(again we put the term $Fe^{-ikx}=0$ for physical reasons, in analogy with the classical case studied). The coefficients can be calculated by considering the boundary conditions.

In particular, we are interested in the probability of transmission of the beam through the barrier and into region III. The transmission coefficient is then the ratio of the outgoing flux in Region III to the incoming flux in Region I (both of these fluxes travel to the Right, so we label them by R):

$$T=\frac{k|\psi_{III}^R|^2}{k|\psi_I^R|^2}=\frac{k|E|^2}{k|A|^2}=\frac{|E|^2}{|A|^2}$$

while the reflection coefficient is the ratio of the reflected (from right to left, labeled L) and incoming (from left to right, labeled R) flux in Region I:

$$R=\frac{k|\psi_I^L|^2}{k|\psi_I^R|^2}=\frac{k|B|^2}{k|A|^2}=\frac{|B|^2}{|A|^2}$$

We can solve explicitly the boundary conditions:

$$\begin{array}{cc}\psi_I(0)=\psi_{II}(0) & \psi_{II}(L)=\psi_{III}(L)\\ \psi_I'(0)=\psi_{II}'(0) & \psi_{II}'(L)=\psi_{III}'(L)\end{array}$$

and find the coefficients B, C, D, E (A is determined from the flux intensity Γ. From the full solution we can verify that T + R = 1, as it should be physically.

Obs. Notice that we could also have found a different solution, e.g. in which we set $F\neq 0$ and A = 0, corresponding to a particle originating from the right.

Negative Energy

In the case where $\Delta E = E - V_H < 0$, in region II we expect as before an imaginary momentum. In fact we find

$$\begin{array}{ccc} \text{Region I} & \text{Region II} & \text{Region III} \\ k=\sqrt{\frac{2mE}{\hbar^2}} & k^{\prime}=i\kappa, \kappa=\sqrt{\frac{2m(V_H-E)}{\hbar^2}} & k=\sqrt{\frac{2mE}{\hbar^2}} \end{array}$$

And the wavefunction is

$$\begin{array}{ccc} \text{Region I} & \text{Region II} & \text{Region III} \\ Ae^{ikx}+Be^{-ikx} & Ce^{-\kappa x}+De^{\kappa x} & Ee^{ikx} \end{array}$$

The difference here is that a finite transmission through the barrier is possible and the transmission coefficient is not zero. Indeed, from the full solution of the boundary condition problem, we can find as in the previous case the coefficients T and R and we have T + R = 1.

There is thus a probability that the particle *tunnels* through the finite barrier and appears in Region III, then continuing to x → ∞.

Obs. Although we have been describing the situation in terms of wave traveling in one direction or the other, what we are describing here is not a time-dependent problem. There is no time-dependence at all in this problem (all the solutions are only a function of x, not of time). This is the same situation as stationary waves for example in a rope. The state of the system is not evolving. It is always (at any time) described by the same waves and thus at any time we will have the same outcomes and probability outcomes for any measurement.

Estimates and Scaling

Instead of solving exactly the problem for the second case, we try to make some estimates in the case there is a very small tunneling probability. In this case we have the following approximations for the coefficients A, B, C and D.

- Assuming $T \ll 1$ we expect $D \approx 0$ since if there is a very small probability for the particle to be in region III, the probability of coming back from it through the barrier must be even smaller (in other words, if $D \neq 0$ we would have an increasing probability to have a wave coming out of the barrier).
- Also, $T \ll 1$ implies $R \approx 1$. This means that $B/A \approx 1$ or $B \approx A$.
- Matching the wavefunction at x = 0, we have $C = A + B \approx 2A$.
- Finally matching the wavefunction at x = L we obtain:

$$\psi(L)=Ce^{-\kappa L}=2Ae^{-\kappa L}=Ee^{ikL}$$

We can then calculate the transmission probability T from $T=\frac{k\left|\psi_{III}^R\right|^2}{k\left|\psi_I^R\right|^2}$, with these assumptions. We obtain

$$T=\frac{k|E|^2}{k|A|^2}=\frac{|E|^2}{|A|^2}=\frac{4|A|^2e^{-2\kappa L}}{|A|^2}\rightarrow T=4e^{-2\kappa L}$$

Thus the transmission probability depends on the length of the potential barrier (the longer the barrier the less transmission we have, as it is intuitive) and on the coefficient κ. Notice that κ depends on the difference between the particle energy and the potential strength: If the particle energy is near the edge of the potential barrier (that is, ΔE ≈ 0) then $\kappa \approx 0$ and there's a high probability of tunneling. This case is however against our first assumptions of small tunneling (that's why we obtain the unphysical result that T ≈ 4!!). The case we are considering is instead where the particle energy is small compared to the potential, so that κ is large, and the particle has a very low probability of tunneling through.

3.3: Alpha Decay

If we go back to the binding energy per mass number plot (B/A vs. A) we see that there is a bump (a peak) for $A \sim 60-100$. This means that there is a corresponding minimum (or energy optimum) around these numbers. Then the heavier nuclei will want to decay toward this lighter nuclides, by shedding some protons and neutrons. More specifically, the decrease in binding energy at high A is due to Coulomb repulsion. Coulomb repulsion grows in fact as Z^2, much faster than the nuclear force which is proportional to A.

This could be thought as a similar process to what happens in the fission process: from a parent nuclide, two daughter nuclides are created. In the α decay we have specifically:

$${}^{\mathrm{A}}_{\mathrm{Z}}\mathrm{XN} \longrightarrow {}^{\mathrm{A}-4}_{\mathrm{Z}-2}\mathrm{X}'_{\mathrm{N}-2} + \alpha$$

where α is the nucleus of $\mathrm{He}-4$: ${}^{4}_{2}\mathrm{He}_2$.

The α decay should be competing with other processes, such as the fission into equal daughter nuclides, or into pairs including ${}^{12}\mathrm{C}$ or ${}^{16}\mathrm{O}$ that have larger B/A then α. However α decay is usually favored. In order to understand this, we start by looking at the energetic of the decay, but we will need to study the quantum origin of the decay to arrive at a full explanation.

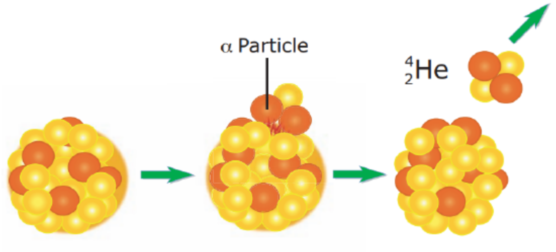


Image by MIT OpenCourseWare.

Figure 3.3.1: Alpha decay schematics (CC BY-NC-ND; Paola Cappellaro)

Energetics

In analyzing a radioactive decay (or any nuclear reaction) an important quantity is Q, the net energy released in the decay: $Q=\left(m_X-m_{X'}-m_\alpha\right)c^2$. This is also equal to the total kinetic energy of the fragments, here $Q=T_{X'}+T_\alpha$ (here assuming that the parent nuclide is at rest).

When $Q > 0$ energy is released in the nuclear reaction, while for $Q < 0$ we need to provide energy to make the reaction happen. As in chemistry, we expect the first reaction to be a spontaneous reaction, while the second one does not happen in nature without intervention. (The first reaction is exo-energetic the second endo-energetic). Notice that it's no coincidence that it's called Q. In practice given some reagents and products, Q give the quality of the reaction, i.e. how energetically favorable, hence probable, it is. For example in the alpha-decay $\log\left(t_{1/2}\right) \propto \frac{1}{\sqrt{Q_\alpha}}$, which is the Geiger-Nuttall rule (1928).

The alpha particle carries away most of the kinetic energy (since it is much lighter) and by measuring this kinetic energy experimentally it is possible to know the masses of unstable nuclides.

We can calculate Q using the SEMF. Then:

$$Q_\alpha = B\left(\begin{array}{c}A-4\\ Z-2\end{array} X'_{N-2}\right) + B\left({}^{4}He\right) - B\left({}^{A}_{Z}X_N\right) = B(A-4, Z-2) - B(A, Z) + B\left({}^{4}He\right)$$

We can approximate the finite difference with the relevant gradient:

$$\begin{aligned} Q_\alpha &= [B(A-4, Z-2) - B(A, Z-2)] + [B(A, Z-2) - B(A, Z)] + B\left({}^{4}He\right) && (3.3.1)\\ &\approx -4\frac{\partial B}{\partial A} - 2\frac{\partial B}{\partial Z} + B\left({}^{4}He\right) && (3.3.2)\\ &= 28.3 - 4a_v + \frac{8}{3}a_s A^{-1/3} + 4a_c\left(1-\frac{Z}{3A}\right)\left(\frac{Z}{A^{1/3}}\right) - 4a_{sym}\left(1-\frac{2Z}{A}+3a_pA^{-7/4}\right)^2 && (3.3.3)\end{aligned}$$

Since we are looking at heavy nuclei, we know that $Z \approx 0.41A$ (instead of $Z \approx A/2$) and we obtain

$$Q_\alpha \approx -36.68 + 44.9 A^{-1/3} + 1.02 A^{2/3},$$

where the second term comes from the surface contribution and the last term is the Coulomb term (we neglect the pairing term, since a priori we do not know if a_p is zero or not).

Then, the Coulomb term, although small, makes Q increase at large A. We find that $Q \geq 0$ for $A \gtrsim 150$, and it is Q ≈ 6MeV for A = 200. Although Q > 0, we find experimentally that α decay only arise for $A \geq 200$.

Further, take for example Francium-200 (${}_{87}^{200}\mathrm{Fr}_{113}$). If we calculate Q_α from the experimentally found mass differences we obtain $Q_\alpha \approx 7.6\mathrm{MeV}$ (the product is ^{196}At). We can do the same calculation for the hypothetical decay into a ^{12}C and remaining fragment (${}_{81}^{188}\mathrm{TI}_{107}$):

$$Q_{12} C = c^2 \left[m \left({A \atop Z} X_N \right) - m \left({A-12 \atop Z-6} X'_{N-6} \right) - m \left({}^{12}C \right) \right] \approx 28 MeV$$

Thus this second reaction seems to be more energetic, hence more favorable than the alpha-decay, yet it does not occur (some decays involving C-12 have been observed, but their branching ratios are much smaller).

Thus, looking only at the energetic of the decay does not explain some questions that surround the alpha decay:

- Why there’s no ^{12}C-decay? (or to some of this tightly bound nuclides, e.g O-16 etc.)
- Why there’s no spontaneous fission into equal daughters?
- Why there’s alpha decay only for $A \geq 200$?
- What is the explanation of Geiger-Nuttall rule? $\log t_{1/2} \propto \frac{1}{\sqrt{Q_\alpha}}$

Quantum mechanics description of alpha decay

We will use a semi-classical model (that is, combining quantum mechanics with classical physics) to answer the questions above.

In order to study the quantum mechanical process underlying alpha decay, we consider the interaction between the daughter nuclide and the alpha particle. Just prior to separation, we can consider this pair to be already present *inside* the parent nuclide, in a bound state. We will describe this pair of particles in their *center of mass* coordinate frames: thus we are interested in the relative motion (and kinetic energy) of the two particles. As often done in these situations, we can describe the relative motion of two particles as the motion of a single particle of reduced mass $\mu = \frac{m_\alpha m'}{m_\alpha + m'}$ (where m' is the mass of the daughter nuclide).

Consider for example the reaction ${}^{238}\mathrm{U} \rightarrow {}^{234}\mathrm{Th} + \alpha$. What is the interaction between the Th and alpha particle in the bound state?

- At short distance we have the nuclear force binding the ^{238}U.
- At long distances, the coulomb interaction predominates

The nuclear force is a very strong, attractive force, while the Coulomb force among protons is repulsive and will tend to expel the alpha particle.

Since the final state is known to have an energy $Q_\alpha = 4.3$ MeV, we will take this energy to be as well the initial energy of the two particles in the potential well (we assume that $Q_\alpha = E$ since Q is the kinetic energy while the potential energy is zero). The size of the potential well can be calculated as the sum of the daughter nuclide (^{234}Th) and alpha radii:

$$R = R' + R_\alpha = R_0 \left((234)^{1/3} + 4^{1/3} \right) = 9.3\mathrm{fm}$$

On the other side, the Coulomb energy at this separation is $V_{Coul} = e^2 Z' Z_\alpha / R = 28 MeV \gg Q_\alpha$ (here Z' = Z − 2). Then, the particles are inside a well, with a high barrier (as $V_{\mathrm{Coul}} \gg Q$) but there is some probability of tunneling, since Q > 0 and the state is not stably bound.

Thus, if the parent nuclide, ^{238}U, was really composed of an alpha-particle and of the daughter nuclide, ^{234}Th, then with some probability the system would be in a bound state and with some probability in a decayed state, with the alpha particle outside the potential barrier. This last probability can be calculated from the tunneling probability P_T we studied in the previous section, given by the amplitude square of the wavefunction outside the barrier, $P_T = |\psi(R_{\mathrm{out}})|^2$.

How do we relate this probability to the decay rate?

We need to multiply the probability of tunneling P_T by the frequency f at which ^{238}U could actually be found as being in two fragments $^{234}\mathrm{Th}+\alpha$ (although still bound together inside the potential barrier). The decay rate is then given by $\lambda_\alpha = f P_T$.

To estimate the frequency f, we equate it with the frequency at which the compound particle in the center of mass frame is at the well boundary: $f = v_{in}/R$, where v_{in} is the velocity of the particles when they are inside the well (see cartoon in Figure 3.3.3). We have $\frac{1}{2} m v_{in}^2 = Q_\alpha + V_0 \approx 40\mathrm{MeV}$, from which we have $v_{in} \approx 4\times 10^{22}\mathrm{fm/s}$. Then the frequency is $f \approx 4.3\times 10^{21}$.

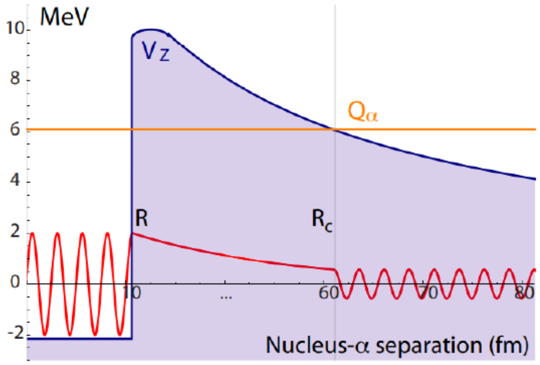


Figure 3.3.2: Potential well for alpha decay tunneling. The inner radius is R while the intersection of Q_α with the potential is R_c> (not to scale). (CC BY-NC-ND; Paola >Cappellaro>)

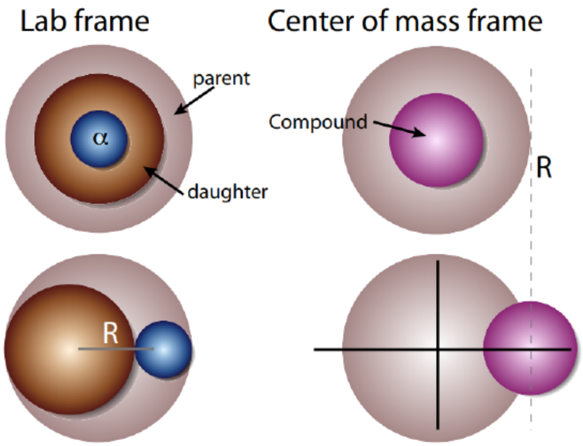


Figure 3.3.3: Positions of daughter and alpha particles in the nucleus, as seen in (left) the laboratory frame and (right) in the center of mass frame. When the relative distance is zero, this correspond to a undivided (parent) nuclide. When the relative distance is R, it corresponds to a separate alpha and daughter nuclide inside the nucleus. (CC BY-NC-ND; Paola Cappellaro)

The probability of tunneling is given by the amplitude square of the wavefunction just outside the barrier, $P_T = |\psi(R_c)|^2$, where R_c is the coordinate at which $V_{\mathrm{Coul}}(R_c) = Q_\alpha$, such that the particle has again a positive kinetic energy:

$$R_c = \frac{e^2 Z_\alpha Z'}{Q_\alpha} \approx 63\mathrm{fm}$$

Recall that in the case of a square barrier, we expressed the wavefunction inside a barrier (in the classically forbidden region) as a plane wave with imaginary momentum, hence a decaying exponential $\psi_{in}(r) \sim e^{-\kappa r}$. What is the relevant momentum $\hbar\kappa$ here? Since the potential is no longer a square barrier, we expect the momentum (and kinetic energy) to be a function of position.

The total energy is given by $E = Q_\alpha$ and is the sum of the potential (Coulomb) and kinetic energy. As we've seen that the Coulomb energy is higher than Q, we know that the kinetic energy is negative:

$$Q_\alpha = T + V_{Coul} = \frac{\hbar^2 k^2}{2\mu} + \frac{Z_\alpha Z' e^2}{r}$$

with μ the reduced mass

$$\mu = \frac{m_\alpha m'}{m_\alpha + m'}$$

and $k^2=-\kappa^2(with\backslash(\kappa\in R)$. This equation is valid at any position inside the barrier:

$$\kappa(r)=\sqrt{\frac{2\mu}{\hbar^2}[V_{Coul}(r)-Q_\alpha]}=\sqrt{\frac{2\mu}{\hbar^2}\left(\frac{Z_\alpha Z' e^2}{r}-Q_\alpha\right)}$$

If we were to consider a small slice of the barrier, from r to $r+dr$, then the probability to pass through this barrier would be $dP_T(r)=e^{-2\kappa(r)dr}$. If we divide then the total barrier range into small slices, the final probability is the product of the probabilities dP_T^k of passing through all of the slices. Then $\log(P_T)=\sum_k\log\left(dP_T^k\right)$ and taking the continuous limit $\log(P_T)=\int_R^{R_c}\log[dP_T(r)]=-2\int_R^{R_c}\kappa(r)dr$.

Finally the probability of tunneling is given by $P_T=e^{-2G}$, where G is calculated from the integral

$$G=\int_R^{R_C}dr\kappa(r)=\int_R^{R_C}dr\sqrt{\frac{2\mu}{\hbar^2}\left(\frac{Z_\alpha Z' e^2}{r}-Q_\alpha\right)}$$

We can solve the integral analytically, by letting $r=R_c y=y\frac{Z_\alpha Z' e^2}{Q_\alpha}$, then

$$G=\frac{Z_\alpha Z_0 e^2}{\hbar c}\sqrt{\frac{2\mu c^2}{Q_\alpha}}\int_{R/R_C}^1 dy\sqrt{\frac{1}{y}-1}$$

which yields

$$G=\frac{Z_\alpha Z' e^2}{\hbar c}\sqrt{\frac{2\mu c^2}{Q_\alpha}}\left[\arccos\left(\sqrt{\frac{R}{R_c}}\right)-\sqrt{\frac{R}{R_c}}\sqrt{1-\frac{R}{R_c}}\right]=\frac{Z_\alpha Z' e^2}{\hbar c}\sqrt{\frac{2\mu c^2}{Q_\alpha}}\frac{\pi}{2}g\left(\sqrt{\frac{R}{R_c}}\right)$$

where to simplify the notation we used the function

$$g(x)=\frac{2}{\pi}\left(\arccos(x)-x\sqrt{1-x^2}\right).$$

Finally the decay rate is given by

$$\boxed{\lambda_\alpha=\frac{v_{in}}{R}e^{-2G}}$$

where G is the so-called **Gamow factor**.

In order to get some insight on the behavior of G we consider the approximation R ≪ R_c:

$$G=\frac{1}{2}\sqrt{\frac{E_G}{Q_\alpha}}g\left(\sqrt{\frac{R}{R_c}}\right)\approx\frac{1}{2}\sqrt{\frac{E_G}{Q_\alpha}}\left[1-\frac{4}{\pi}\sqrt{\frac{R}{R_c}}\right]$$

where E_G is the Gamow energy:

$$\boxed{E_G=\left(\frac{2\pi Z_\alpha Z e^2}{\hbar c}\right)^2\frac{\mu c^2}{2}}$$

For example for the ^{238}U decay studied E_G = 122, 000MeV (huge!) so that $\sqrt{E_G/Q_\alpha}=171$ while $g\left(\sqrt{\frac{R}{R_c}}\right)\approx 0.518$. The exponent is thus a large number, giving a very low tunneling probabily: $e^{-2G}=e^{-89}=4\times 10^{-39}$. Then, $\lambda_\alpha=1.6\times 10^{-17}$ s or $t_{1/2}=4.5\times 10^9$ years, close to what observed.

These results finally give an answer to the questions we had regarding alpha decay. The decay probability has a very strong dependence on not only Q_α but also on Z_1Z_2 (where Z_i are the number of protons in the two daughters). This leads to the following observations:

- Other types of decay are less likely, because the Coulomb energy would increase considerably, thus the barrier becomes too high to be overcome.
- The same is true for spontaneous fission, despite the fact that Q is much higher (∼ 200MeV).

- We thus find that alpha decay is the optimal mechanism. Still, it can happen only for A ≥ 200 exactly because otherwise the tunneling probability is very small.
- The Geiger-Nuttall law is a direct consequence of the quantum tunneling theory. Also, the large variations of the decay rates with Q are a consequence of the exponential dependence on Q.

A final word of caution about the model: the semi-classical model used to describe the alpha decay gives quite accurate predictions of the decay rates over many order of magnitudes. However it is not to be taken as an indication that the parent nucleus is really already containing an alpha particle and a daughter nucleus (only, it behaves as if it were, as long as we calculate the alpha decay rates).

CHAPTER OVERVIEW

4: Energy Levels

4.1: Bound Problems

In the previous chapter we studied stationary problems in which the system is best described as a (time-independent) wave, “scattering” and “tunneling” (that is, showing variation on its intensity) because of obstacles given by changes in the potential energy.

Although the potential determined the space-dependent wavefunction, there was no limitation imposed on the possible wavenumbers and energies involved. An infinite number of *continuous* energies were possible solutions to the time- independent Schrödinger equation.

In this chapter, we want instead to describe systems which are best described as particles confined inside a potential. This type of system well describe atoms or nuclei whose constituents are bound by their mutual interactions. We shall see that because of the particle confinement, the solutions to the energy eigenvalue equation (i.e. the time- independent Schrödinger equation) are now only a *discrete* set of possible values (a discrete set os energy levels). The energy is therefore **quantized**. Correspondingly, only a *discrete* set of eigenfunctions will be solutions, thus the system, if it’s in a stationary state, can only be found in one of these allowed eigenstates.

We will start to describe simple examples. However, after learning the relevant concepts (and mathematical tricks) we will see how these same concepts are used to predict and describe the energy of atoms and nuclei. This theory can predict for example the discrete emission spectrum of atoms and the nuclear binding energy.

Energy in Square infinite well (particle in a box)

The simplest system to be analyzed is a particle in a box: classically, in 3D, the particle is stuck inside the box and can never leave. Another classical analogy would be a ball at the bottom of a well so deep that no matter how much kinetic energy the ball possess, it will never be able to exit the well.

We consider again a particle in a 1D space. However now the particle is no longer free to travel but is confined to be between the positions 0 and L. In order to confine the particle there must be an infinite force at these boundaries that repels the particle and forces it to stay only in the allowed space. Correspondingly there must be an infinite potential in the forbidden region.

Thus the potential function is as depicted in Figure 4.1.2: V(x) = ∞ for x < 0 and x > L; and V(x) = 0 for 0 ≤ x ≤ L. This last condition means that the particle behaves as a free particle inside the well (or box) created by the potential.

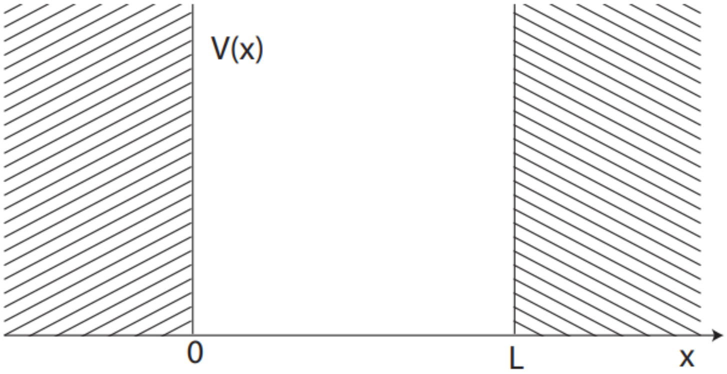


Figure 4.1.1: Potential of an infinite well (CC BY-NC-ND; Paola Cappellaro)

We can then write the energy eigenvalue problem inside the well:

$$\mathcal{H}\left[w_n\right]=-\frac{\hbar^2}{2m}\frac{\partial^2 w_n(x)}{\partial x^2}=E_n w_n(x)$$

Outside the well we cannot write a proper equation because of the infinities. We can still set the values of $w_n(x)$ at the boundaries 0, L. Physically, we expect $w_n(x)=0$ in the forbidden region. In fact, we know that $\psi(x)=0$ in the forbidden region (since the particle has zero probability of being there)[6]. Then if we write any $\psi(x)$ in terms of the energy eigenfunctions, $\psi(x)=\sum_n c_n w_n(x)$ this has to be zero $\forall c_n$ in the forbidden region, thus the w_n have to be zero.

At the boundaries we can thus write the boundary conditions[7]:

$$w_n(0)=w_n(L)=0$$

We can solve the eigenvalue problem inside the well as done for the free particle, obtaining the eigenfunctions

$$w_n'(x)=A'e^{ik_nx}+B'e^{-ik_nx},$$

with eigenvalues $E_n=\frac{\hbar^2k_n^2}{2m}$.
It is easier to solve the boundary conditions by considering instead:

$$w_n(x)=A\sin(k_nx)+B\cos(k_nx)$$

We have:

$$w_n(0)=A\times 0+B\times 1=B=0$$

Thus from $w_n(0)=0$ we have that B = 0. The second condition states that

$$w_n(L)=A\sin(k_nL)=0$$

The second condition thus does not set the value of A (that can be done by the normalization condition). In order to satisfy the condition, instead, we have to set

$$k_nL=n\pi\rightarrow k_n=\frac{n\pi}{L}$$

for integer n. This condition then in turns sets the allowed values for the energies:

$$E_n=\frac{\hbar^2k_n^2}{2m}=\frac{\hbar^2\pi^2}{2mL^2}n^2\equiv E_1n^2$$

where we set $E_1=\frac{\hbar^2\pi^2}{2mL^2}$ and n is called a **quantum number** (associated with the energy eigenvalue). From this, we see that only some values of the energies are allowed. There are still an infinite number of energies, but now they are not a continuous set. We say that the energies are **quantized**. The quantization of energies (first the photon energies in black-body radiation and photoelectric effect, then the electron energies in the atom) is what gave *quantum* mechanics its name. However, as we saw from the scattering problems in the previous chapter, the quantization of energies is not a general property of quantum mechanical systems. Although this is common (and the rule any time that the particle is *bound*, or confined in a region by a potential) the quantization is always a consequence of a particular characteristic of the potential. There exist potentials (as for the free particle, or in general for unbound particles) where the energies are not quantized and do form a continuum (as in the classical case).

Note

6 Note that this is true because the potential is infinite. The energy eigenvalue function (for the Hamiltonian operator) is always valid. The only way for the equation to be valid outside the well it is if $w_n(x)=0$.

7 Note that in this case we cannot require that the first derivative be continuous, since the potential becomes infir boundary. In the cases we examined to describe scattering, the potential had only discontinuity of the first kind.

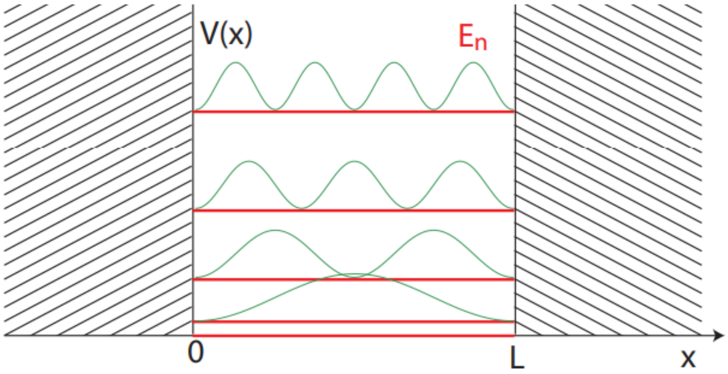


Figure 4.1.2: Quantized energy levels (E_n for n = 0 − 4) in red. Also, in green the position probability distribution $|w_n(x)|^2$ (CC BY-NC-ND; Paola Cappellaro)

Finally we calculate the normalization of the energy eigenfunctions:

$$\int_{-\infty}^{\infty} dx|w_n|^2 = 1 \rightarrow \int_0^L A^2 \sin{(k_n x)}^2 dx = \frac{L}{2}A^2 = 1 \quad \rightarrow \quad A = \sqrt{\frac{2}{L}}$$

Notice that because the system is bound inside a well defined region of space, the normalization condition has now a very clear physical meaning (and thus we must always apply it): if the system is represented by one of the eigenfunctions (and it is thus stationary) we know that it must be found somewhere between 0 and L. Thus the probability of finding the system somewhere in that region must be one. This corresponds to the condition $\int_0^L p(x)dx = 1$ or $\int_0^L |\psi(x)|^2 dx = 1$.

Finally, we have

$$\boxed{w_n(x) = \sqrt{\frac{2}{L}}\sin{k_n x}, \quad k_n = \frac{n\pi}{L}, \quad E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2}$$

Now assume that a particle is in an energy eigenstate, that is $\psi(x) = w_n(x)$ for some n: $\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$. We plot in Figure 4.1.3 some possible wavefunctions.

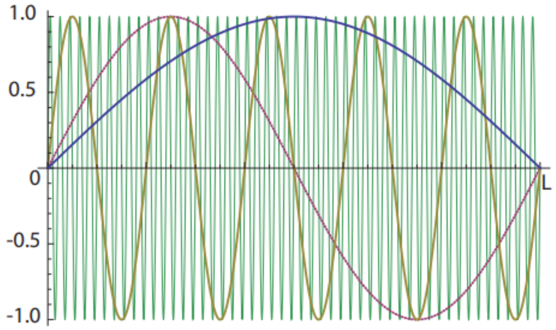


Figure 4.1.3: Energy eigenfunctions. Blue: n=1, Mauve n=2, Brown n=10, Green n=100 (CC BY-NC-ND; Paola Cappellaro)

Consider for example n = 1

Exercise 4.1.1

What does an energy measurement yield? What is the probability of this measurement?

Answer

($E = \frac{\hbar^2\pi^2}{2m}$ with probability 1)

Exercise 4.1.2

what does a postion measurement yield? What is the probability of finding the particle at 0 ≤ x ≤ L? and at x = 0, L?

Exercise 4.1.3

What is the difference in energy between n and n + 1 when n → ∞? And what about the position probability $|w_n|^2$ at large n? What does that say about a possible classical limit?

Answer

> In the limit of large quantum numbers or small deBroglie wavelength $\lambda \propto 1/k$ on average the quantum mechanical description recovers the classical one (*Bohr correspondence principle*).

Finite Square Well

We now consider a potential which is very similar to the one studied for scattering (compare Figure 3.2.2 to Figure 4.1.4), but that represents a completely different situation. The physical picture modeled by this potential is that of a bound particle. Specifically if we consider the case where the total energy of the particle $E_2 < 0$ is negative, then classically we would expect the particle to be trapped inside the potential well. This is similar to what we already saw when studying the infinite well. Here however the height of the well is finite, so that we will see that the quantum mechanical solution allows for a finite penetration of the wavefunction in the classically forbidden region.

Exercise 4.1.4

What is the expect behavior of a classical particle? (consider for example a snowboarder in a half-pipe. If she does not have enough speed she's not going to be able to jump over the slope, and will be confined inside)

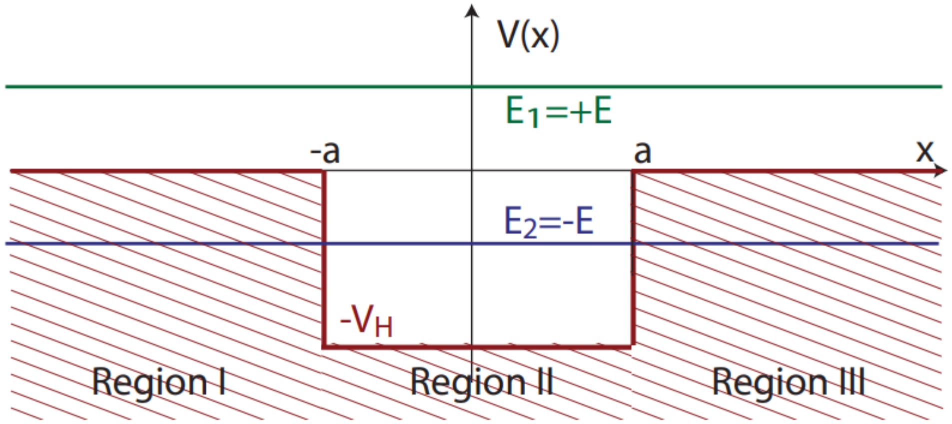


Figure 4.1.4: Potential of a finite well. The potential is non-zero and equal to $-V_H$ in the region $-a \leq x \leq a$. (CC BY-NC-ND; Paola Cappellaro)

For a quantum mechanical particle we want instead to solve the Schrödinger equation. We consider two cases. In the first case, the kinetic energy is always positive:

$$\mathcal{H}\psi(x) = -\frac{{}^2 d^2}{2m dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \rightarrow \begin{cases} -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \text{ in Region I} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = (E + V_H)\,\psi(x) \text{ in Region II} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \text{ in Region III} \end{cases}$$

so we expect to find a solution in terms of traveling waves. This is not so interesting, we only note that this describes the case of an unbound particle. The solutions will be similar to scattering solutions (see mathematica demonstration). In the second case, the kinetic energy is greater than zero for $|x| \leq a$ and negative otherwise (since the total energy is negative). Notice that I set E to be a positive quantity, and the system's energy is −E. We also assume that $E < V_H$. The equations are thus rewritten as:

$$\mathcal{H}\psi(x)=-\frac{{}^2d^2}{2mdx^2}\psi(x)+V(x)\psi(x)=E\psi(x)\rightarrow\begin{cases}-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=-E\psi(x)\text{ in Region I}\\-\frac{\hbar^2}{2m}\frac{d^2\psi^2\psi(x)}{dx^2}=(V_H-E)\,\psi(x)\text{ in Region II}\\-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=-E\psi(x)\text{ in Region III}\end{cases}$$

Then we expect waves inside the well and an imaginary momentum (yielding exponentially decaying probability of finding the particle) in the outside regions. More precisely, in the 3 regions we find:

$$\begin{array}{lll}\text{Region I} & \text{Region II} & \text{Region III}\\ k'=i\kappa, & k=\sqrt{\frac{2m(V_H+E_2)}{\hbar^2}} & k'=i\kappa\\ \kappa=\sqrt{\frac{-2mE_2}{\hbar^2}}=\sqrt{\frac{2mE}{\hbar^2}} & =\sqrt{\frac{2m(V_H-E)}{\hbar^2}} & \kappa=\sqrt{\frac{2mE}{\hbar^2}}\end{array}$$

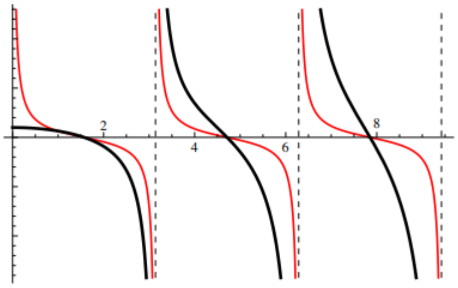


Figure 4.1.5: cot z (Red) and z cot z (Black) (CC BY-NC-ND; Paola Cappellaro)

And the wavefunction is

$$\begin{array}{ccc}\text{Region I} & \text{Region II} & \text{Region III}\\ C'e^{-\kappa|x|} & A'e^{ikx}+B'e^{-ikx} & D'e^{-\kappa x}\end{array}$$

(Notice that in the first region I can write either $C'e^{-\kappa|x|}$ or $C'e^{\kappa x}$. The first notation makes it clear that we have an exponential decay). We now want to match the boundary conditions in order to find the coefficients. Also, we remember from the infinite well that the boundary conditions gave us not the coefficient A, B but a condition on the allowed values of the energy. We expect something similar here, since the infinite case is just a limit of the present case.

First we note that the potential is an even function of x. The differential operator is also an even function of x. Then the solution has to either be odd or even for the equation to hold. This means that A and B have to be chosen so that $\psi(x)=A'e^{ikx}+B'e^{-ikx}$ is either even or odd. This is arranged by setting $\psi(x)=A\cos(kx)$ [even solution] or $\psi(x)=A\sin(kx)$ [odd solution]. Here I choose the odd solution, $\psi(-x)=-\psi(x)$. That also sets $C'=-D'$ and we rewrite this constant as $-C'=D'=C$.

We then have:

$$\begin{array}{ccc}\text{Region I} & \text{Region II} & \text{Region III}\\ \psi(x)=-Ce^{\kappa x} & \psi(x)=A\sin(kx) & \psi(x)=Ce^{-\kappa x}\\ \psi'(x)=-\kappa Ce^{\kappa x} & \psi'(x)=kA\cos(kx) & \psi'(x)=-\kappa Ce^{-\kappa x}\end{array}$$

Since we know that $\psi(-x)=-\psi(x)$ (odd solution) we can consider the boundary matching condition only at x = a.

The two equations are:

$$\begin{cases}A\sin(ka)=Ce^{-\kappa a}\\ Ak\cos(ka)=-\kappa Ce^{-\kappa a}\end{cases}$$

Substituting the first equation into the second we find: $Ak\cos(ka)=-\kappa A\sin(ka)$. Then we obtain an equation not for the coefficient A (as it was the case for the infinite well) but a constraint on the eigenvalues k and κ:

$$\boxed{\kappa=-k\cot(ka)}$$

This is a condition on the eigenvalues that allows only a subset of solutions. This equation cannot be solved analytically, we thus search for a solution graphically (it could be done of course numerically!).

To do so, we first make a change of variable, multiplying both sides by a and setting $ka = z, \kappa a = z_1$. Notice that $z_1^2 = \frac{2mE}{\hbar^2}a^2$ and $z^2 = \frac{2m(V_H-E)}{\hbar^2}a^2$. Setting $z_0^2 = \frac{2mV_Ha^2}{\hbar^2}$, we have $z_1^2 = z_0^2 - z^2$ or $\kappa a = \sqrt{z_0^2 - z^2}$. Then we can

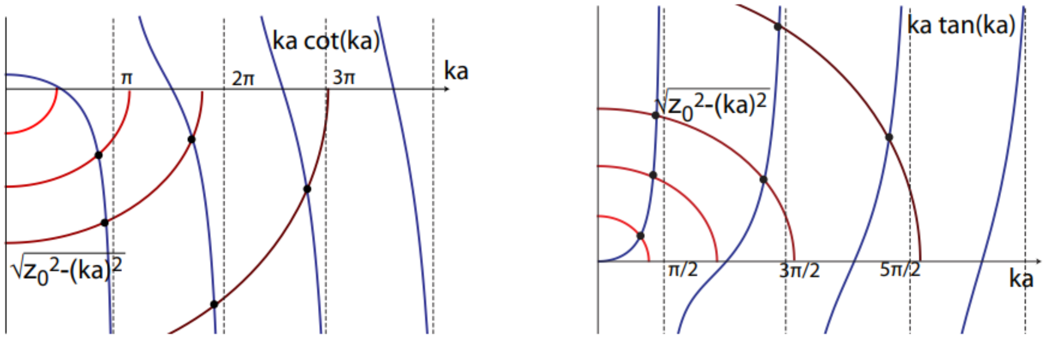


Figure 4.1.6: Graphic solution of the eigenvalue equation. Left: **odd** solutions; Right: **even** solutions. The red curves of different tone are the function $-\sqrt{z_0^2 - z^2}$ (left) or $\sqrt{z_0^2 - z^2}$ (right) for different (increasing) values of z_0. Crossings (solutions) are marked by a black dot. (CC BY-NC-ND; Paola Cappellaro)

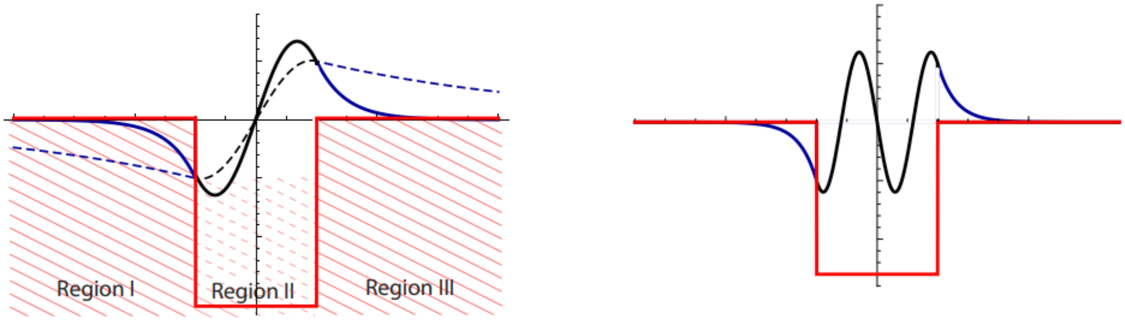


Figure 4.1.7: Left: Odd solution for the finite barrier potential, for two potential depth. Ground state of the wavefunction. The wavefunction is a sinusoidal in Region II (Black) and an exponential decay in regions I and III (Blue). Notice that for the shallower potential (dashed lines) the wavefunction just barely “fit” inside the well. Right: Odd solution, for larger k vector (higher quantum number), allowing two oscillations. (CC BY-NC-ND; Paola Cappellaro)

rewrite the equation $\kappa a = -ka\cot(ka) \rightarrow z_1 = -z\cot(z)$ as $\sqrt{z_0^2 - z^2} = -z\cot(z)$, or:

$$\sqrt{z_0^2 - z^2} = -z\cot(z)$$

This is a transcendental equation for z (and hence E) as a function of z_0, which gives the depth of the well (via V_H). To find solutions we plot both sides of the equation and look for crossings. That is, we plot $y_1(z) = -\sqrt{z_0^2 - z^2}$, which represent a quarter circle (as z is positive) of radius $z_0 = \sqrt{\frac{2mV_Ha^2}{\hbar^2}}$ and $y_2(z) = z\cot(z)$.

Observation 1

The coefficient A (and thus C and D) can be found (once the eigenfunctions have been found numerically or graphically) by imposing that the eigenfunction is normalized.

Observation 2

Notice that the first red curve never crosses the blue curves. That means that there are no solutions. If $z_0 < \pi/2$ there are no solutions (That is, if the well is too shallow there are no bound solutions, the particle can escape). Only if $V_H > \frac{\hbar^2}{ma^2}\frac{\pi^2}{8}$ there’s a bound solution.

Observation 3

There’s a finite number of solutions, given a value of $z_0 > \pi/2$. For example, for $\pi/2 \leq z_0 \leq 3\pi/2$ there’s only one solution, 2 for $3\pi/2 \leq z_0 \leq 5\pi/2$, etc.

Remember however that we only considered the *odd* solutions. A bound solution is always possible if we consider the even solutions., since the equation to be solved is

$$\kappa a = ka \tan(ka) = \sqrt{z_0^2 - z^2}.$$

Importantly, we found that for the odd solution there is a minimum size of the potential well (width and depth) that supports bound states. How can we estimate this size? A bound state requires a negative total energy, or a kinetic energy smaller than the potential: $E_{kin} = \frac{\hbar^2 k^2}{2m} < V_H$. This poses a constraint on the wavenumber k and thus the wavelength, $\lambda = \frac{2\pi}{k}$.

$$\lambda \geq \frac{2\pi\hbar}{\sqrt{2mV_H}}$$

However, in order to satisfy the boundary conditions (that connect the oscillating wavefunction to the exponentially decay one) we need to *fit* at least half of a wavelength inside the $2a$ width of the potential, $\frac{1}{2}\lambda \leq 2a$. Then we obtain

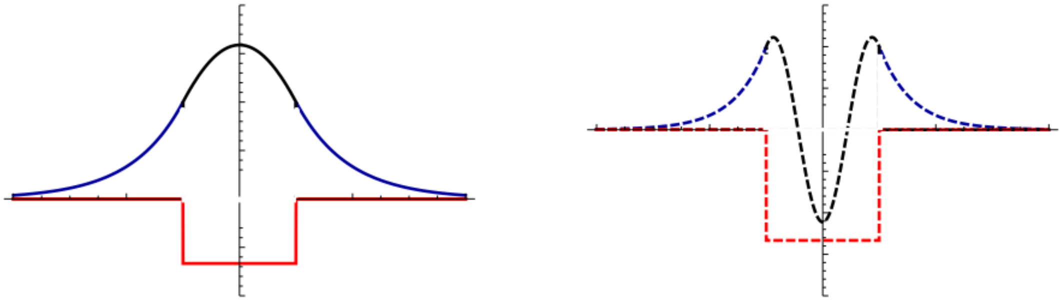


Figure 4.1.8: Even solution for the finite barrier potential. The wavefunction is $\propto \cos(kx)$ in Region II (Black) and an exponential decay in regions I and III (Blue). Left: any wavefunction can “fit” in the well and satisfy the boundary condition (there’s no minimum well depth and width). Right, wavefunction with a higher quantum number, showing two oscillations a relationship between the minimum potential depth and width

$$\frac{2\pi\hbar}{\sqrt{2mV_H}} \leq \lambda \leq 4a \quad \rightarrow \quad V_H \geq \frac{\hbar^2}{ma^2}\frac{\pi^2}{8}$$

Although we solved a 1D problem, the square well represents a 3D problem as well. Consider for example a spherical well in 3D: The potential is zero inside a region of radius a and is V_H for r > a. Then we can rewrite the timeindependent Schrödinger equation in 3D for this potential in spherical coordinates and use separation of variables $(\{r, \vartheta, \varphi\})$. Because of symmetry, the wavefunction is a constant in ϑ and φ, thus we will have to solve just a single differential equation for the radial variable, very similar to what found here. We must then choose the odd-parity solution in order to obtain a finite wavefunction at r = 0. Thus in 3D, only the odd solutions are possible and we need a minimum potential well depth in order to find a bound state. (CC BY-NC-ND; Paola Cappellaro)

4.2: Quantum Mechanics in 3D - Angular momentum

Schrödinger equation in spherical coordinates

We now go back to the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V(x,y,z)\right)\psi(x)=E\psi(x)$$

We have already studied some solutions to this equations – for specific potentials in *one dimension*. Now we want to solve QM problems in 3D. Specifically, we look at 3D problems where the potential $V(\vec{x})$ is isotropic, that is, it only depends on the distance from the origin. Then, instead of using cartesian coordinates $\vec{x}=\{x,y,z\}$, it is convenient to use spherical coordinates $\vec{x}=\{r,\vartheta,\varphi\}$:

$$\left\{\begin{array}{l} x=r\sin\vartheta\cos\varphi \\ y=r\sin\vartheta\sin\varphi \\ x=r\cos\vartheta \end{array}\right. \Leftrightarrow \left\{\begin{array}{l} r=\sqrt{x^2+y^2+z^2} \\ \vartheta=\arctan\left(z/\sqrt{x^2+y^2}\right) \\ \varphi=\arctan(y/x) \end{array}\right.$$

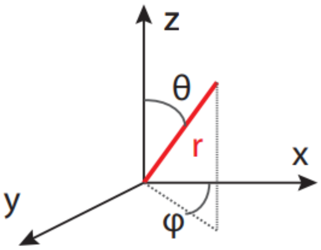


Figure 4.2.1: Spherical Coordinates (CC BY-NC-ND; Paola Cappellaro)

First, we express the Laplacian ∇^2 in spherical coordinates:

$$\nabla^2=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right)+\frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$$

To look for solutions, we use again the separation of variable methods, writing $\psi(\vec{x})=\psi(r,\vartheta,\varphi)=R(r)Y(\vartheta,\varphi)$:

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{R}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right)+\frac{R}{r^2\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2}\right]+V(r)RY=ERY$$

We then divide by RY/r^2 and rearrange the terms as

$$-\frac{\hbar^2}{2m}\left[\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\right]+r^2(V-E)=\frac{\hbar^2}{2mY}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2}\right]$$

Each side is a function of r only and ϑ,φ, so they must be independently equal to a constant C that we set (for reasons to be seen later) equal to $C=-\frac{\hbar^2}{2m}l(l+1)$. We obtain two equations:

$$\boxed{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{2}(V-E)=l(l+1)}$$

and

$$\boxed{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2}=-l(l+1)Y}$$

This last equation is the angular equation. Notice that it can be considered an eigenvalue equation for an operator $\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$. What is the meaning of this operator?

Angular momentum operator

We take one step back and look at the angular momentum operator. From its classical form $\vec{L}=\vec{r}\times\vec{p}$ we can define the QM operator:

$$\hat{\vec{L}}=\hat{\vec{r}}\times\hat{\vec{p}}=-i\hat{\vec{r}}\times\hat{\vec{\nabla}}$$

In cartesian coordinates this reads

$$\begin{aligned}\hat{L}_x&=\hat{y}\hat{p}_z-\hat{p}_y\hat{z}=-i\hbar\left(y\frac{\partial}{\partial z}-\frac{\partial}{\partial y}z\right)\\ \hat{L}_y&=\hat{z}\hat{p}_x-\hat{p}_z\hat{x}=-i\hbar\left(z\frac{\partial}{\partial x}-\frac{\partial}{\partial z}x\right)\\ \hat{L}_z&=\hat{x}\hat{p}_y-\hat{p}_x\hat{y}=-i\hbar\left(z\frac{\partial}{\partial y}-\frac{\partial}{\partial x}y\right)\end{aligned}$$

Some very important properties of this vector operator regard its commutator. Consider for example $\left[\hat{L}_x,\hat{L}_y\right]$:

$$\left[\hat{L}_x,\hat{L}_y\right]=\left[\hat{y}\hat{p}_z-\hat{p}_y\hat{z},\hat{z}\hat{p}_x-\hat{p}_z\hat{x}\right]=\left[\hat{y}\hat{p}_z,\hat{z}\hat{p}_x\right]-\left[\hat{p}_y\hat{z},\hat{z}\hat{p}_x\right]-\left[\hat{y}\hat{p}_z,\hat{p}_z\hat{x}\right]+\left[\hat{p}_y\hat{z},\hat{p}_z\hat{x}\right]$$

Now remember that $[x_i,x_j]=[p_i,p_j]=0$ and $[x_i,p_j]=i\delta_{ij}$. Also $[AB,C]=A[B,C]+[A,C]B$. This simplifies matters a lot

$$\left[\hat{L}_x,\hat{L}_y\right]=\hat{y}\left[\hat{p}_z,\hat{z}\right]\hat{p}_x-\cancel{\left[\hat{p}_y\hat{z},\hat{z}\hat{p}_x\right]}-\cancel{\left[\hat{y}\hat{p}_z,\hat{p}_z\hat{x}\right]}+\hat{p}_y\left[\hat{z},\hat{p}_z\right]\hat{x}=i\hbar\left(\hat{x}\hat{p}_y-\hat{y}\hat{p}_x\right)=i\hbar\hat{L}_z$$

By performing a cyclic permutation of the indexes, we can show that this holds in general:

$$\boxed{\left[\hat{L}_a,\hat{L}_b\right]=i\hbar\hat{L}_c}$$

Obs

Since the different components of the angular momentum do not commute, they do not possess common eigenvalues and there is an uncertainty relation for them. If for example I know with absolute precision the angular momentum along the z direction, I cannot have any knowledge of the components along x and y.

Exercise 4.2.1

What is the uncertainty relation for the x and y components?

$$\Delta L_x\Delta L_y\geq\frac{\hbar}{2}|\langle L_z\rangle|$$

Exercise 4.2.2

Assume we know with certainty the angular momentum along the z direction. What is the uncertainty in the angular momentum in the x and y directions?

Answer

From the uncertainty relations, $\Delta L_x\Delta L_z\geq\frac{\hbar}{2}|\langle L_y\rangle|$ and $\Delta L_y\Delta L_z\geq\frac{\hbar}{2}|\langle L_x\rangle|$, we have that if $\Delta L_z=0$ (perfect knowledge) then we have a complete uncertainty in L_x and L_y.

Obs.

Consider the squared length of the angular momentum vector $\hat{L}^2=\hat{L}_x^2+\hat{L}_y^2+\hat{L}_z^2$. We can show that $\left[\hat{L}_a,\hat{L}^2\right]=0$ (for $a=\{x,y,z\}$). Thus we can always know the length of the angular momentum plus one of its components.

> For example, choosing the z-component, we can represent the angular momentum as a cone, of length $\langle L\rangle$, projection on the z-axis $\langle L_z\rangle$ and with complete uncertainty of its projection along x and y.

We now express the angular momentum using spherical coordinates. This simplifies particularly how the azimuthal angular momentum $\hat{L}_z$ is expressed:

$$\hat{L}_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\vartheta} + \cot\vartheta\cos\varphi\frac{\partial}{\partial\varphi}\right),$$

$$\hat{L}_y = -i\hbar\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right),$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}$$

The form of $\hat{L}^2$ should be familiar:

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right]$$

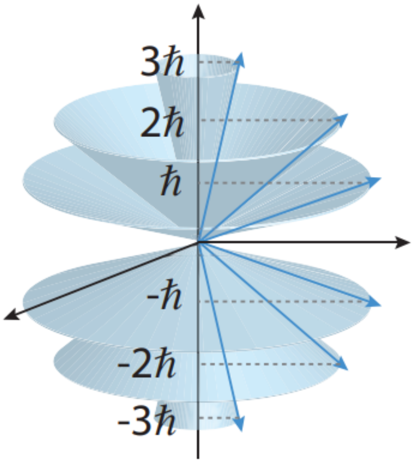


Figure 4.2.2: Graphical representation of the angular momentum, with fixed L_z and L^2, but complete uncertainty in L_x and L_y. (CC BY-NC-ND; Paola Cappellaro)

as you should recognize the angular part of the 3D Schrödinger equation. We can then write the eigenvalue equations for these two operators:

$$\hat{L}^2\Phi(\vartheta,\varphi) = \hbar^2 l(l+1)\Phi(\vartheta,\varphi)$$

and

$$\hat{L}_z\Phi(\vartheta,\varphi) = \hbar m_z\Phi(\vartheta,\varphi)$$

where we already used the fact that they share common eigenfunctions (then, we can label these eigenfunctions by l and $m_z : \Phi_{l,m_z}(\vartheta,\varphi)$.

The allowed values for l and m_z are integers such that $l = 0, 1, 2, \ldots$ and $m_z = -l, \ldots, l-1, l$. This result can be inferred from the commutation relationship. For interested students, the derivation is below.

Derivation of the eigenvalues. Assume that the eigenvalues of L^2 and L_z are unknown, and call them λ and μ. We introduce two new operators, the raising and lowering operators $L_+ = L_x + iL_y$ and $L_- = L_x - iL_y$. The commutator with L_z is $[L_z, L_\pm] = \pm\hbar L_\pm$ (while they of course commute with L^2). Now consider the function $f_\pm = L_\pm f$, where f is an eigenfunction of L^2 and L_z:

$$L^2 f_\pm = L_\pm L^2 f = L_\pm\lambda f = \lambda f_\pm$$

and

$$L_z f_\pm = [L_z, L_\pm] f + L_\pm L_z f = \pm\hbar L_\pm f + L_\pm \mu f = (\mu \pm \hbar) f_\pm$$

Then $f_\pm = L_\pm f$ is also an eigenfunction of L^2 and L_z. Furthermore, we can keep finding eigenfunctions of L_z with higher and higher eigenvalues $\mu' = \mu + \hbar + \hbar + \ldots$, by applying the L_+ operator (or lower and lower with L_-), while the L^2 eigenvalue is fixed. Of course there is a limit, since we want $\mu' \leq \lambda$. Then there is a maximum eigenfunction such that $L_+ f_M = 0$ and we set the corresponding eigenvalue to $\hbar l_M$. Now notice that we can write L^2 instead of by using $L_{x,y}$ by using $L_\pm$:

$$L^2 = L_- L_+ + L_z^2 + \hbar L_z$$

Using this relationship on f_M we find:

$$L^2 f_m = \lambda f_m \quad \rightarrow \quad \left(L_- L_+ + L_z^2 + \hbar L_z\right) f_M = \left[0 + \hbar^2 l_M^2 + \hbar\left(\hbar l_M\right)\right] f_M \quad \rightarrow \quad \lambda = \hbar^2 l_M \left(l_M + 1\right)$$

In the same way, there is also a minimum eigenvalue l_m and eigenfunction s.t. $L_- f_m = 0$ and we can find $\lambda = \hbar^2 l_m \left(l_m - 1\right)$. Since λ is always the same, we also have $l_m \left(l_m - 1\right) = l_M \left(l_M + 1\right)$, with solution $l_m = -l_M$ (the other solution would have $l_m > l_M$). Finally we have found that the eigenvalues of L_z are between $+\hbar l$ and $-\hbar l$ with integer increases, so that $l = -l + N$ giving l = N/2: that is, l is either an integer or an half-integer. We thus set $\lambda = \hbar^2 l(l+1)$ and $\mu = \hbar m, m = -l, -l+1, \ldots, l$. □

We can gather some intuition about the eigenvalues if we solve first the second equation, finding

$$-i\hbar \frac{\partial \Phi_{l,m}}{\partial \varphi} = \hbar m_z \Phi(\vartheta, \varphi), \quad \Phi_{l,m}(\vartheta, \varphi) = \Theta_l(\vartheta) e^{i m_z \varphi}$$

where, because of the periodicity in φ, m_z can only take on integer values (positive and negative) so that $\Phi_{lm}(\vartheta, \varphi + 2\pi) = \Phi_{lm}(\vartheta, \varphi)$.

If we solve the first equation, we would find for each eigenvalue l there are many eigenfunctions. What is the degeneracy of the eigenvalue l? We know that given l, m_z can take many values (between $-l$ and l), in particular $2l$ + 1 values. This is the degeneracy of l.

Exercise 4.2.3

What are the possible values of $\hat{L}_x$ if l = 7 and m_z = 5?

We know that we can define quantum numbers $m_{x(y)}$ such that they take integer numbers $m_{x(y)} = -l, \ldots, l-1, l$. Also, we have the relation among the expectation values:

$$\left\langle \hat{L}^2 \right\rangle = \left\langle \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \right\rangle \rightarrow l(l+1) = m_z^2 + \left\langle \hat{L}_x^2 + \hat{L}_y^2 \right\rangle / \hbar^2$$

so in general

$$\left\langle \hat{L}_x^2 \right\rangle \leq \hbar^2 \left[l(l+1) - m_z^2 \right]$$

Then here we have

$$\left\langle \hat{L}_x^2 \right\rangle \leq \hbar^2 (56 - 25) = 31\hbar^2$$

If $\hat{L}_x$ could only take its maximum value (with probability one) we would have $\left\langle \hat{L}_x^2 \right\rangle = \sum P_i L_{x,i}^2 = L_{x,\max}^2$ thus we have $L_{x,\max} \leq 5\hbar$ (with 5 the closest integer to $\sqrt{31}$). Often, because of symmetry, we have $\left\langle \hat{L}_x^2 \right\rangle = \left\langle \hat{L}_y^2 \right\rangle$ and,

$$\left\langle \hat{L}_x^2 \right\rangle = \hbar^2 \left[l(l+1) - m_z^2 \right] / 2$$

thus restricting even further the maximum value of L_x.

Spin angular momentum

The quantization of angular momentum gave the result that the angular momentum quantum number was defined by integer values. There is another quantum operator that has the same commutation relationship as the angular momentum but has no classical counterpart and can assume half-integer values. It is called the intrinsic spin angular momentum $\hat{\vec{S}}$ (or for short, spin). Because it is not a classical properties, we cannot write spin in terms of position and momentum operator. The spin is defined in an abstract spin space (not the usual phase space). Every elementary particle has a specific and immutable value of the intrinsic spin quantum number s (with s determining the eigenvalues of $\hat{\vec{S}}^2, \hbar^2 s(s+1)$), which we call the spin of that particular species: pi mesons have spin 0; electrons have spin 1/2; photons have spin 1; gravitons have spin 2; and so on. By contrast, the orbital angular momentum quantum number l of a particle can a priori take on any (integer) value, and l will change when the system is perturbed.

The eigenvectors of the spin operators are not spherical harmonics. Actually, since the spin is not defined in terms of position and momentum, they are not a function of position and are not defined on the usual phase space. The eigenstates are instead described by linear vectors, for example, two-dimensional vectors for the spin-$\frac{1}{2}$. Thus the operators will be as well represented by matrices.

We already saw the operators describing the spin-$\frac{1}{2}$ operators and we even calculated their eigenvalues and eigenvectors (see section 2.2).

We can then also define the total angular momentum, which is the sum of the usual angular momentum (called the *orbital* angular momentum) and the spin:

$$\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$$

What is the meaning of the sum of two angular momentum operators and what are the eigenvalues and eigenfunctions of the resulting operators?

Addition of angular momentum

We have seen above that any elementary particle posses an intrinsic spin. Then, we can always define the total angular momentum as the sum of the orbital angular momentum and the intrinsic spin. This is an example of addition of angular momentum. Then of course we could also consider two distinct particles and ask what is the total orbital angular momentum of the two particles (or of more particles). There are thus many cases of addition of angular momentum, for example:

1. $\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$
2. $\hat{\vec{L}} = \hat{\vec{L}}_1 + \hat{\vec{L}}_2$
3. $\hat{\vec{J}} = \hat{\vec{J}}_1 + \hat{\vec{J}}_2 = \hat{\vec{L}}_1 + \hat{\vec{S}}_1 + \hat{\vec{L}}_2 + \hat{\vec{S}}_2$
4. $\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2 + \hat{\vec{S}}_3$
5. ...

Consider for example the second case. A possible state of the two particles can be described by the eigenvalues/eigenfunctions of each particle angular momentum. For example we could specify l_1 and m_z^1 as well as l_2 and m_z^2 (I will from now on just write m_1 and m_z^1 etc.). Then a state could be for example written in Dirac's notation as $|l_1, m_1, l_2, m_2\rangle$. This however does not tell us anything about the total system and its angular momentum. Sometime this quantity is more interesting (for example if the two particles are interacting, their total angular momentum is bound to determine their energy, and not the state of each particle alone).

Coupled and uncoupled representations

The sum of angular momentum satisfy the general commutation rules, $[L^2, L_z] = 0, [L_x, L_y] = iL_z$ etc. We can then also define the eigenvalues (and eigenfunctions) of the total angular momentum $\hat{\vec{L}}$, for example l (for L^2) and m (for L_z). However, since we only have 2 quantum numbers, we expect the eigenfunctions to be degenerate and we still need to find two more quantum numbers. Equivalently, what we need to do is to find a complete set of commuting observables, such that an eigenfunction (common to all these observables) is well defined –no ambiguity in it– by the set of eigenvalues (or quantum numbers) of the observables.

The first question we can ask is : are these eigenfunctions going to be in common with the single particle operators? To determine this, we need to look at the commutation of the operators.

Now we know that $[L_1^2, L_{z,1}] = 0$, but what about $[L^2, L_{z,1}]$?

We first express L^2 explicitly: $L^2 = \left|\hat{\vec{L}}_1 + \hat{\vec{L}}_2\right|^2 = L_1^2 + L_2^2 + 2\hat{\vec{L}}_1 \cdot \hat{\vec{L}}_2$. Then the commutator is:

$$\left[L^2, L_{z,1}\right] = \left[L_1^2 + L_2^2 + 2\left(L_{x,1}L_{x,2} + L_{y,1}L_{y,2} + L_z^1 L_z^2\right), L_{z,1}\right]$$

$$= \left[2\left(L_{x,1}L_{x,2} + L_{y,1}L_{y,2}\right), L_{z,1}\right] = 2i\left(\left(L_{y,1}L_{x,2} - L_{x,1}L_{y,2}\right) \neq 0\right.$$

Thus the two operators do not commute and do not share common eigenfunctions. What about L_1^2?

$$\left[L^2, L_1^2\right] = \left[L_1^2 + L_2^2 + 2\left(L_{x,1}L_{x,2} + L_{y,1}L_{y,2} + L_z^1 L_z^2\right), L_1^2\right] = 0$$

since $\left[L_1^2, L_{a,1}\right] = 0$. This means that there are common eigenfunctions of L_1^2, L_2^2, L^2 and L_z. These operators are a complete set of commuting observables. An eigenfunction is thus well defined by the set of eigenvalues l, m, l_1 and l_2 and we can write the eigenstates as $\psi_{l,m,l_\mathrm{i},l_2}$ or $|l, m, l_1, l_2\rangle$.

There are then two possible representations of the combined system (two possible basis to represent a general state):

Representation	**Eigenstates**	**Complete set of commuting observables**
Uncoupled	$\|l_1, m_1, l_2, m_2\rangle$,	$L_1^2, L_2^2, L_{1,z}$ and $L_{2,z}$
Coupled	$\|l, m, l_1, l_2\rangle$,	L_1^2, L_2^2, L^2 and L_z

How do we go from one basis to the other? As usual this is done by expressing each vector in one basis as a linear combination of vectors in the other basis:

$$|l, m, l_1, l_2\rangle = \sum_{m_1, m_2} c_{m_1, m_2}^l |l_1, m_1, l_2, m_2\rangle$$

Notice that since the total angular momentum in the z direction must be m, we limit the sum to terms s.t. $m_1 + m_2 = m$.

What are the coefficients c_{m_1,m_2}^l?

Since the two representations are two orthogonal basis, we have that $\langle l_1', m_1', l_2', m_2' \mid l_1, m_1, l_2, m_2\rangle = 0$ unless all the indexes are equal. Then the coefficient can be calculated (as usual!) from the inner product of $|l_1, m_1, l_2, m_2\rangle$ and $|l, m, l_1, l_2\rangle$:

$$c_{m_1,m_2}^l = \langle l_1, m_1, l_2, m_2 \mid l, m, l_1, l_2\rangle$$

These coefficients are called the **Clebsch-Gordon** coefficients.

Addition rules: Two particles

In describing the energy levels of atoms and nuclei it is very convenient to be able to find the allowed values of (l, m) given the values of (l_1, l_2) for two given particles (e.g. electrons, protons or neutrons). Indeed, we saw that the operator $\hat{L}^2$ appears in the Hamiltonian of the system. Thus its eigenvalue $\hbar^2 l(l+1)$ will be important in determining the system energy.

Even if we cannot fix the value of l if we only know l_1, m_1, l_2 and m_2 we can at least restrict the possible values of l. In order to do so, one has to analyze the possible maximum length of the total angular momentum and the degeneracy of the eigenvalues.

1. **Maximum** l: For two particles with quantum numbers l_1 and l_2 we know that in the coupled representation we cannot fix the values of m_1 and m_2. However, we know that given l_1 and l_2 only some values of m_1 and m_2 are allowed (e.g. $m_1 = -l_1, -l_1 + 1, \ldots, l_1$. Then the maximum values of m_1 and m_2 are $m_1 = l_1$ and $m_2 = l_2$. This also determines the maximum value of $m : m_{\max} = l_1 + l_2$. But m itself can only take values $m = -l, \ldots, l-1, l$.
   Then the maximum value of l is $m_{\max} = l_{\max}$.
   Thus, what we just proved is that $l \leq l_1 + l_2$.
2. **Minimum** l: To find the minimum l value we need to look at the degeneracy of the state $|l, m, l_1, l_2\rangle$. Since this state could be also written (in the uncoupled representation) as $\sum_{m_1+m_2=m} c_{m_1,m_2}^l |l_1, m_1, l_2, m_2\rangle$, the degeneracy of the state must be the same. What are the two degeneracies?
   We know that for a given angular momentum operator $\hat{L}$ with total angular momentum quantum number l, there are 2l + 1 states with the same angular momentum $\hbar^2 l(l+1)$.
   Then, considering the uncoupled representation we have $\mathcal{D} = (2l_1 + 1)(2l_2 + 1)$ possible states with l_1 and l_2. In the coupled representation instead we have to consider all the states that have an allowed $l : \mathcal{D} = \sum_{l=l_{\min}}^{l_1+l_2} (2l+1)$. We want these two

quantities to be equal. Now remember that $\sum_{k=1}^{K} k = \frac{K(K+1)}{2}$. Then $\sum_{l=l_{min}}^{l_1+l_2}(2l+1) = (1+l_1+l_2)^2 - l_{\min}^2$, so that $l_{\min}^2 = (1+l_1+l_2)^{\ 2} - (2l_1+1)(2l_2+1) = (l_1-l_2)^{\ 2}$.
Using the degeneracy condition we thus proved that $l \geq |l_1 - l_2|$.

The addition rule states thus that

$$\boxed{\text{The total angular momentum quantum number is bounded by } |l_1 - l_2| \leq l \leq l_1 + l_2}$$

✓ Example 4.2.1

Consider two spins-1/2 particles (for example two electrons with zero orbital angular momentum). Since we choose spin-$\frac{1}{2}$ we have only 1 possible value s = $\frac{1}{2}$ and two values for $m_z : m_z = \pm\frac{1}{2}$. We can omit writing explicitly the s quantum number (since it's always $\frac{1}{2}$, and we write $\left|+\frac{1}{2},+\frac{1}{2}\right\rangle = \left|+\frac{1}{2}\right\rangle$ and $\left|+\frac{1}{2},-\frac{1}{2}\right\rangle = \left|-\frac{1}{2}\right\rangle$. A basis for the uncoupled representation is then given by:

$$|s_1, m_1, s_2, m_2\rangle = \begin{cases} \left|+\frac{1}{2},+\frac{1}{2},+\frac{1}{2},+\frac{1}{2}\right\rangle = \left|+\frac{1}{2},+\frac{1}{2}\right\rangle \\ \left|+\frac{1}{2},+\frac{1}{2},+\frac{1}{2},-\frac{1}{2}\right\rangle = \left|+\frac{1}{2},-\frac{1}{2}\right\rangle \\ \left|+\frac{1}{2},-\frac{1}{2},+\frac{1}{2},+\frac{1}{2}\right\rangle = \left|-\frac{1}{2},+\frac{1}{2}\right\rangle \\ \left|+\frac{1}{2},-\frac{1}{2},+\frac{1}{2},-\frac{1}{2}\right\rangle = \left|-\frac{1}{2},-\frac{1}{2}\right\rangle \end{cases}$$

Consider now the coupled representation. The possible values for s are 1 or 0. In the first case, we have 3 possible values for m = −1, 0, 1. While the second only has m = 0. Again, since the values of s_1 and s_2 are fixed we do not write them:

$$|s, m, s_1, s_2\rangle = \begin{cases} 0, 0, \frac{1}{2}, \frac{1}{2}\rangle = |0, 0\rangle \\ 1, -1, \frac{1}{2}, \frac{1}{2}\rangle = |1, -1\rangle \\ 1, 0, \frac{1}{2}, \frac{1}{2}\rangle = |1, 0\rangle \\ 1, 1, \frac{1}{2}, \frac{1}{2}\rangle = |1, 1\rangle \end{cases}$$

In this particular example it is easy to calculate the Clebsch-Gordon coefficients and we find the relations between the two representations:

$$\begin{aligned} |0,0\rangle = &\quad \frac{\left|+\frac{1}{2},-\frac{1}{2}\right\rangle - \left|-\frac{1}{2},+\frac{1}{2}\right\rangle}{\sqrt{2}} \\ |1,-1\rangle = &\quad \left|-\frac{1}{2},-\frac{1}{2}\right\rangle \\ |1,0\rangle = &\quad \frac{\left|+\frac{1}{2},-\frac{1}{2}\right\rangle + \left|-\frac{1}{2},+\frac{1}{2}\right\rangle}{\sqrt{2}} \\ |1,1\rangle = &\quad \left|+\frac{1}{2},+\frac{1}{2}\right\rangle \end{aligned}$$

Addition rules: many particles

The addition rules can be generalized to many particles, by just repetitively applying the two-particle rules. We then find for N particles:

- $l_{\max} = \sum_{k=1}^{N} l_k$
- $l_{\min} = \max\{0, 2l_N - l_{\max}\}$

where l_N is the largest of the $\{l_k\}$.

4.3: Solutions to the Schrödinger Equation in 3D

We now go back to the Schrödinger equation in spherical coordinates and we consider the angular and radial equation separately to find the energy eigenvalues and eigenfunctions.

Angular Equation

The angular equation was found to be:

$$\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y_l^m(\vartheta,\varphi)}{\partial\vartheta}\right)+\frac{1}{\sin^2\vartheta}\frac{\partial^2 Y_l^m(\vartheta,\varphi)}{\partial\varphi^2}=-l(l+1)Y_l^m(\vartheta,\varphi)$$

Notice that this equation does not depend at all on the potential, thus it will be common to all problems with an isotropic potential.

We can solve the equation by using again separation of variables: $Y(\vartheta,\varphi)=\Theta(\vartheta)\Phi(\varphi)$. By multiplying both sides of the equation by $\sin^2(\vartheta)/Y(\vartheta,\varphi)$ we obtain:

$$\frac{1}{\Theta(\vartheta)}\left[\sin\vartheta\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)\right]+l(l+1)\sin^2\vartheta=-\frac{1}{\Phi(\varphi)}\frac{d^2\Phi}{d\varphi^2}$$

As usual we separate the two equations in the different variables and introduce a constant C = m^2:

$$\frac{d^2\Phi}{d\varphi^2}=-m^2\Phi(\varphi)$$

$$\sin\vartheta\frac{d}{d\vartheta}\left(\sin\vartheta\frac{d\Theta}{d\vartheta}\right)=\left[m^2-l(l+1)\sin^2\vartheta\right]\Theta(\vartheta)$$

The first equation is easily solved to give $\Phi(\varphi)=e^{im\varphi}$ with $m=0,\pm1,\pm2,\ldots$ since we need to impose the periodicity of Φ, such that $\Phi(\varphi+2\pi)=\Phi(\varphi)$.

The solutions to the second equations are associated Legendre Polynomials: $\Theta(\vartheta)=AP_l^m(\cos\vartheta)$, the first few of l which are in table 1. Notice that, as previously found when solving for the eigenvalues of the angular momentum, we have that $m=-l,-l+1,\ldots,l$, with l = 0, 1, ...

$_l\backslash^m$	0	1	2	3
0	$P_0^0=1$			
1	$P_1^0=\cos\vartheta$	$P_1^1=\sin\vartheta$		
2	$P_2^0=\frac{1}{2}(3\cos^2\vartheta-1)$	$P_2^1=3\cos\vartheta\sin\vartheta$	$P_2^2=3\sin^2\vartheta$	
3	$P_3^0=\frac{1}{2}(5\cos^3\vartheta-3\cos\vartheta)$	$P_3^1=\frac{3}{2}(5\cos^2\vartheta-1)\sin\vartheta$	$P_3^2=15\cos\vartheta\sin^2\vartheta$	$P_3^3=15\sin^3\vartheta$

Table 4.3.1: Legendre Polynomials

The normalized angular eigenfunctions are then Spherical Harmonic functions, given by the normalized Legendre polynomial times the solution to the equation in φ (see also Table 2)

$$Y_l^m(\vartheta,\varphi)=\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\vartheta)e^{im\varphi}$$

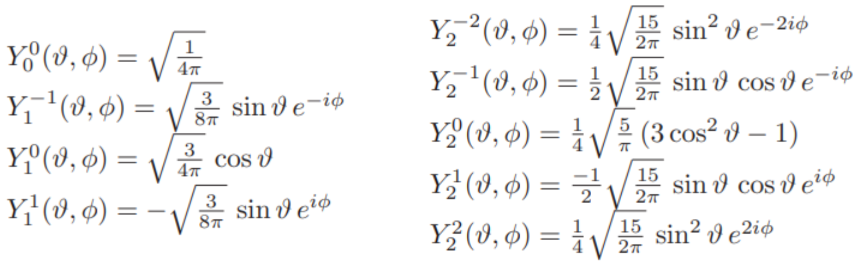
As we expect from eigenfunctions, the Spherical Harmonics are orthogonal:

$$\int_{4\pi}d\Omega Y_l^m(\vartheta,\varphi)Y_{l'}^{m'}(\vartheta,\varphi)=\delta_{l,l'}\delta_{m,m'}$$

The radial equation

We now turn to the radial equation:

$$\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)-\frac{2mr^2}{\hbar^2}(V-E)=l(l+1)R(r)$$



$$Y_0^0(\vartheta,\phi)=\sqrt{\frac{1}{4\pi}}$$
$$Y_1^{-1}(\vartheta,\phi)=\sqrt{\frac{3}{8\pi}}\,\sin\vartheta\,e^{-i\phi}$$
$$Y_1^0(\vartheta,\phi)=\sqrt{\frac{3}{4\pi}}\,\cos\vartheta$$
$$Y_1^1(\vartheta,\phi)=-\sqrt{\frac{3}{8\pi}}\,\sin\vartheta\,e^{i\phi}$$

$$Y_2^{-2}(\vartheta,\phi)=\frac{1}{4}\sqrt{\frac{15}{2\pi}}\,\sin^2\vartheta\,e^{-2i\phi}$$
$$Y_2^{-1}(\vartheta,\phi)=\frac{1}{2}\sqrt{\frac{15}{2\pi}}\,\sin\vartheta\,\cos\vartheta\,e^{-i\phi}$$
$$Y_2^0(\vartheta,\phi)=\frac{1}{4}\sqrt{\frac{5}{\pi}}\,(3\cos^2\vartheta-1)$$
$$Y_2^1(\vartheta,\phi)=\frac{-1}{2}\sqrt{\frac{15}{2\pi}}\,\sin\vartheta\,\cos\vartheta\,e^{i\phi}$$
$$Y_2^2(\vartheta,\phi)=\frac{1}{4}\sqrt{\frac{15}{2\pi}}\,\sin^2\vartheta\,e^{2i\phi}$$

Table 4.3.2: Spherical Harmonics

To simplify the solution, we introduce a different function $u(r)=rR(r)$. Then the equation reduces to:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[V+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u(r)=Eu(r)$$

This equation is very similar to the Schrödinger equation in 1D if we define an *effective potential* $V'(r)=V(r)+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$. The second term in this effective potential is called the **centrifugal** term.

Solutions can be found for some forms of the potential V (r), by first calculating the equation solutions $u_{n,l}(r)$, then finding $R_{n,l}(r)=u_{n,l}(r)/r$ and finally the wavefunction

$$\Psi_{n,l,m}(r,\vartheta,\varphi)=R_{n,l}(r)Y_l^m(\vartheta,\varphi).$$

Notice that we need 3 quantum numbers (n, l, m) to define the eigenfunctions of the Hamiltonian in 3D.

For example we can have a simple spherical well: V (r) = 0 for $r<r_0$ and $V(r)=V_0$ otherwise. In the case of l = 0, this is the same equation as for the square well in 1D. Notice however that since the boundary conditions need to be such that R(r) is finite for all r, we need to impose that $u(r=0)=0$, hence only the odd solutions are acceptable (as we had anticipated). For l > 0 we can find solutions in terms of Bessel functions.

Two other important examples of potential are the harmonic oscillator potential $V(r)=V_0\frac{r^2}{r_0^2}-V_0$ (which is an approximation for any potential close to its minimum) and the Coulomb potential $V(r)=-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$, which describes the atomic potential and in particular the Hydrogen atom.

The Hydrogen atom

We want to solve the radial equation for the Coulomb potential, or at least find the eigenvalues of the equation. Notice we are looking for bound states, thus the total energy is negative E < 0. Then we define the real quantity $\kappa=\sqrt{\frac{-2mE}{\hbar^2}}$, and the quantities[8]:

$$\text{Bohr radius: } a_0=\frac{4\pi\epsilon_0\hbar^2}{m_e e^2},\qquad \text{Rydberg constant:}\quad \mathbb{R}=\frac{\hbar^2}{2ma_0^2}$$

and $\lambda^2=\frac{\mathbb{R}}{|E|}$. The values of the two constants are $a_0=5.29\times10^{-11}\text{ m}$ and $\mathbb{R}=13.6\text{eV}$ (thus λ is a dimensionless parameter). The Bohr radius gives the distance at which the kinetic energy of an electron (classically) orbiting around the nucleus equals the Coulomb interaction: $\frac{1}{2}m_ev^2=\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$. In the semi-classical Bohr model, the angular momentum $L=m_evr$ is quantized, with lowest value $L=\hbar$, then by inserting in the equation above, we find $r=a_0$. We will see that the Rydberg energy gives instead the minimum energy for the hydrogen.

We further apply a change of variable$\rho=2\kappa r$, and we rewrite the radial equation as:

$$\frac{d^2u}{d\rho^2}=\left[\frac{1}{4}-\frac{\lambda}{\rho}+\frac{l(l+1)}{\rho^2}\right]u(\rho)$$

There are two limiting cases:

For $\rho\to0$, the equation reduces to $\frac{d^2u}{d\rho^2}=\frac{l(l+1)}{\rho^2}u$, with solution $u(\rho)\sim\rho^{l+1}$.

For $\rho \to \infty$ we have $\frac{d^2u}{d\rho^2} = \frac{u(\rho)}{4}$, giving $u(\rho) \sim e^{-\rho/2}$.

Note

8 Note that the definition of the Bohr radius is slightly different if the Coulomb potential is not expressed in SI units but in cgs units

A general solution can then be written as $u(\rho) = e^{-\rho/2}\rho^{l+1}S(\rho)$ (with S to be determined). We then expand $S(\rho)$ in series as $S(\rho) = \sum_{j=0}^{\infty} s_j \rho^j$ and try to find the coefficients s_j. By inserting $u(\rho) = e^{-\rho/2}\rho^{l+1}\sum_{j=0}^{\infty} s_j\rho^j$ in the equation we have:

$$\left[\rho\frac{d^2}{d\rho^2} + (2l+2-\rho)\frac{d}{d\rho} - (l+1-\lambda)\right] S(\rho) = 0$$

From which we obtain:

$$\sum_j \left[\rho\left\{j(j+1)s_{j+1}\rho^{j-1}\right\} + (2l+2-\rho)\left\{(j+1)s_{j+1}\rho^j\right\} - (l+1-\lambda)\left\{s_j\rho^j\right\}\right] = 0$$

(where the terms in brackets correspond to the derivatives of $S(\rho)$). This equation defines a recursive equation for the coefficients s_j:

$$s_{j+1} = \frac{j+l+1-\lambda}{j(j+1)+(2l+2)(j+1)} s_j$$

If we want the function $u(\rho)$ to be well defined, we must impose that $u(\rho) \to 0$ for $\rho \to \infty$. This imposes a maximum value for j, $j_{\max}$, such that all the higher coefficients $s_j > j_{\max}$ are zero.

Then we have that $j_{\max} + l + 1 - \lambda = 0$. But this is an equation for λ, which in turns determines the energy eigenvalue:

$$\lambda = j_{\max} + l + 1.$$

We then rename the parameter λ the principal quantum number n since it is an integer (as j and l are integers). Then the energy is given by $E = -\frac{\mathbb{R}}{n^2}$ and the allowed energies are given by the famous **Bohr formula**:

$$\boxed{E_n = -\frac{1}{n^2}\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2}$$

Obs.

Note that the energy is only determined by the principal quantum number. What is the degeneracy of the$n$quantum number? We know that the full eigenfunction is specified by knowing the angular momentum L^2 and one of its components (e.g. L_z). From the equation above, $n = j_{\max} + l + 1$, we see that for each n, l can vary from l = 0 to l =n− 1. Then we also have 2l + 1 m values for each l (and 2 spin states for each m). Finally, the degeneracy is then given by

$$\sum_{l=0}^{n-1} 2(2l+1) = 2n^2$$

Atomic periodic structure

We calculated the energy levels for the Hydrogen atom. This will give us spectroscopy information about the excited states that we can excite using, for example, laser light. How can we use this information to infer the structure of the atoms?

A neutral atom, of atomic number Z, consists of a heavy nucleus, with electric charge Ze, surrounded by Z electrons (mass m and charge -e). The Hamiltonian for this system is

$$\mathcal{H} = \sum_{j=1}^{Z}\left[-\frac{\hbar^2}{2m}\nabla_j^2 - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_j}\right] + \frac{1}{2}\frac{1}{4\pi\epsilon_0}\sum_{j\neq k}^{Z}\frac{e^2}{|\vec{r}_j - \vec{r}_k|}$$

The first term is simply the kinetic energy of each electron in the atom. The second term is the potential energy of the jth electron in the electric field created by the nucleus. Finally the last sum (which runs over all values of j and k except j = k) is the potential energy associated with the mutual repulsion of the electrons (the factor of 1/2 in front corrects for the fact that the summation counts each pair twice).

Given this Hamiltonian, we want to find the energy levels (and in particular the ground state, which will give us the stable atomic configuration). We then need to solve Schrödinger 's equation. But what would an eigenstate of this equation now be?

Consider for example Helium, an atom with only two electrons. Neglecting for the moment spin, we can write the wavefunction as $\Psi\left(\vec{r}_1, \vec{r}_2, t\right)$ (and stationary wavefunctions, $\psi\left(\vec{r}_1, \vec{r}_2\right)$), that is, we have a function of the spatial coordinates of both electrons. The physical interpretation of the wavefunction is a simple extension of the one-particle wavefunction: $\left|\psi\left(\vec{r}_1, \vec{r}_2\right)\right|^2 d^3\vec{r}_1 d^3\vec{r}_2$ is the probability of finding contemporaneously the two electrons at the positions $\vec{r}_1$ and $\vec{r}_2$, respectively. The wavefunction must then be normalized as $\int\left|\psi\left(\vec{r}_1, \vec{r}_2\right)\right|^2 d^3\vec{r}_1 d^3\vec{r}_2 = 1$. The generalization to many electrons (or more generally to many particles) is then evident.

To determine the ground state of an atom we will then have to solve the Schrödinger equation

$$\mathcal{H}\psi\left(\vec{r}_1, \ldots, \vec{r}_Z\right) = E\psi\left(\vec{r}_1, \ldots, \vec{r}_Z\right)$$

This equation has not been solved (yet) except for the case Z=1 of the Hydrogen atom we saw earlier. What we can do is to make a very crude approximation and ignore the Coulomb repulsion among electrons. Mathematically this simplifies tremendously the equation, since now we can simply use separation of variables to write many equations for each independent electron. Physically, this is often a good enough approximation because mutual repulsion of electron is not as strong as the attraction from all the protons. Then the Schrödinger equation becomes:

$$\sum_{j=1}^{Z}\left[-\frac{\hbar^2}{2m}\nabla_j^2 - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_j}\right]\psi\left(\vec{r}_1, \ldots, \vec{r}_Z\right) = E\psi\left(\vec{r}_1, \ldots, \vec{r}_Z\right)$$

and we can write $\psi\left(\vec{r}_1, \ldots, \vec{r}_Z\right) = \psi\left(\vec{r}_1\right)\psi\left(\vec{r}_2\right)\ldots\psi\left(\vec{r}_Z\right)$

Then, we can solve for each electron separately, as we did for the Hydrogen atom equation, and find for each electron the same level structure as for the Hydrogen, except that the since the potential energy is now $\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_j}$ the electron energy (Bohr's formula) is now multiplied by Z. The solutions to the time-independent Schrödinger equations are then the same eigenfunctions we found for the hydrogen atom, $\psi\left(\vec{r}_j = \psi_{lmn}(r, \vartheta, \varphi)\right.$.

Thus if we ignore the mutual repulsion among electrons, the individual electrons occupy one-particle hydrogenic states (n, l, m), called **orbitals**, in the Coulomb potential of a nucleus with charge Ze.

There are $2n^2$ hydrogenic wave functions (all with the same energy E_n) for a given value of n. Looking at the Periodic Table we see this periodicity, with two elements in the$n$= 1 shell, 8 in the$n$= 2 shell, 18 in the third shell. Higher shells however are more influenced by the electron-electron repulsion that we ignored, thus simple considerations from this model are no longer valid.

However, we would expect instead the electrons in the atoms to occupy the state with lowest energy. The ground state would then be a situation were all the electron occupy their own ground state (n = 0, l = 0, m = 0). But is this correct? This is not what is observed in nature, otherwise all the atom would show the same chemical properties. So what happens?

To understand, we need to analyze the statistical properties of identical particles. But before that, we will introduce the solution for another central potential, the harmonic oscillator potential $V(r) = V_0\frac{r^2}{r_0^2} - V_0$ (which is an approximation for any potential close to its minimum).

The Harmonic Oscillator Potential

The quantum h.o. is a model that describes systems with a characteristic energy spectrum, given by a ladder of evenly spaced energy levels. The energy difference between two consecutive levels is ΔE. The number of levels is infinite, but there must exist a minimum energy, since the energy must always be positive. Given this spectrum, we expect the Hamiltonian will have the form

$$\mathcal{H}|n\rangle = \left(n + \frac{1}{2}\right) \quad \omega|n\rangle,$$

where each level in the ladder is identified by a number n. The name of the model is due to the analogy with characteristics of classical h.o., which we will review first.

Classical harmonic oscillator and h.o. model

A classical h.o. is described by a potential energy $V=\frac{1}{2}kx^2$ (the radial potential considered above, $V(r)=V_0\frac{r^2}{r_0^2}-V_0$, has this form). If the system has a finite energy E, the motion is bound by two values $\pm x_0$, such that $V\left(x_0\right)=E$. The equation of motion is given by

$$\left\{\begin{array}{l}\frac{dx}{dt}=\frac{p(t)}{m}, \\ \frac{dp}{dt}=-kx\end{array}\right. \quad \rightarrow \quad m\frac{d^2x}{dx^2}=-kx\,,$$

and the kinetic energy is of course

$$T=\frac{1}{2}m\dot{x}^2=\frac{p^2}{2m}.$$

The energy is constant since it is a conservative system, with no dissipation. Most of the time the particle is in the position x_0 since there the velocity is zero, while at x = 0 the velocity is maximum.

The h.o. oscillator in QM is an important model that describes many different physical situations. It describes e.g. the electromagnetic field, vibrations of solid-state crystals and (a simplified model of) the nuclear potential. This is because any potential with a local minimum can be locally described by an h.o.. Provided that the energy is low enough (or x close to x_0), any potential can in fact be expanded in series, giving: $V(x)\approx V\left(x_0\right)+b\left(x-x_0\right)^2+\ldots$ where $b=\left.\frac{d^2V}{dx^2}\right|_{x_0}$.

It is easy to solve the equation of motion. Instead of just solving the usual equation, we follow a slightly different route. We define dimensionless variables,

$$P=\frac{p}{\sqrt{m\omega}}, \quad X=x\sqrt{m\omega}$$

where we defined a parameter with units of frequency: $\omega=\sqrt{k/m}$ and we introduce a complex classical variable (following Roy J. Glauber –Phys. Rev. 131, 2766–2788 (1963))

$$\alpha=\frac{1}{\sqrt{2}}(X+iP).$$

The classical equations of motion for x and p define the evolution of the variable α:

$$\left\{\begin{array}{l}\frac{dx}{dt}=\frac{p(t)}{m}, \\ \frac{dp}{dt}=-kx\end{array}\right. \quad \rightarrow \quad \frac{d\alpha}{dt}=-i\omega\alpha(t)$$

The evolution of α is therefore just a rotation in its phase space: $\alpha(t)=\alpha(0)e^{-i\omega t}$.

Since $X=\sqrt{2}\operatorname{Re}(\alpha)$ and $P=\sqrt{2}operatornameIm(\alpha), X$ and P oscillate, as usual in the classical case:

$$\begin{aligned}X&=\frac{1}{\sqrt{2}}\left(\alpha_0e^{-i\omega t}+\alpha_0^*e^{i\omega t}\right)\\ P&=\frac{-i}{\sqrt{2}}\left(\alpha_0e^{-i\omega t}-\alpha_0^*e^{i\omega t}\right)\end{aligned}$$

The classical energy, given by $\omega/2\left(X^2+P^2\right)=\omega\alpha_0^2$, is constant at all time.

Oscillator Hamiltonian: Position and momentum operators

Using the operators associated with position and momentum, the Hamiltonian of the quantum h.o. is written as:

$$\mathcal{H}=\frac{p^2}{2m}+\frac{kx^2}{2}=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2.$$

In terms of the dimensionless variables, P and X, the Hamiltonian is $\mathcal{H}=\frac{\omega}{2}\left(X^2+P^2\right)$.

In analogy with the classical variable a(t) [and its complex conjugate a*(t), which simplified the equation of motion, we introduce two operators, a, a†, hoping to simplify the eigenvalue equation (time-independent Schrödinger equation):

$$\begin{aligned} a &= \tfrac{1}{\sqrt{2\hbar}}(X+iP) = \tfrac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega}x + \tfrac{i}{\sqrt{m\omega}}p\right) \\ a^\dagger &= \tfrac{1}{\sqrt{2\hbar}}(X-iP) = \tfrac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega}x - \tfrac{i}{\sqrt{m\omega}}p\right), \end{aligned}$$

Also, we define the number operator as N = a†a, with eigenvalues n and eigenfunctions $|n\rangle$. The Hamiltonian can be written in terms of these operators. We substitute a, a† at the place of X and P, yielding $\mathcal{H} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) = \hbar\omega\left(N + \frac{1}{2}\right)$ and the minimum energy $\omega/2$ is called the zero point energy.

The commutation properties are: $\left[a, a^\dagger\right] = 1$ and $[N, a] = -a$, $\left[N, a^\dagger\right] = a^\dagger$. Also we have:

$$\begin{aligned} x &= \sqrt{\tfrac{\hbar}{2m\omega}}\left(a^\dagger + a\right) \\ p &= i\sqrt{\tfrac{m\omega\hbar}{2}}\left(a^\dagger - a\right) \end{aligned}$$

☐ Prove the commutation relationships of the raising and lowering operators.

$$\left[a, a^\dagger\right] = \frac{1}{2}[X+iP, X-iP] = \frac{1}{2}([X, -iP] + [iP, X]) = -\frac{i}{\hbar}[X, P] = -\frac{i}{\hbar}[x, p] = 1$$

So we also have $aa^\dagger = \left[a, a^\dagger\right] + a^\dagger a = 1 + a^\dagger a = 1 + N$.

$$[N, a] = \left[a^\dagger a, a\right] = \left[a^\dagger, a\right]a = -a \quad \text{and} \quad \left[N, a^\dagger\right] = \left[a^\dagger a, a^\dagger\right] = a^\dagger\left[a, a^\dagger\right] = a^\dagger$$

☐

From the commutation relationships we have:

$$a|n\rangle = [a, N]|n\rangle = an|n\rangle - Na|n\rangle \to N(a|n\rangle) = (n-1)(a|n\rangle),$$

that is, $a|n\rangle$ is also an eigenvector of the N operator, with eigenvalue (n − 1). Thus we confirm that this is the lowering operator: $a|n\rangle = c_n|n-1\rangle$. Similarly, $a^\dagger|n\rangle$ is an eigenvector of N with eigenvalue n + 1:

$$a^\dagger|n\rangle = \left[N, a^\dagger\right]|n\rangle = Na^\dagger|n\rangle - a^\dagger n|n\rangle \to N\left(a^\dagger|n\rangle\right) = (n+1)(a|n\rangle).$$

We thus have $a|n\rangle = c_n|n-1\rangle$ and $a^\dagger|n\rangle = d_n|n+1\rangle$. What are the coefficients c_n, d_n?

Since

$$\langle n|N|n\rangle = \left\langle n\left|a^\dagger a\right|n\right\rangle = n$$

and

$$\left\langle n\left|a^\dagger a\right|n\right\rangle = (\langle an|)(a|n\rangle)) = \langle n-1 \mid n-1\rangle c_n^2,$$

we must have $c_n = \sqrt{n}$. Analogously, since $aa^\dagger = N+1$, as seen from the commutation relationship:

$$d_n^2\langle n+1 \mid n+1\rangle = \left\langle a^\dagger n \mid a^\dagger n\right\rangle = \left\langle n\left|aa^\dagger\right|n\right\rangle\langle n|(N+1)|n\rangle = n+1$$

So in the end we have :

$$\boxed{a|n\rangle = \sqrt{n}|n-1\rangle; \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.}$$

All the n eigenvalues of N have to be non-negative since $n = \langle n|N|n\rangle = \left\langle\psi_{n_1} \mid \psi_{n_1}\right\rangle \geq 0$ (this follows from the properties of the inner product and the fact that $\left|\psi_{n_1}\right\rangle = a|n\rangle$ is just a regular state vector). However, if we apply over and over the a (lowering) operator, we could arrive at negative numbers n: we therefore require that $a|0\rangle = 0$ to truncate this process. The action of the raising operator a† can then produce any eigenstate, starting from the 0 eigenstate:

$$|n\rangle = \frac{\left(a^\dagger\right)^n}{\sqrt{n!}}|0\rangle.$$

The matrix representation of these operator in the $|n\rangle$ basis (with infinite-dimensional matrices) is particularly simple, since $\langle n|a|n'\rangle=\delta_{n',n-1}\sqrt{n}$ and $\left\langle n\left|a^{\dagger}\right|n'\right\rangle=\delta_{n',n+1}\sqrt{n+1}$:

$$a=\begin{bmatrix}0 & \sqrt{1} & 0 & \ldots\\ 0 & 0 & \sqrt{2} & \ldots\\ 0 & 0 & 0 & \ldots\end{bmatrix} \qquad a^{\dagger}=\begin{bmatrix}0 & 0 & 0 & \ldots\\ \sqrt{1} & 0 & 0 & \ldots\\ 0 & \sqrt{2} & 0 & \ldots\end{bmatrix}$$

Position representation

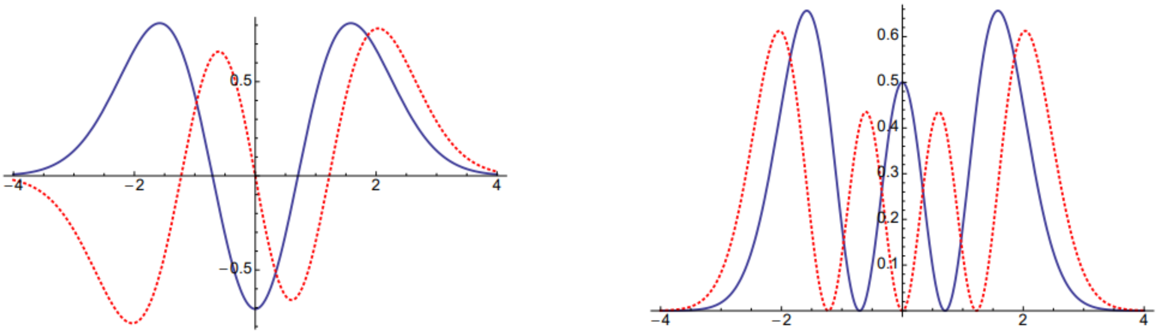


Figure 4.3.1: Left: Harmonic oscillator wavefunction. Right: corresponding probability distribution function for n = 2 (blue) and n = 3 (Red, dotted). (Copyright; author via source)

We have now started from a (physical) description of the h.o. Hamiltonian and made a change of basis in order to arrive at a simple diagonal form of it. Now that we know its eigenkets, we would like to go back to a more intuitive picture of position and momentum. We thus want to express the eigenkets $|n\rangle$ in terms of the position representation.

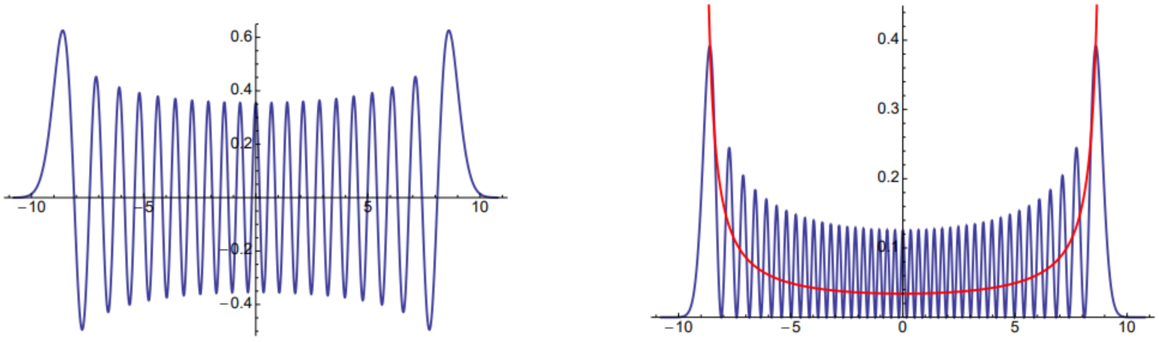


Figure 4.3.2: Left: Harmonic oscillator wavefunction. Right: corresponding probability distribution function for n = 40. In Red, the classical probability. (Copyright; author via source)

The position representation corresponds to expressing a state vector $|\psi\rangle$ in the position basis: $|\psi\rangle=\int dx\langle x\mid\psi\rangle|x\rangle=\int dx\psi(x)|x\rangle$ (where $|x\rangle$ is the eigenstate of the position operator that is a continuous variable, hence the integral). This defines the wavefunction $\psi(x)=\langle x\mid\psi\rangle$.

The wave function description in the x representation of the quantum h.o. can be found by starting with the ground state wavefunction. Since $a|0\rangle=0$ we have $\frac{1}{\sqrt{2\hbar}}(X+iP)|0\rangle=\frac{1}{\sqrt{2\hbar}}\left(\sqrt{m\omega}x+\frac{ip}{\sqrt{m\omega}}\right)|0\rangle=0$. In the x representation, given $\psi_0(x)=\langle x\mid 0\rangle$

$$\frac{1}{\sqrt{2\hbar}}\left\langle x\left|\left(\sqrt{m\omega}x+\frac{ip}{\sqrt{m\omega}}\right)\right|0\right\rangle=0 \quad\rightarrow\quad \left(m\omega x+\frac{d}{dx}\right)\psi_0(x)=0 \quad\rightarrow\quad \psi_0(x)\propto e^{-m\omega x^2/2}$$

The other eigenstates are built using Hermite Polynomials $H_n(x)$, using the formula[9] $|n\rangle=\frac{\left(a^{\dagger}\right)^n}{\sqrt{n!}}|0\rangle$ to derive differential equations:

$$\psi_n(x)=\langle x\mid n\rangle=\frac{1}{\sqrt{n!2^n}}\left[\sqrt{m\omega}x-\frac{1}{\sqrt{m\omega}}\frac{d}{dx}\right]^n\psi_0(x)$$

with solutions $\psi_n(x) = \langle x \mid n\rangle = \frac{1}{\sqrt{2^n n!}} H_n(x)\psi_0(x)$. The n = 2 and n = 3 wavefunctions are plotted in the following figure, while the second figure displays the probability distribution function. Notice the different parity for even and odd number and the number of zeros of these functions. Classically, the probability that the oscillating particle is at a given value of x is simply the fraction of time that it spends there, which is inversely proportional to its velocity $v(x) = x_0\omega\sqrt{1-\frac{x^2}{x_0^2}}$ at that position. For large n, the probability distribution becomes close to the classical one (see Fig. 4.3.2).

Note

9 For more details on Hermite Polynomials and their generator function, look on Cohen-Tannoudji. Online information from: Eric W. Weisstein. Hermite Polynomial. From MathWorld–A Wolfram Web Resource.

4.4: Identical Particles

We start first with the simplest case of a two-particle system. The wavefunction is then: $\psi\left(\vec{r}_1, \vec{r}_2\right)$ and if we assume that there is no interaction between the two particles, we will be able to describe the states using separation of variables:

$$\psi\left(\vec{r}_1, \vec{r}_2\right)=\psi_a\left(\vec{r}_1\right) \psi_b\left(\vec{r}_2\right)$$

where a and b label two different single-particle states. Implicit in this expression is the assumption that I can distinguish the two particles by some mean, and link particle one to the position 1 and the state a. However, if we consider two identical particles (2 electrons, two photons, two neutrons) there is no physical mean to distinguish them. Even if we try to measure them in order to keep track of which one is which, we know that in the process we destroy the state (by the wavefunction collapse) so not even this is a possibility.

Bosons, fermions

In quantum mechanics identical particle are fundamentally indistinguishable. Then the expression above does not correctly describe the state anymore. In order to faithfully describe a state in which we cannot know if particle a or b is at r_1 or r_2, we can take a linear combination of these two possibilities: $\psi\left(\vec{r}_1, \vec{r}_2\right)=A_1 \psi_a\left(\vec{r}_1\right) \psi_b\left(\vec{r}_2\right)+A_2 \psi_b\left(\vec{r}_1\right) \psi_a\left(\vec{r}_2\right)$. Now, since the two possibilities have the same probability, we have $\left|A_1\right|=\left|A_2\right|=\frac{1}{\sqrt{2}}$. Then there are two possible combinations:

$$\psi\left(\vec{r}_1, \vec{r}_2\right)=\frac{1}{\sqrt{2}}\left[\psi_a\left(\vec{r}_1\right) \psi_b\left(\vec{r}_2\right) \pm \psi_b\left(\vec{r}_1\right) \psi_a\left(\vec{r}_2\right)\right]$$

These two combinations describe two types of particle. The combination with the plus sign describes **bosons**, particles that are invariant under exchange of a particle pair. The combination with the minus sign describes **fermions**:

- all particles with integer spin are **bosons**
- all particles with half-integer spin are **fermions**

(This can be proved in relativistic QM).

Exchange operator

We can define an operator $\hat{P}$ that interchanges the two particles:

$$\hat{P}\left[\psi\left(\vec{r}_1, \vec{r}_2\right)\right]=\psi\left(\vec{r}_2, \vec{r}_1\right)$$

Since of course $\hat{P}\left[\hat{P}\left[\psi\left(\vec{r}_1, \vec{r}_2\right)\right]\right]=\psi\left(\vec{r}_1, \vec{r}_2\right)$, we have that $\hat{P}^2=1$. Then the eigenvalues of $\hat{P}$ must be ± 1. [If φ_n is an eigenfunction of $\hat{P}$ with eigenvalue p_n, we have $\hat{P}^2 \varphi_n=p_n^2 \varphi_n=\varphi_n$, from which $p_n^2=1$.] If two particles are identical, then the Hamiltonian is invariant with respect to their exchange and $[\mathcal{H}, \hat{P}]=0$. Then we can find energy eigenfunctions that are common eigenfunctions of the exchange operator, or $\psi\left(\vec{r}_1, \vec{r}_2\right)=\pm \psi\left(\vec{r}_2, \vec{r}_1\right)$. Then if the system is initially in such a state, it will be always be in a state with the same exchange symmetry. For the considerations above, however, we have seen that the wavefunction is not only allowed, but it must be in a state with a definite symmetry:

$$\psi\left(\vec{r}_1, \vec{r}_2\right)=\left\{\begin{array}{ll}\psi\left(\vec{r}_2, \vec{r}_1\right) & \text{bosons} \\ -\psi\left(\vec{r}_2, \vec{r}_1\right) & \text{fermions}\end{array}\right.$$

Pauli exclusion principle

From the form of the allowed wavefunction for fermions, it follows that two fermions cannot occupy the same state. Assume that $\psi_a(\vec{r})=\psi_b(\vec{r})$, then we always have that

$$\psi_f\left(\vec{r}_1, \vec{r}_2\right)=\frac{1}{\sqrt{2}}\left[\psi_a\left(\vec{r}_1\right) \psi_b\left(\vec{r}_2\right)-\psi_b\left(\vec{r}_1\right) \psi_a\left(\vec{r}_2\right)\right]=0 .$$

This is the well-known Pauli exclusion principle. Notice that of course it applies to any fermions. For example, it applies to electrons, and this is the reason why electrons do not pile up in the lowest energy level of the atomic structure, but form a shell model. We will see that the same applies as well to protons and neutrons, giving rise to the shell model for nuclei.

CHAPTER OVERVIEW

5: Nuclear Structure

5.1: Characteristics of the Nuclear Force

In this part of the course we want to study the structure of nuclei. This in turns will give us insight on the energies and forces that bound nuclei together and thus of the phenomena (that we'll study later on) that can break them apart or create them.

In order to study the nuclear structure we need to know the constituents of nuclei (the nucleons, that is, protons and neutrons) and treat them as QM objects. From the point of view of QM as we studied until now, we want first to know what is the state of the system (at equilibrium). Thus we want to solve the time-independent Schrödinger equation. This will give us the energy levels of the nuclei.

The exact nature of the forces that keep together the nucleus constituents are the study of quantum chromodynamics, that describes and look for the source of the strong interaction, one of the four fundamental interactions, along with gravitation, the electromagnetic force and the weak interaction. This theory is well-beyond this course. Here we want only to point out some of the properties of the nucleon-nucleon interaction:

- At short distances is stronger than the Coulomb force: we know that nuclei comprise tightly packed protons, thus to keep these protons together the nuclear force has to beat the Coulomb repulsion.
- The nuclear force is short range. This is supported by the fact that interactions among e.g. two nuclei in a molecule are only dictated by the Coulomb force and no longer by the nuclear force.
- Not all the particles are subjected to the nuclear force (a notable exception are electrons)
- The nuclear force does not depend at all on the particle charge, e.g. it is the same for protons and neutrons.
- The nuclear force does depend on spin, as we will prove in the case of the deuteron.
- Experiments can reveal other properties, such as the fact that there is a repulsive term at very short distances and that there is a component that is angular-dependent (the force is then not *central* and angular momentum is not conserved, although we can neglect this to a first approximation).

We will first see how these characteristics are reflected into the Hamiltonian of the simplest (non-trivial) nucleus, the deuteron. This is the only nucleus that we can attempt to solve analytically by forming a full model of the interaction between two nucleons. Comparing the model prediction with experimental results, we can verify if the characteristics of the nuclear force we described are correct. We will then later study how the nuclear force properties shape the nature and composition of stable and unstable nuclei.

5.2: The Deuteron

Reduced Hamiltonian in the center-of-mass frame

We start with the simplest problem, a nucleus formed by just one neutron and one proton: the **deuteron**. We will at first neglect the spins of these two particles and solve the energy eigenvalue problem (time-independent Schrödinger equation) for a bound p-n system. The Hamiltonian is then given by the kinetic energy of the proton and the neutron and by their mutual interaction.

$$\mathcal{H}=\frac{1}{2m_n}\hat{p}_n^2+\frac{1}{2m_p}\hat{p}_p^2+V_{nuc}\left(|x_p-x_n|\right)$$

Here we stated that the interaction depends only on the distance between the two particles (and not for example the angle...)

We could try to solve the Schrödinger equation for the wavefunction $\Psi=\Psi\left(\vec{x}_p,\vec{x}_n,t\right)$. This is a wavefunction that treats the two particles as fundamentally independent (that is, described by independent variables). However, since the two particles are interacting, it might be better to consider them as one single system. Then we can use a different type of variables (position and momentum).

We can make the transformation from $\{\vec{x}_p,\vec{x}_n\}\rightarrow\{\vec{R},\vec{r}\}$ where $\vec{R}$ describes the *average* position of the two particles (i.e. the position of the total system, to be accurately defined) and $\vec{r}$ describes the relative position of one particle wrt the other:

$$\begin{cases}\vec{R}=\frac{m_p\vec{x}_p+m_n\vec{x}_n}{m_p+m_n} & \text{center of mass}\\ \vec{r}=\vec{x}_p-\vec{x}_n & \text{relative position}\end{cases}$$

We can also invert these equations and define $\vec{x}_p=x_p(\vec{R},\vec{r})$ and $\vec{x}_n=x_n(\vec{R},\vec{r})$. Also, we can define the center of mass momentum and relative momentum (and velocity):

$$\begin{cases}\vec{p}_{cm}=\vec{p}_p+\vec{p}_n\\ \vec{p}_r=\left(m_n\vec{p}_p-m_p\vec{p}_n\right)/M\end{cases}$$

Then the (classical) Hamiltonian, using these variables, reads

$$H=\frac{1}{2M}p_{cm}^2+\frac{1}{2\mu}p_r^2+V_{nuc}(|r|)$$

where $M=m_p+m_n$ and $\mu=\frac{m_pm_n}{m_p+m_n}$ is the reduced mass. Now we can just write the quantum version of this classical Hamiltonian, using

$$\hat{p}_{cm}=-i\hbar\frac{\partial}{\partial\vec{R}}\qquad\hat{p}_r=-i\hbar\frac{\partial}{\partial\vec{r}}$$

in the equation

$$\mathcal{H}=\frac{1}{2M}\hat{p}_{cm}^2+\frac{1}{2\mu}\hat{p}_r^2+V_{nuc}(|\hat{r}|)$$

Now, since the variables r and R are independent (same as r_p and r_n) they commute. This is also true for p_{cm} and r (and p_r and R). Then, p_{cm} commutes with the whole Hamiltonian, $\left[\hat{\vec{p}}_{cm},\mathcal{H}\right]=0$. This implies that $\hat{\vec{p}}_{cm}$ is a constant of the motion. This is also true for $E_{cm}=\frac{1}{2M}\hat{\vec{p}}_{cm}^2$, the energy of the center of mass. If we solve the problem in the center-of-mass frame, then we can set $E_{cm}=0$ and this is not ever going to change. In general, it means that we can ignore the first term in the Hamiltonian and just solve

$$\mathcal{H}_D=-\frac{\hbar^2}{2\mu}\nabla_r^2+V_{nuc}(|\vec{r}|)$$

In practice, this corresponds to having applied separation of variables to the original total Schrödinger equation. The Hamiltonian $\mathcal{H}_D$ (the deuteron Hamiltonian) is now the Hamiltonian of a single-particle system, describing the motion of a reduced mass particle in a central potential (a potential that only depends on the distance from the origin). This motion is the motion of a neutron and a proton relative to each other. In order to proceed further we need to know the shape of the central potential.

Ground state

What are the most important characteristics of the nuclear potential? It is known to be very **strong** and **short range**. These are the only characteristics that are of interest now; also, if we limit ourselves to these characteristics and build a simple, fictitious potential based on those, we can hope to be able to solve exactly the problem.

If we looked at a more complex, albeit more realistic, potential, then most probably we cannot find an exact solution and would have to simplify the problem. Thus, we just take a very simple potential, a nuclear square well of range $R_0 \approx 2.1 fm$ and of depth $-V_0 = -35 \text{ MeV}$.

We need to write the Hamiltonian in spherical coordinates (for the reduced variables). The kinetic energy term is given by:

$$-\frac{\hbar^2}{2\mu}\nabla_r^2 = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hbar^2}{2\mu r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right] = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2\mu r^2}$$

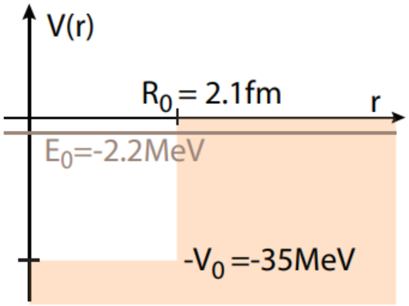


Figure 5.2.1: Nuclear potential (CC BY-NC-ND; Paola Cappellaro)

where we used the angular momentum operator (for the reduced particle) $\hat{L}^2$.

The Schrödinger equation then reads

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2\mu r^2} + V_{nuc}(r)\right]\Psi_{n,l,m}(r,\vartheta,\varphi) = E_n\Psi_{n,l,m}(r,\vartheta,\varphi)$$

We can now also check that $\left[\hat{L}^2, \mathcal{H}\right] = 0$. Then $\hat{L}^2$ is a constant of the motion and it has common eigenfunctions with the Hamiltonian.

We have already solved the eigenvalue problem for the angular momentum. We know that solutions are the spherical harmonics $Y_l^m(\vartheta,\varphi)$:

$$\hat{L}^2 Y_l^m(\vartheta,\varphi) = \hbar^2 l(l+1) Y_l^m(\vartheta,\varphi)$$

Then we can solve the Hamiltonian above with the separation of variables methods, or more simply look for a solution $\Psi_{n,l,m} = \psi_{n,l}(r)Y_l^m(\vartheta,\varphi)$:

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi_{n,l}(r)}{\partial r}\right)Y_l^m(\vartheta,\varphi) + \psi_{n,l}(r)\frac{\hat{L}^2\left[Y_l^m(\vartheta,\varphi)\right]}{2\mu r^2} = \left[E_n - V_{nuc}(r)\right]\psi_{n,l}(r)Y_l^m(\vartheta,\varphi)$$

and then we can eliminate Y_l^m to obtain:

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi_{n,l}(r)}{dr}\right) + \left[V_{nuc}(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}\right]\psi_{n,l}(r) = E_n\psi_{n,l}(r)$$

Now we write $\psi_{n,l}(r) = u_{n,l}(r)/r$. Then the radial part of the Schrödinger equation becomes

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2}+\left[V_{nuc}(r)+\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\right]u(r)=Eu(r)$$

with boundary conditions

$$\begin{aligned} u_{nl}(0)=0 &\quad\rightarrow\quad \psi(0) \text{ is finite} \\ u_{nl}(\infty)=0 &\quad\rightarrow\quad \text{bound state} \end{aligned}$$

This equation is just a 1D Schrödinger equation in which the potential $V(r)$ is replaced by an **effective potential**

$$V_{eff}(r)=V_{nuc}(r)+\frac{\hbar^2 l(l+1)}{2\mu r^2}$$

that presents the addition of a centrifugal potential (that causes an outward force).

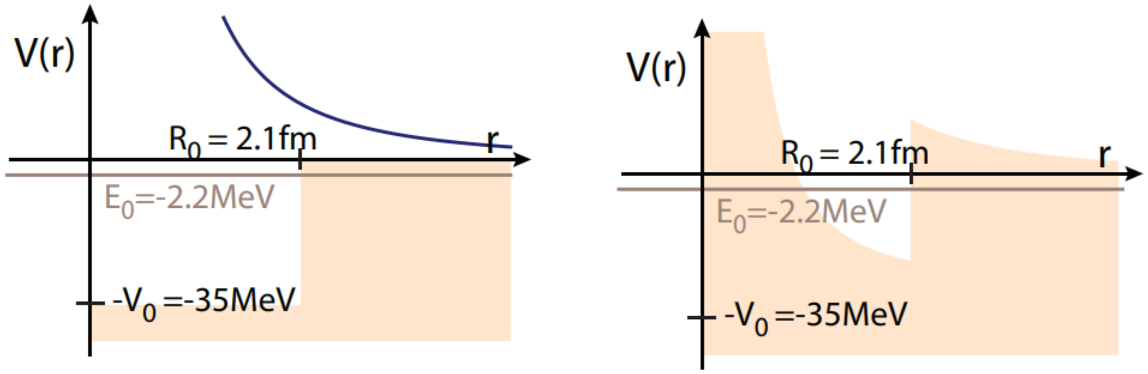


Figure 5.2.2: Nuclear potential for $l\neq 0$. Left, nuclear potential and centrifugal potential. Right, the effective potential (CC BY-NC-ND; Paola Cappellaro)

Notice that if l is large, the centrifugal potential is higher. The ground state is then found for l = 0. In that case there is no centrifugal potential and we only have a square well potential (that we already solved).

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r}+V_{nuc}(r)\right]u_0(r)=E_0u_0(r)$$

This gives the eigenfunctions

$$u(r)=A\sin(kr)+B\cos(kr),\quad 0<r<R_0$$

and

$$u(r)=Ce^{-\kappa r}+De^{\kappa r},\quad r>R_0$$

The allowed eigenfunctions (as determined by the boundary conditions) have eigenvalues found from the odd-parity solutions to the equation

$$-\kappa=k\cot(kR_0)$$

with

$$k^2=\frac{2\mu}{\hbar^2}(E_0+V_0)\quad \kappa^2=-\frac{2\mu}{\hbar^2}E_0$$

(with $E_0<0$).

Recall that we found that there was a minimum well depth and range in order to have a bound state. To satisfy the continuity condition at $r=R_0$ we need $\lambda/4\leq R_0$ or $kR_0\geq\frac{1}{4}2\pi=\frac{\pi}{2}$. Then $R_0\geq\frac{\pi}{2k}$.

In order to find a bound state, we need the potential energy to be higher than the kinetic energy $V_0>E_{kin}$. If we know R_0 we can use $k\geq\frac{\pi}{2R_0}$ to find

$$V_0 > \frac{\hbar^2\pi^2}{2\mu 4R_0^2} = \frac{\pi^2}{8}\frac{\hbar^2 c^2}{\mu c^2 R_0^2} = \frac{\pi^2}{8}\frac{(191MeV fm)^2}{469MeV(2.1fm)^2} = 23.1MeV$$

We thus find that indeed a bound state is possible, but the binding energy $E_0 = E_{kin} - V_0$ is quite small. Solving numerically the trascendental equation for E_0 we find that

$$\boxed{E_0 = -2.2\text{MeV}}$$

Notice that in our procedure we started from a model of the potential that includes the range R_0 and the strength V_0 in order to find the ground state energy (or binding energy). Experimentally instead we have to perform the inverse process. From scattering experiments it is possible to determine the binding energy (such that the neutron and proton get separated) and from that, based on our theoretical model, a value of V_0 can be inferred.

Deuteron excited state

Are bound excited states for the deuteron possible?

Consider first $l = 0$. We saw that the binding energy for the ground state was already small. The next odd solution would have $k = \frac{3\pi}{2R_0} = 3k_0$. Then the kinetic energy is 9 times the ground state kinetic energy or $E^1_{kin} = 9E^0_{kin} = 9\times 32.8MeV = 295.2MeV$. . The total energy thus becomes positive, the indication that the state is no longer bound (in fact, we then have no longer a discrete set of solutions, but a continuum of solutions).

Consider then $l > 0$. In this case the potential is increased by an amount $\frac{\hbar^2 l(l+1)}{2\mu R_0^2} \geq 18.75MeV$ (for $l = 1$). The potential thus becomes shallower (and narrower). Thus also in this case the state is no longer bound. **The deuteron has only one bound state.**

Spin dependence of nuclear force

Until now we neglected the fact that both neutron and proton possess a spin. The question remains how the spin influences the interaction between the two particles.

The total angular momentum for the deuteron (or in general for a nucleus) is usually denoted by I. Here it is given by

$$\hat{\vec{I}} = \hat{\vec{L}} + \hat{\vec{S}}_p + \hat{\vec{S}}_n$$

For the bound deuteron state $l = 0$ and $\hat{\vec{I}} = \hat{\vec{S}}_p + \hat{\vec{S}}_n = \hat{\vec{S}}$. A priori we can have $\hat{\vec{S}} = 0$ or 1 (recall the rules for addition of angular momentum, here $\hat{\vec{S}}_{p,n} = \frac{1}{2}$).

There are experimental signatures that the nuclear force depends on the spin. In fact the deuteron is only found with $\hat{\vec{S}} = 1$ (meaning that this configuration has a lower energy).

The simplest form that a spin-dependent potential could assume is $V_{\text{spin}} \propto \hat{\vec{S}}_p \cdot \hat{\vec{S}}_n$ (since we want the potential to be a scalar). The coefficient of proportionality $V_1(r)/\hbar^2$ can have a spatial dependence. Then, we guess the form for the spin-dependent potential to be $V_{spin} = V_1(r)/\hbar^2 \hat{\vec{S}}_p \cdot \hat{\vec{S}}_n$. What is the potential for the two possible configurations of the neutron and proton spins?

The configuration are either $\hat{\vec{S}} = 1$ or $\hat{\vec{S}} = 0$. Let us write $\hat{\vec{S}}^2 = \hbar S(S+1)$ in terms of the two spins:

$$\hat{\vec{S}}^2 = \hat{\vec{S}}_p^2 + \hat{\vec{S}}_n^2 + 2\hat{\vec{S}}_p \cdot \hat{\vec{S}}_n$$

The last term is the one we are looking for:

$$\hat{\vec{S}}_p \cdot \hat{\vec{S}}_n = \frac{1}{2}\left(\hat{\vec{S}}^2 - \hat{\vec{S}}_p^2 - \hat{\vec{S}}_n^2\right)$$

Because $\hat{S}^2$ and $\hat{\vec{S}}_p^2, \hat{\vec{S}}_n^2$ commute, we can write an equation for the expectation values wrt eigenfunctions of these operators[10]:

$$\left\langle \hat{\vec{S}}_p \cdot \hat{\vec{S}}_n \right\rangle = \left\langle S, S_p, S_n, S_z \middle| \hat{\vec{S}}_p \cdot \hat{\vec{S}}_n \middle| S, S_p, S_n, S_z \right\rangle = \frac{\hbar^2}{2}\left(S(S+1) - S_p\left(S_p+1\right) - S_n\left(S_n+1\right)\right)$$

since $S_{p,n}=\frac{1}{2}$, we obtain

$$\left\langle \hat{\vec{S}}_p \cdot \hat{\vec{S}}_n \right\rangle = \frac{\hbar^2}{2}\left(S(S+1)-\frac{3}{2}\right) = \begin{matrix} +\frac{\hbar^2}{4} & \text{Triplet State, } \left|S=1,\frac{1}{2}\frac{1}{2},m_z\right\rangle \\ -\frac{3\hbar^2}{4} & \text{singlet State, } \left|S=0,\frac{1}{2},\frac{1}{2},0\right\rangle \end{matrix}$$

If V_1(r) is an attractive potential (< 0), the total potential is $V_{nuc}|_{S=1}=V_T=V_0+\frac{1}{4}V_1$ for a triplet state, while its strength is reduced to $V_{nuc}|_{S=0}=V_S=V_0-\frac{3}{4}V_1$ for a singlet state. How large is V_1?

We can compute V_0 and V_1 from knowing the binding energy of the triplet state and the energy of the unbound *virtual* state of the singlet (since this is very close to zero, it can still be obtained experimentally). We have $E_T=-2.2\text{MeV}$ (as before, since this is the experimental data) and $E_S=77\text{keV}$. Solving the eigenvalue problem for a square well, knowing the binding energy E_T and setting $E_S \approx 0$, we obtain V_T = −35MeV and V_S = −25MeV (Notice that of course V_T is equal to the value we had previously set for the deuteron potential in order to find the correct binding energy of 2.2MeV, we just –wrongly– neglected the spin earlier on). From these values by solving a system of two equations in two variables:

$$\begin{cases} V_0+\frac{1}{4}V_1=V_T \\ V_0-\frac{3}{4}V_1=V_S \end{cases}$$

we obtain V_0 = −32.5MeV V_1 = −10MeV. Thus the spin-dependent part of the potential is weaker, but not negligible.

Note

[10] Note that of course we use the *coupled* representation since the properties of the deuteron, and of its spin-dependent energy, are set by the common state of proton and neutron

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5.3: Nuclear Models

In the case of the simplest nucleus (the deuterium, with 1p-1n) we have been able to solve the time independent Schrödinger equation from first principles and find the wavefunction and energy levels of the system —of course with some approximations, simplifying for example the potential. If we try to do the same for larger nuclei, we soon would find some problems, as the number of variables describing position and momentum increases quickly and the math problems become very complex.

Another difficulty stems from the fact that the exact nature of the nuclear force is not known, as there’s for example some evidence that there exist also 3-body interactions, which have no classical analog and are difficult to study via scattering experiments.

Then, instead of trying to solve the problem exactly, starting from a microscopic description of the nucleus constituents, nuclear scientists developed some models describing the nucleus. These models need to yield results that agree with the already known nuclear properties and be able to predict new properties that can be measured in experiments. We are now going to review some of these models.

Shell structure

The atomic shell model

You might already be familiar with the atomic shell model. In the atomic shell model, shells are defined based on the atomic quantum numbers that can be calculated from the atomic Coulomb potential (and ensuing the eigenvalue equation) as given by the nuclear’s protons.

Shells are filled by electrons in order of increasing energies, such that each orbital (level) can contain at most 2 electrons (by the Pauli exclusion principle). The properties of atoms are then mostly determined by electrons in a non-completely filled shell. This leads to a periodicity of atomic properties, such as the atomic radius and the ionization energy, that is reflected in the periodic table of the elements. We have seen when solving for the hydrogen atom that a quantum state is described by the quantum numbers: $|\psi = |n, l, m$ where n is the principle quantum number (that in the hydrogen atom was giving the energy). l is the angular momentum quantum number (or azimuthal quantum number) and m the magnetic quantum number. This last one is $m = -l, \ldots, l-1, l$ thus together with the spin quantum number, sets the degeneracy of each orbital (determined by n and $l < n$) to be $D(l) = 2(2l+1)$. Historically, the orbitals have been called with the spectroscopic notation as follows:

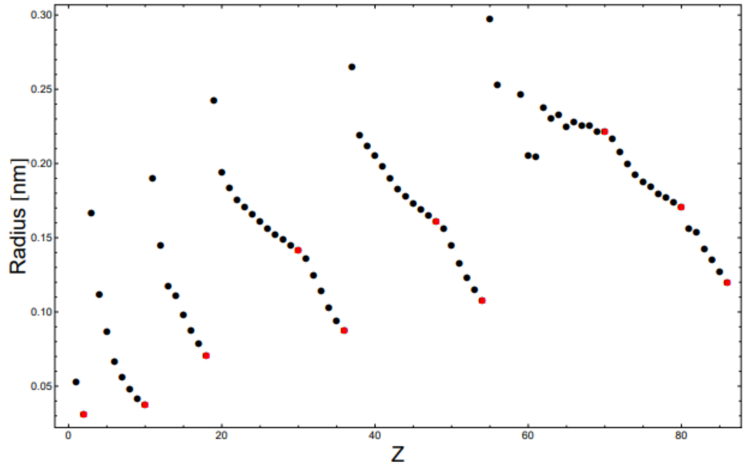
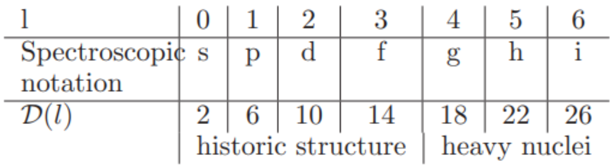


Figure 5.3.1: Atomic Radius vs Z. (CC BY-NC-ND; Paola Cappellaro)



l	0	1	2	3	4	5	6
Spectroscopic notation	s	p	d	f	g	h	i
$\mathcal{D}(l)$	2	6	10	14	18	22	26
	historic structure				heavy nuclei		

The historical notations come from the description of the observed spectral lines:

$$\mathbf{s} = \text{sharp} \quad \mathbf{p} = \text{ principal} \quad \mathbf{d} = \text{ diffuse} \quad \mathbf{f} = \text{ fine}$$

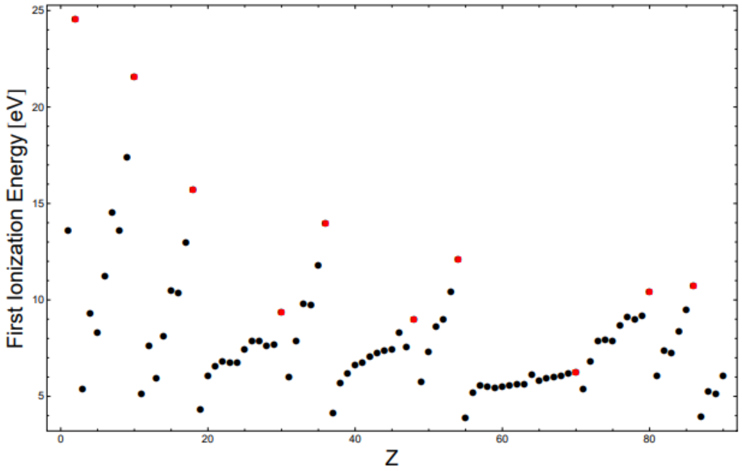


Figure 5.3.2: Ionization energy vs Z. (CC BY-NC-ND; Paola Cappellaro)

Orbitals (or energy eigenfunctions) are then collected into groups of similar energies (and similar properties). The degeneracy of each orbital gives the following (cumulative) occupancy numbers for each one of the energy group:

$$\boxed{2, \quad 10, \quad 18, \quad 36, \quad 54, \quad 70, \quad 86}$$

Notice that these correspond to the well known groups in the periodic table.

There are some difficulties that arise when trying to adapt this model to the nucleus, in particular the fact that the potential is not external to the particles, but created by themselves, and the fact that the size of the nucleons is much larger than the electrons, so that it makes much less sense to speak of orbitals. Also, instead of having just one type of particle (the electron) obeying Pauli's exclusion principle, here matters are complicated because we need to fill shells with two types of particles, neutrons and protons.

In any case, there are some compelling experimental evidences that point in the direction of a shell model.

Evidence of nuclear shell structure: Two-nucleon separation energy

The two-nucleon separation energy (2p- or 2n-separation energy) is the equivalent of the ionization energy for atoms, where nucleons are taken out in pair to account for a term in the nuclear potential that favor the *pairing* of nucleons. From this first set of data we can infer that there exist shells with occupation numbers

$$\boxed{8, \quad 20, \quad 28, \quad 50, \quad 82, \quad 126}$$

These are called **Magic numbers** in nuclear physics. Comparing to the size of the atomic shells, we can see that the atomic magic numbers are quite different from the nuclear ones (as expected since there are two-types of particles and other differences.) Only the guiding principle is the same. The atomic shells are determined by solving the energy eigenvalue equation. We can attempt to do the same for the nucleons.

Nucleons Hamiltonian

The Hamiltonian for the nucleus is a complex many-body Hamiltonian. The potential is the combination of the nuclear and coulomb interaction:

$$\mathcal{H} = \sum_i \frac{\hat{p}_i^2}{2m_i} + \sum_{j,i\leq j} V_{nuc}\left(|\vec{x}_i - \vec{x}_j|\right) + \underbrace{\sum_{j,i\leq j} \frac{e^2}{|\vec{x}_i - \vec{x}_j|}}_{\text{sum on protons only}}$$

There is not an external potential as for the electrons (where the protons create a strong external central potential for each electron). We can still simplify this Hamiltonian by using **mean field theory**[11].

Note

11 This is a concept that is relevant in many other physical situations

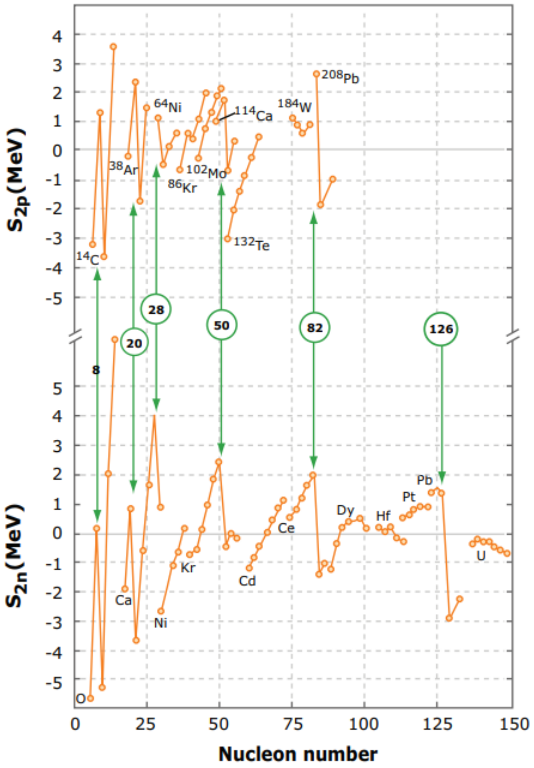


Image by MIT OpenCourseWare. After Krane.

Figure 5.3.3: Top: Two-proton separation energies of isotones (constant N). Bottom: two-neutron separation energies of isotopes (constant Z). On the x-axis: nucleon number. The sudden changes at the magic number are apparent. From Krane, fig 5.2

We can rewrite the Hamiltonian above by picking 1 nucleon, e.g. the j^{th} neutron:

$$\mathcal{H}_j^n=\frac{\hat{p}_j^2}{2m_n}+\sum_{i\leq j} V_{nuc}\left(\left|\vec{x}_i-\vec{x}_j\right|\right)$$

or the k^{th} proton:

$$\mathcal{H}_k^p=\frac{\hat{p}_k^2}{2m_n}+\sum_{i\leq k} V_{nuc}\left(\left|\vec{x}_i-\vec{x}_k\right|\right)+\underbrace{\sum_{i\leq k}\frac{e^2}{\left|\vec{x}_i-\vec{x}_k\right|}}_{\text{sum on protons only}}$$

then the total Hamiltonian is just the sum over these one-particle Hamiltonians:

$$\mathcal{H}=\sum_{j\,(\text{neutrons})}\mathcal{H}_j^n+\sum_{k(\text{ protons })}\mathcal{H}_k^p$$

The Hamiltonians $\mathcal{H}_j^n$ and $\mathcal{H}_j^p$ describe a single nucleon subjected to a potential $V_{nuc}^j\left(\left|\vec{x}_j\right|\right)$ — or $V^j\left(\left|\vec{x}_j\right|\right)=V_{nuc}^j\left(\left|\vec{x}_j\right|\right)+V_{coul}^j\left(\left|\vec{x}_j\right|\right)$ for a proton. These potentials are the effect of all the other nucleons on the nucleon we picked, and only their sum comes into play. The nucleon we focused on is then evolving in the mean field created by all the other nucleons. Of course this is a simplification, because the field created by the other nucleons depends also on the j^{th} nucleon, since this nucleon influences (for example) the position of the other nucleons. This kind of back-action is ignored in the mean-field approximation, and we considered the mean-field potential as fixed (that is, given by nucleons with a fixed position).

We then want to adopt a model for the mean-field V_{nuc}^j and V_{coul}^j. Let's start with the nuclear potential. We modeled the interaction between two nucleons by a square well, with depth $-\mathrm{V}_0$ and range R_0. The range of the nuclear well is related to the nuclear radius, which is known to depend on the nuclear mass number A, as $R \sim 1.25 A^{1/3}\mathrm{fm}$. Then V_{nuc}^j is the sum of many of these square wells, each with a different range (depending on the separation of the nucleons). The depth is instead almost constant at V_0 = 50MeV, when we consider large-A nuclei (this correspond to

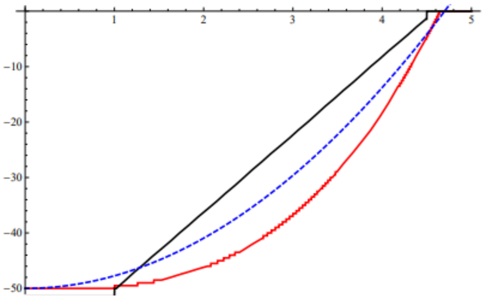


Figure 5.3.4: Potential obtained from the sum of many rectangular potential wells. Black, the potential range increases proportionally to the number of nucleons considered. Red, $R \sim A^{1/3}$. Blue, harmonic potential, that approximates the desired potential. (CC BY-NC-ND; Paola Cappellaro)

the average strength of the total nucleon potential). What is the sum of many square wells? The potential smooths out. We can approximate this with a parabolic potential. [Notice that for any continuous function, a minimum can always be approximated by a parabolic function, since a minimum is such that the first derivative is zero]. This type of potential is useful because we can find an analytical solution that will give us a classification of nuclear states. Of course, this is a crude approximation. This is the *oscillator* potential model:

$$V_{nuc} \approx -V_0\left(1-\frac{r^2}{R_0^2}\right)$$

Now we need to consider the Coulomb potential for protons. The potential is given by: $V_{\text{coul}} = \frac{(Z-1)e^2}{R_0}\left[\frac{3}{2}-\frac{r^2}{2R_0^2}\right]$ for $r \leq R_0$, which is just the potential for a sphere of radius R_0 containing a uniform charge $(Z-1)e$. Then we can write an effective (mean-field, in the parabolic approximation) potential as

$$V_{\text{eff}} = \underbrace{r^2\left(\frac{V_0}{R_0^2}-\frac{(Z-1)e^2}{2R_0^3}\right)}_{\equiv\frac{1}{2}m\omega^2r^2}\underbrace{-V_0+\frac{3}{2}\frac{(Z-1)e^2}{R_0}}_{\equiv -V_0'}$$

We defined here a modified nuclear square well potential $V_0' = V_0 \quad \frac{3}{2}\frac{(Z-1)e^2}{R_0}$ for protons, which is shallower than for neutrons. Also, we defined the harmonic oscillator frequencies $\omega^2 = \frac{2}{m}\left(\frac{V_0}{R_0^2}-\frac{(Z-1)e^2}{2R_0^3}\right)$.

The proton well is thus slightly shallower and wider than the neutron well because of the Coulomb repulsion. This potential model has limitations but it does predict the lower magic numbers.

The eigenvalues of the potential are given by the sum of the harmonic potential in 3D (as seen in recitation) and the square well:

$$E_N = \hbar\omega\left(N+\frac{3}{2}\right)-V_0'.$$

(where we take $\mathrm{V}_0{}' = \mathrm{V}_0$ for the neutron).

Note that solving the equation for the harmonic oscillator potential is not equivalent to solve the full radial equation, where the centrifugal term $\hbar^2\frac{l(l+1)}{2mr^2}$ must be taken into account. We could have solved that total equation and found the energy eigenvalues labeled by the radial and orbital quantum numbers. Comparing the two solutions, we find that the h.o. quantum number N can be expressed in terms of the radial and orbital quantum numbers as

$$N = 2(n-1)+l$$

Since $l = 0, 1, \ldots n-1$ we have the selection rule for l as a function of $N : l = N, N-2, \ldots$ (with $l \geq 0$). The degeneracy of the E_N eigenvalues is then $\mathcal{D}'(N) = \sum_{l=N,N-2,\ldots}(2l+1) = \frac{1}{2}(N+1)(N+2)$ (ignoring spin) or $\mathcal{D}(N) = (N+1)(N+2)$ when including the spin.

We can now use these quantum numbers to fill the nuclear levels. Notice that we have separate levels for neutrons and protons. Then we can build a table of the levels occupations numbers, which predicts the first 3 magic numbers.

N	l	Spectroscopic Notation	$\frac{1}{2}\mathcal{D}(N)$	$\mathcal{D}(N)$	Cumulative of nucleons#
0	0	1 s	1	2	2
1	1	1p	3	6	8
2	0, 2	2 s, 1 d	6	12	20
3	1, 3	2p, 1f	10	20	40
4	0, 2, 4	3 s, 2 d, 1 g	15	30	70

For higher levels there are discrepancies thus we need a more precise model to obtain a more accurate prediction. The other problem with the oscillator model is that it predicts only 4 levels to have lower energy than the 50MeV well potential (thus only 4 bound energy levels). The separation between oscillator levels is in fact $\hbar\omega = \sqrt{\frac{2\hbar^2 V_0}{mR_0^2} - \frac{(Z-1)e^2}{2R_0^3}} \approx \sqrt{\frac{2\hbar^2 c^2 V_0}{mc^2 R_0^2}}$. Inserting the numerical values we find $\hbar\omega = \sqrt{\frac{2(200MeVfm)^2 \times 50MeV}{938MeV\left(1.25fmA^{1/3}\right)^2}} \approx 51.5A^{-1/3}$. Then the separation between oscillator levels is on the order of 10-20MeV.

Spin orbit interaction

In order to predict the higher magic numbers, we need to take into account other interactions between the nucleons. The first interaction we analyze is the spin-orbit coupling.

The associated potential can be written as

$$\frac{1}{\hbar^2} V_{so}(r)\hat{\vec{l}} \cdot \hat{\vec{s}}$$

where $\hat{\vec{s}}$ and $\hat{\vec{l}}$ are spin and angular momentum operators for a single nucleon. This potential is to be added to the single-nucleon mean-field potential seen before. We have seen previously that in the interaction between two nucleons there was a spin component. This type of interaction motivates the form of the potential above (which again is to be taken in a mean-field picture).

We can calculate the dot product with the same trick already used:

$$\langle\hat{\vec{l}} \cdot \hat{\vec{s}}\rangle = \frac{1}{2}\left(\hat{\vec{j}}^2 - \hat{\vec{l}}^2 - \hat{\vec{s}}^2\right) = \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right]$$

where $\hat{\vec{j}}$ is the total angular momentum for the nucleon. Since the spin of the nucleon is $s = \frac{1}{2}$, the possible values of j are $j = l \pm \frac{1}{2}$. Then $j(j+1) - l(l+1) = \left(l \pm \frac{1}{2}\right)\left(l \pm \frac{1}{2} + 1\right) - l(l+1)$, and we obtain

$$\langle\hat{\vec{l}} \cdot \hat{\vec{s}}\rangle = \begin{cases} l\frac{\hbar^2}{2} & \text{for j} = \text{l} + \frac{1}{2} \\ -(l+1)\frac{\hbar^2}{2} & \text{for j} = \text{l} - \frac{1}{2} \end{cases}$$

and the total potential is

$$V_{nuc}(r) = \begin{cases} V_0 + V_{so}\frac{l}{2} & \text{for j} = 1 + \frac{1}{2} \\ V_0 - V_{so}\frac{t+1}{2} & \text{for j} = \text{l} - \frac{1}{2} \end{cases}$$

Now recall that both V_0 is negative and choose also V_{so} negative. Then:

- when the spin is **aligned** with the angular momentum ($j=l+\frac{1}{2}$) the potential becomes more negative, i.e. the well is deeper and the state more tightly bound.
- when spin and angular momentum are **anti-aligned** the system's energy is higher.

The energy levels are thus split by the spin-orbit coupling (see figure 5.3.5). This splitting is directly proportional to the angular momentum l (is larger for higher l): $\Delta E=\frac{\hbar^2}{2}(2l+1)$. The two states in the same energy configuration but with the spin aligned or anti-aligned are called a doublet.

Example 5.3.1

Consider the N = 3 h.o. level. The level $1f_{7/2}$ is pushed far down (because of the high l). Then its energy is so different that it makes a shell on its own. We had found that the occupation number up to N = 2 was 20 (the 3rd magic number). Then if we take the degeneracy of , , we obtain the 4th magic number 28.

[Notice that since here j already includes the spin, $D(j)=2j+1$.]

Since the $1f_{7/2}$ level now forms a shell on its own and it does not belong to the N = 3 shell anymore, the residual degeneracy of N = 3 is just 12 instead of 20 as before. To this degeneracy, we might expect to have to add the lowest level of the N = 4 manifold. The highest l possible for N = 4 is obtained with n = 1 from the formula $N=2(n-1)+l\rightarrow l=4$ (this would be 1g). Then the lowest level is for $j=l+1/2=4+1/2=9/2$ with degeneracy D = 2(9/2 + 1) = 10. This new combined shell comprises then 12 + 10 levels. In turns this gives us the magic number 50.

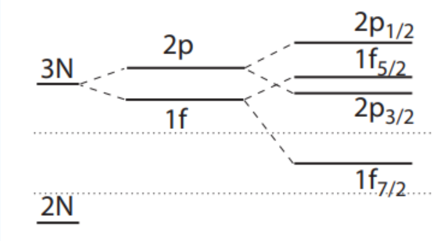


Figure 5.3.5: The energy levels from the harmonic oscillator level (labeled by N) are first shifted by the angular momentum potential (2p, 1f). Each l level is then split by the spin-orbit interaction, which pushes the energy up or down, depending on the spin and angular momentum alignment (CC BY-NC-ND; Paola Cappellaro)

Using these same considerations, the splittings given by the spin-orbit coupling can account for all the magic numbers and even predict a new one at 184:

- N = 4, 1 g $\rightarrow 1g_{7/2}$ and $1g_{9/2}$. Then we have 20 − 8 = 12 +D(9/2) = 10. From 28 we add another 22 to arrive at the magic number 50.
- N = 5, 1 h $\rightarrow 1h_{9/2}$ and $1h_{11/2}$. The shell thus combines the N = 4 levels not already included above, and the $D\left(1h_{11/2}\right)=12$ levels obtained from the $N=51h_{11/2}$. The degeneracy of N = 4 was 30, from which we subtract the 10 levels included in N = 3. Then we have $(30-10)+D\left(1h_{11/2}\right)=20+12=32$. From 50 we add arrive at the magic number 82.
- N = 6, 1i $\rightarrow 1i_{11/2}$ and $1i_{13/2}$. The shell thus have $D(N=5)-D\left(1h_{11/2}\right)+D\left(1i_{13/2}\right)=42-12+14=44$ levels (D(N) = (N + 1)(N + 2)). The predicted magic number is then 126.
- $N=7\rightarrow 1j_{15/2}$ is added to the N = 6 shell, to give $D(N=6)-D\left(1i_{13/2}\right)+D\left(1j_{15/2}\right)=56-14+16=58$, predicting a yet not-observed 184 magic number.

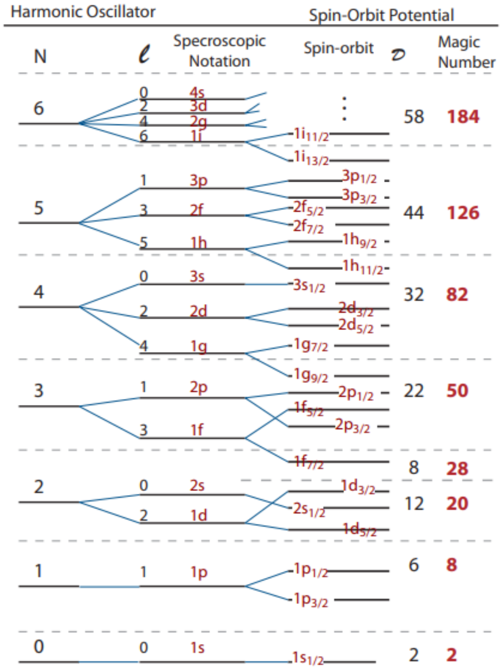


Figure 5.3.6: Shell Model prediction of the magic numbers. Level splittings due to h.o. levels, l-quantum number and spin-orbit coupling. Notice that further variations in the position of the levels are actually present (see Krane Fig. 5.6). Here only the shiftings leading to new shell groupings are shown. (CC BY-NC-ND; Paola Cappellaro)

These predictions do not depend on the exact shape of the square well potential, but only on the spin-orbit coupling and its relative strength to the nuclear interaction V_0 as set in the harmonic oscillator potential (we had seen that the separation between oscillator levels was on the order of 10MeV.) In practice, if one studies in more detail the potential well, one finds that the oscillator levels with higher l are lowered with respect to the others, thus enhancing the gap created by the spin-orbit coupling.

The shell model that we have just presented is quite a simplified model. However it can make many predictions about the nuclide properties. For example it predicts the nuclear spin and parity, the magnetic dipole moment and electric quadrupolar moment, and it can even be used to calculate the probability of transitions from one state to another as a result of radioactive decay or nuclear reactions.

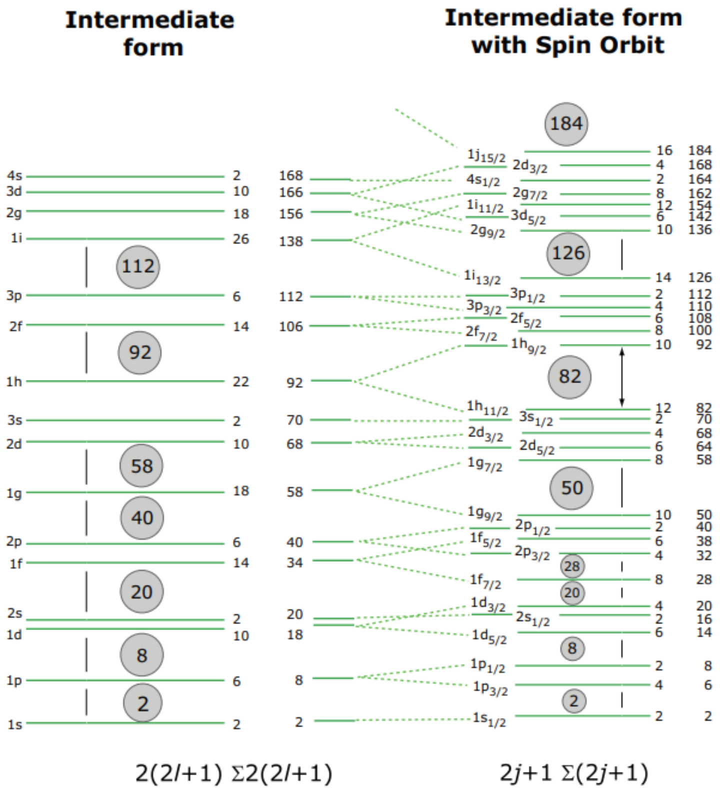


Image by MIT OpenCourseWare. After Krane.

Figure 5.3.7: Shell Model energy levels (from Krane Fig. 5.6). Left: Calculated energy levels based on potential. To the right of each level are its capacity and cumulative number of nucleons up to that level. The spin-orbit interaction splits the levels with l > 0 into two new levels. Note that the shell effect is quite apparent, and magic numbers are reproduced exactly.

Spin pairing and valence nucleons

In the extreme shell model (or extreme independent particle model), the assumption is that only the last unpaired nucleon dictates the properties of the nucleus. A better approximation would be to consider all the nucleons above a filled shell as contributing to the properties of a nucleus. These nucleons are called the valence nucleons.

Properties that can be predicted by the characteristics of the valence nucleons include the magnetic dipole moment, the electric quadrupole moment, the excited states and the spin-parity (as we will see). The shell model can be then used not only to predict excited states, but also to calculate the rate of transitions from one state to another due to radioactive decay or nuclear reactions.

As the proton and neutron levels are filled the nucleons of each type pair off, yielding a zero angular momentum for the pair. This pairing of nucleons implies the existence of a *pairing force* that lowers the energy of the system when the nucleons are paired-off.

Since the nucleons get paired-off, the total spin and parity of a nucleus is only given by the last unpaired nucleon(s) (which reside(s) in the highest energy level). Specifically we can have either one neutron or one proton or a pair neutron-proton.

The parity for a single nucleon is $(-1)^l$, and the overall parity of a nucleus is the product of the single nucleon parity. (The parity indicates if the wavefunction changes sign when changing the sign of the coordinates. This is of course dictated by the angular part of the wavefunction – as in spherical coordinates Then if you look back at the angular wavefunction for a central potential it is easy to see that the spherical harmonics change sign iff l is odd).

Obs.

The shell model with pairing force predicts a nuclear spin I = 0 and parity Π = even (or $I^{\Pi} = 0^{+}$) for all even-even nuclides.

Odd-Even nuclei

Despite its crudeness, the shell model with the spin-orbit correction describes well the spin and parity of all odd-A nuclei. In particular, all odd-A nuclei will have half-integer spin (since the nucleons, being fermions, have half-integer spin).

Example 5.3.2

${}_{8}^{15}\mathrm{O}_{7}$ and ${}_{8}^{17}\mathrm{O}_{9}$. (of course ${}^{16}\mathrm{O}$ has spin zero and even parity because all the nucleons are paired). The first ({ }_{8}^{15} \mathrm{O}_{7}\)) has an unpaired neutron in the $p_{1/2}$ shell, than l = 1, s = 1/2 and we would predict the isotope to have spin 1/2 and odd parity. The ground state of ${}_{8}^{17}\mathrm{O}_{9}$ instead has the last unpaired neutron in the $\mathrm{d}_{5/2}$ shell, with l = 2 and s = 5/2, thus implying a spin 5/2 with even parity. Both these predictions are confirmed by experiments.

Example 5.3.3

These are even-odd nuclides (i.e. with A odd).

$\rightarrow\ {}_{51}^{123}Sb_{72}$ has 1proton in 1 $\mathrm{g}_{7/2} :\rightarrow\ \frac{7}{2}^{+}$.

$\rightarrow\ {}_{51}^{123}Sb_{72}$ has 1proton in 1 $\mathrm{g}_{7/2} :\rightarrow\ \frac{7}{2}^{+}$.

$\rightarrow\ {}_{17}^{35}Cl$ has 1proton in 1 $\mathrm{d}_{3/2} :\rightarrow\ \frac{3}{2}^{+}$.

$\rightarrow\ {}_{14}^{29}Si$ has 1 neutron in 2 $\mathrm{s}_{1/2} :\rightarrow\ \frac{1}{2}^{+}$.

$\rightarrow\ {}_{14}^{28}Si$ has paired nucleons: $\rightarrow\ 0^{+}$.

Example 5.3.4

There are some nuclides that seem to be exceptions:

$\rightarrow\ {}_{51}^{121}Sb_{70}$ has last proton in 2 $\mathrm{d}_{5/2}$ instead of 1 $\mathrm{g}_{7/2} :\rightarrow\ \frac{5}{2}^{+}$ (details in the potential could account for the inversion of the two level order)

$\rightarrow {}_{62}^{147}\mathrm{Sn}_{85}$ has last proton in $2\mathrm{f}_{7/2}$ instead of 1 $\mathrm{h}_{9/2} :\rightarrow\ \frac{7}{2}^{-}$.

$\rightarrow {}_{35}^{79}\mathrm{Br}_{44}$ has last neutron in $2\mathrm{p}_{3/2}$ instead of $1\mathrm{f}_{5/2} :\rightarrow\ \frac{3}{2}^{-}$.

$\rightarrow {}_{82}^{207}Pb_{125}$. Here we invert $1\mathrm{i}_{13/2}$ with $3\mathrm{p}_{1/2}$. This seems to be wrong because the 1i level must be quite more energetic than the 3p one. However, when we move a neutron from the 3p to the 1i all the neutrons in the 1i level are now paired, thus lowering the energy of this new configuration.

$\rightarrow\ {}_{28}^{61}Ni_{33}\ 1\mathrm{f}_{5/2} \longleftrightarrow 2\mathrm{p}_{3/2} \rightarrow \left(\frac{3}{2}^{-}\right)$

$\rightarrow\ {}_{79}^{197}Au_{118}\ 1\mathrm{f}_{5/2} \longleftrightarrow 3\mathrm{p}_{3/2} \rightarrow \left(\frac{3}{2}^{+}\right)$

Odd-Odd nuclei

Only five stable nuclides contain both an odd number of protons and an odd number of neutrons: the first four odd-odd nuclides ${}_{1}^{2}\mathrm{H}, {}_{3}^{6}\mathrm{Li}, {}_{5}^{10}$ B, and ${}_{7}^{14}$ N. These nuclides have two unpaired nucleons (or odd-odd nuclides), thus their spin is more complicated to calculate. The total angular momentum can then take values between $|j_1 - j_2|$ and $j_1 + j_2$.

Two processes are at play:

1. the nuclei tends to have the smallest angular momentum, and
2. the nucleon spins tend to align (this was the same effect that we saw for example in the deuteron In any case, the resultant nuclear spin is going to be an integer number.

Nuclear Magnetic Resonance

The nuclear spin is important in chemical spectroscopy and medical imaging. The manipulation of nuclear spin by radiofrequency waves is at the basis of nuclear magnetic resonance and of magnetic resonance imaging. Then, the spin property of a particular isotope can be predicted when you know the number of neutrons and protons and the shell model. For example, it is easy to predict that hydrogen, which is present in most of the living cells, will have spin 1/2. We already saw that deuteron instead has spin 1. What about Carbon, which is also commonly found in biomolecules? ${}_{6}^{12}\mathrm{C}$ is of course and even-even nucleus, so we expect it to have spin-0. ${}_{6}^{13}\mathrm{C}_{7}$ instead has one unpaired neutron. Then ${}^{13}\mathrm{C}$ has spin-$\frac{1}{2}$.

Why can nuclear spin be manipulated by electromagnetic fields? To each spin there is an associated magnetic dipole, given by:

$$\mu=\frac{g\mu_N}{\hbar}I=\gamma_N I$$

where γ_N is called the gyromagnetic ratio, g is the g-factor (that we are going to explain) and μ_N is the nuclear magneton $\mu_N=\frac{e\hbar}{2m}\approx 3\times 10^{-8}\mathrm{eV/T}$ (with m the proton mass). The g factor is derived from a combination of the angular momentum g-factor and the spin g-factor. For protons $g_l=1$, while it is $g_l=0$ for neutrons as they don't have any charge. The spin g-factor can be calculated by solving the relativistic quantum mechanics equation, so it is a property of the particles themselves (and a dimensionless number). For protons and neutrons we have: $g_{s,p}=5.59$ and $g_{s,n}=-3.83$.

In order to have an operational definition of the magnetic dipole associated to a given angular momentum, we define it to be the expectation value of $\hat{\mu}$ when the system is in the state with the maximum z angular momentum:

$$\langle\mu\rangle=\frac{\mu_N}{\hbar}\langle g_l l_z+g_s s_z\rangle=\frac{\mu_N}{\hbar}\langle g_l j_z+(g_s-g_l)\,s_z\rangle$$

Then under our assumptions $j_z=j\hbar$ (and of course $l_z=\hbar m_z$ and $s_z=\hbar m_s$) we have

$$\langle\mu\rangle=\frac{\mu_N}{\hbar}\left(g_l j\hbar+(g_s-g_l)\,\langle s_z\rangle\right)$$

How can we calculate s_z? There are two cases, either $j=l+\frac{1}{2}$ or $j=l-\frac{1}{2}$. And notice that we want to find the projection of $\hat{\vec{S}}$ in the state which is aligned with $\hat{\vec{J}}$, so we want the expectation value of $\frac{|\hat{S}\cdot\hat{J}|\hat{J}}{|\hat{J}|^2}$. By replacing the operators with their expectation values (in the case where $j_z=j\hbar$), we obtain

$\langle s_z\rangle=+\frac{\hbar}{2}$ for $j=l+\frac{1}{2}$.

$\langle s_z\rangle=-\frac{\hbar}{2}\frac{j}{j+1}$ for $j=l-\frac{1}{2}$.

(thus we have a small correction due to the fact that we are taking an expectation value with respect to a tilted state and not the usual state aligned with $\hat{S}_z$. Remember that the state is well defined in the coupled representation, so the uncoupled representation states are no longer good eigenstates).

Finally the dipole is

$$\langle\mu\rangle=\mu_N\left[g_l\left(j-\frac{1}{2}\right)+\frac{g_s}{2}\right]$$

for $j=l+\frac{1}{2}$ and

$$\langle\mu\rangle=\mu_N g_l\left[g_l\frac{j\,(j+\frac{3}{2})}{j+1}-\frac{g_s}{2}\frac{1}{j+1}\right]$$

otherwise. Notice that the exact g-factor or gyromagnetic ratio of an isotope is difficult to calculate: this is just an approximation based on the last unpaired nucleon model, interactions among all nucleons should in general be taken into account.

More complex structures

Other characteristics of the nuclear structure can be explained by more complex interactions and models. For example all even-even nuclides present an anomalous 2^+ excited state (Since all even-even nuclides are 0^+ we have to look at the excited levels to learn more about the spin configuration.) This is a hint that the properties of all nucleons play a role into defining the nuclear structure. This is exactly the terms in the nucleons Hamiltonian that we had decided to neglect in first approximation. A different model would then to consider all the nucleons (instead of a single nucleons in an external potential) and describe their property in a collective way. This is similar to a liquid drop model. Then important properties will be the vibrations and rotations of this model.

A different approach is for example to consider not only the effects of the last unpaired nucleon but also all the nucleons outside the last closed shell. For more details on these models, see Krane.

CHAPTER OVERVIEW

6: Time Evolution in Quantum Mechanics

Until now we used quantum mechanics to predict properties of atoms and nuclei. Since we were interested mostly in the equilibrium states of nuclei and in their energies, we only needed to look at a *time-independent* description of quantum-mechanical systems. To describe dynamical processes, such as radiation decays, scattering and nuclear reactions, we need to study how quantum mechanical systems evolve in time.

6.1: Time-dependent Schrödinger Equation

When we first introduced quantum mechanics, we saw that the fourth postulate of QM states that: *The evolution of a closed system is unitary (reversible). The evolution is given by the time-dependent Schrödinger equation*

$$i\hbar\frac{\partial|\psi\rangle}{\partial t}=\mathcal{H}|\psi\rangle$$

where $\mathcal{H}$ is the Hamiltonian of the system (the energy operator) and $\hbar$ is the reduced Planck constant ($\hbar=h/2\pi$ with h the Planck constant, allowing conversion from energy to frequency units).

We will focus mainly on the Schrödinger equation to describe the evolution of a quantum-mechanical system. The statement that the evolution of a closed quantum system is unitary is however more general. It means that the state of a system at a later time t is given by , where $U(t)$ is a unitary operator. An operator is unitary if its adjoint $\mathrm{U}^\dagger$ (obtained by taking the transpose and the complex conjugate of the operator, $U^\dagger=(U^*)^T$) is equal to its inverse: $U^\dagger=U^{-1}$ and $UU^\dagger=1$.

Note that the expression $|\psi(t)\rangle=U(t)|\psi(0)\rangle$ is an integral equation relating the state at time zero with the state at time t. For example, classically we could write that $x(t)=x(0)+vt$ (where v is the speed, for constant speed). We can as well write a differential equation that provides the same information: the Schrödinger equation. Classically for example, (in the example above) the equivalent differential equation would be $\frac{dx}{dt}=v$ (more generally we would have Newton's equation linking the acceleration to the force). In QM we have a differential equation that control the evolution of closed systems. This is the Schrödinger equation:

$$\boxed{i\hbar\frac{\partial\psi(x,t)}{\partial t}=\mathcal{H}\psi(x,t)}$$

where $\mathcal{H}$ is the system's Hamiltonian. The solution to this partial differential equation gives the wavefunction $\psi(x,t)$ at any later time, when $\psi(x,0)$ is known.

Solutions to the Schrödinger equation

We first try to find a solution in the case where the Hamiltonian $\mathcal{H}=\frac{\hat{p}^2}{2m}+V(x,t)$ is such that the potential $V(x,t)$ is time independent (we can then write $V(x)$). In this case we can use separation of variables to look for solutions. That is, we look for solutions that are a product of a function of position only and a function of time only:

$$\psi(x,t)=\varphi(x)f(t)$$

Then, when we take the partial derivatives we have that

$$\frac{\partial\psi(x,t)}{\partial t}=\frac{df(t)}{dt}\varphi(x),\quad \frac{\partial\psi(x,t)}{\partial x}=\frac{d\varphi(x)}{dx}f(t)\ \text{and}\ \frac{\partial^2\psi(x,t)}{\partial x^2}=\frac{d^2\varphi(x)}{dx^2}f(t)$$

The Schrödinger equation simplifies to

$$i\hbar\frac{df(t)}{dt}\varphi(x)=-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{x^2}f(t)+V(x)\varphi(x)f(t)$$

Dividing by $\psi(x,t)$ we have:

$$i\hbar\frac{df(t)}{dt}\frac{1}{f(t)}=-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{x^2}\frac{1}{\varphi(x)}+V(x)$$

Now the LHS is a function of time only, while the RHS is a function of position only. For the equation to hold, both sides have then to be equal to a constant (separation constant):

$$i\hbar\frac{df(t)}{dt}\frac{1}{f(t)}=E,-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{x^2}\frac{1}{\varphi(x)}+V(x)=E$$

The two equations we find are a simple equation in the time variable:

$$\frac{df(t)}{dt}=-\frac{i}{\hbar}Ef(t),\ \rightarrow\ f(t)=f(0)e^{-i\frac{Et}{\hbar}}$$

and

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{x^2}\frac{1}{\varphi(x)}+V(x)=E$$

that we have already seen as the time-independent Schrödinger equation. We have extensively studied the solutions of the this last equation, as they are the eigenfunctions of the energy-eigenvalue problem, giving the stationary (equilibrium) states of quantum systems. Note that for these stationary solutions $\varphi(x)$ we can still find the corresponding total wavefunction, given as stated above by $\psi(x,t)=\varphi(x)f(t)$, which does describe also the time evolution of the system:

$$\boxed{\psi(x,t)=\varphi(x)e^{-i\frac{Et}{\hbar}}}$$

Does this mean that the states that up to now we called stationary are instead evolving in time?

The answer is yes, but with a caveat. Although the states themselves evolve as stated above, any measurable quantity (such as the probability density $|\psi(x,t)|^2$ or the expectation values of observable, $\langle A\rangle=\int\psi(x,t)^*A[\psi(x,t)])$ are still time-independent. (Check it!)

Thus we were correct in calling these states **stationary** and neglecting in practice their time-evolution when studying the properties of systems they describe.

Notice that the wavefunction built from one energy eigenfunction, $\psi(x,t)=\varphi(x)f(t)$, is only a particular solution of the Schrödinger equation, but many other are possible. These will be complicated functions of space and time, whose shape will depend on the particular form of the potential $V(x)$. How can we describe these general solutions? We know that in general we can write a basis given by the eigenfunction of the Hamiltonian. These are the functions $\{\varphi(x)\}$ (as defined above by the time-independent Schrödinger equation). The eigenstate of the Hamiltonian do not evolve. However we can write any wavefunction as

$$\psi(x,t)=\sum_k c_k(t)\varphi_k(x)$$

This just corresponds to express the wavefunction in the *basis* given by the energy eigenfunctions. As usual, the coefficients $c_k(t)$ can be obtained at any instant in time by taking the inner product: $\langle\varphi_k\mid\psi(x,t)\rangle$.

What is the evolution of such a function? Substituting in the Schrödinger equation we have

$$i\hbar\frac{\partial\left(\sum_k c_k(t)\varphi_k(x)\right)}{\partial t}=\sum_k c_k(t)\mathcal{H}\varphi_k(x)$$

that becomes

$$i\hbar\sum_k\frac{\partial\left(c_k(t)\right)}{\partial t}\varphi_k(x)=\sum_k c_k(t)E_k\varphi_k(x)$$

For each φ_k we then have the equation in the coefficients only

$$i\hbar\frac{dc_k}{dt}=E_kc_k(t)\ \rightarrow\ c_k(t)=c_k(0)e^{-i\frac{E_kt}{\hbar}}$$

A general solution of the Schrödinger equation is then

$$\psi(x,t)=\sum_k c_k(0)e^{-i\frac{E_kt}{\hbar}}\varphi_k(x)$$

Obs.

We can define the eigen-frequencies $\hbar\omega_k=E_k$ from the eigen-energies. Thus we see that the wavefunction is a superposition of waves φ_k propagating in time each with a different frequency ω_k.

The behavior of quantum systems –even particles– thus often is similar to the propagation of waves. One example is the diffraction pattern for electrons (and even heavier objects) when scattering from a slit. We saw an example in the electron diffraction video at the beginning of the class.

Obs.

What is the probability of measuring a certain energy E_k at a time t? It is given by the coefficient of the φ_k eigenfunction, $\left|c_k(t)\right|^2=\left|c_k(0)e^{-i\frac{E_k t}{\hbar}}\right|^2=\left|c_k(0)\right|^2$. This means that the probability for the given energy is constant, does not change in time. Energy is then a so-called constant of the motion. This is true only for the energy eigenvalues, not for other observables‘.

Example 6.1.1

Consider instead the probability of finding the system at a certain position, $p(x)=|\psi(x,t)|^2$. This of course changes in time. For example, let

$$\psi(x,0)=c_1(0)\varphi_1(x)+c_2(0)\varphi_2(x),$$

with

$$\left|c_1(0)\right|^2+\left|c_2(0)\right|^2=\left|c_1\right|^2+\left|c_2\right|^2=1$$

and $\varphi_{1,2}$ normalized energy eigenfunctions. Then at a later time we have

$$\psi(x,0)=c_1(0)e^{-i\omega_1 t}\varphi_1(x)+c_2(0)e^{-i\omega_2 t}\varphi_2(x).$$

What is $p(x,t)$?

Solution

$$\begin{aligned}&\left|c_1(0)e^{-i\omega_1 t}\varphi_1(x)+c_2(0)e^{-i\omega_2 t}\varphi_2(x)\right|^2\\=&\left|c_1(0)\right|^2\left|\varphi_1(x)\right|^2+\left|c_2(0)\right|^2\left|\varphi_2(x)\right|^2+c_1^*c_2\varphi_1^*\varphi_2e^{-i(\omega_2-\omega_1)t}+c_1c_2^*\varphi_1\varphi_2^*e^{i(\omega_2-\omega_1)t}\\=&\left|c_1\right|^2+\left|c_2\right|^2+2\operatorname{Re}\left[c_1^*c_2\varphi_1^*\varphi_2e^{-i(\omega_2-\omega_1)t}\right]\end{aligned}$$

The last term describes a wave interference between different components of the initial wavefunction.

Obs.

The expressions found above for the time-dependent wavefunction are only valid if the potential is itself time-independent. If this is not the case, the solutions are even more difficult to obtain.

Unitary Evolution

We saw two equivalent formulation of the quantum mechanical evolution, the Schrödinger equation and the Heisenberg equation. We now present a third possible formulation: following the 4th postulate we express the evolution of a state in terms of a unitary operator, called the **propagator**:

$$\psi(x,t)=\hat{U}(t)\psi(x,0)$$

with $\hat{U}^\dagger\hat{U}=1$. (Notice that a priori the unitary operator $\hat{U}$ could also be a function of space). We can show that this is equivalent to the Schrödinger equation, by verifying that $\psi(x,t)$ above is a solution:

$$i\hbar\frac{\partial\hat{U}\psi(x,0)}{\partial t}=\mathcal{H}\hat{U}\psi(x,0)\quad\rightarrow\quad i\hbar\frac{\partial\hat{U}}{\partial t}=\mathcal{H}\hat{U}$$

where in the second step we used the fact that since the equation holds for any wavefunction ψ it must hold for the operator themselves. If the Hamiltonian is time independent, the second equation can be solved easily, obtaining:

$$i\hbar\frac{\partial\hat{U}}{\partial t}=\mathcal{H}\hat{U}\quad\rightarrow\quad\hat{U}(t)=e^{-i\mathcal{H}t/\hbar}$$

where we set $\hat{U}(t=0)=1$. Notice that as desired $\hat{U}$ is unitary, $\hat{U}^\dagger\hat{U}=e^{i\mathcal{H}t/\hbar}e^{-i\mathcal{H}t/\hbar}=1$.

6.2: Evolution of Wave-packets

In Section 6.1.1 we looked at the evolution of a general wavefunction under a time-independent Hamiltonian. The solution to the Schrödinger equation was given in terms of a linear superposition of energy eigenfunctions, each acquiring a time-dependent phase factor. The solution was then the superposition of waves each with a different frequency.

Now we want to study the case where the eigenfunctions form a continuous basis, $\{\varphi_k\}\to\{\varphi(k)\}$. More precisely, we want to describe how a free particle evolves in time. We already found the eigenfunctions of the free particle Hamiltonian ($\mathcal{H}=\hat{p}^2/2m$): they were given by the momentum eigenfunctions e^{ikx} and describe more properly a traveling wave. A particle localized in space instead can be described by wavepacket $\psi(x,0)$ initially well localized in x-space (for example, a Gaussian wavepacket).

How does this wave-function evolve in time? First, following Section 2.2.1, we express the wavefunction in terms of momentum (and energy) eigenfunctions:

$$\psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\bar{\psi}(k)\mathrm{e}^{ikx}dk,$$

We saw that this is equivalent to the Fourier transform of $\bar{\psi}(k)$, then $\psi(x,0)$ and $\bar{\psi}(k)$ are a Fourier pair (can be obtained from each other via a Fourier transform).

Thus the function $\bar{\psi}(k)$ is obtained by Fourier transforming the wave-function at $t=0$. Notice again that the function $\bar{\psi}(k)$ is the continuous-variable equivalent of the coefficients $c_k(0)$.

The second step is to evolve in time the superposition. From the previous section we know that each energy eigenfunction evolves by acquiring a phase $e^{-i\omega(k)t}$, where $\omega(k)=E_k/\hbar$ is the energy eigenvalue. Then the time evolution of the wavefunction is

$$\psi(x,t)=\int_{-\infty}^{\infty}\bar{\psi}(k)\mathrm{e}^{\mathrm{i}\varphi(k)}dk,$$

where

$$\varphi(k)=kx-\omega(k)t.$$

For the free particle we have $\omega_k=\frac{\hbar k^2}{2m}$. If the particle encounters instead a potential (such as in the potential barrier or potential well problems we already saw) ω_k could have a more complex form. We will thus consider this more general case.

Now, if $\bar{\psi}(k)$ is **strongly peaked** around $k=k_0$, it is a reasonable approximation to Taylor expand $\varphi(k)$ about k_0. We can then approximate $\bar{\psi}(k)$ by

$$\bar{\psi}(k)\approx e^{-\frac{(k-k_0)^2}{4(\Delta k)^2}}$$

and keeping terms up to second-order in $k-k_0$, we obtain

$$\psi(x,t)\propto\int_{-\infty}^{\infty}e^{-\frac{(k-k_0)^2}{4(\Delta k)^2}}\exp\left[-\mathrm{i}kx+\mathrm{i}\left\{\varphi_0+\varphi_0^{\prime}\left(k-k_0\right)+\frac{1}{2}\varphi_0^{\prime\prime}\left(k-k_0\right)^2\right\}\right],$$

where

$$\begin{aligned}
\varphi_0 &=\varphi\left(k_0\right)=k_0x-\omega_0t,\\
\varphi_0^{\prime} &=\frac{d\varphi\left(k_0\right)}{dk}=x-v_gt,\\
\varphi_0^{\prime\prime} &=\frac{d^2\varphi\left(k_0\right)}{dk^2}=-\alpha t,\\
-\mathrm{i}kx+\mathrm{i}&\left\{k_0x-\omega_0t+\left(x-v_gt\right)\left(k-k_0\right)+\frac{1}{2}\varphi_0^{\prime\prime}\left(k-k_0\right)^2\right\}
\end{aligned}$$

with

$$\omega_0=\omega\left(k_0\right),\quad v_g=\frac{d\omega\left(k_0\right)}{dk},\quad \alpha=\frac{d^2\omega\left(k_0\right)}{dk^2},$$

As usual, the variance of the initial wavefunction and of its Fourier transform are relates: $\Delta k=1/(2\Delta x)$, where Δx is the initial width of the wave-packet and Δk the spread in the momentum. Changing the variable of integration to $y=(k-k_0)/(2\Delta k)$, we get

$$\psi(x,t)\propto \mathrm{e}^{\mathrm{i}(k_0x-\omega_0t)}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\beta_1y-(1+\mathrm{i}\beta_2)y^2}dy$$

where

$$\begin{aligned}\beta_1 &=2\Delta k\left(x-x_0-v_gt\right),\\ \beta_2 &=2\alpha(\Delta k)^2t,\end{aligned}$$

The above expression can be rearranged to give

$$\psi(x,t)\propto e^{i(k_0x-\omega_0t)-(1+i\beta_2)\beta^2/4}\int_{-\infty}^{\infty}e^{-(1+i\beta_2)(y-y_0)^2}dy,$$

where $y_0=\mathrm{i}\beta/2$ and $\beta=\beta_1/\left(1+\mathrm{i}\beta_2\right)$.

Again changing the variable of integration to $z=\left(1+\mathrm{i}\beta_2\right)^{1/2}\left(y-y_0\right)$, we get

$$\psi(x,t)\propto\left(1+\mathrm{i}\beta_2\right)^{-1/2}\mathrm{e}^{\mathrm{i}(k_0x-\omega_0t)-(1+\mathrm{i}\beta_2)\beta^2/4}\int_{-\infty}^{\infty}\mathrm{e}^{-z^2}dz.$$

The integral now just reduces to a number. Hence, we obtain

$$\psi(x,t)\propto\frac{e^{i(k_0x-\omega_0t)}\,e^{-\frac{(x-x_0-v_gt)^2\left[1-i2\alpha\Delta k^2t\right]}{4\sigma(t)^2}}}{\sqrt{1+i2\alpha(\Delta k)^2t}},$$

where

$$\sigma^2(t)=(\Delta x)^2+\frac{\alpha^2t^2}{4(\Delta x)^2}.$$

Note that even if we made an approximation earlier by Taylor expanding the phase factor $\varphi(k)$ about $k=k_0$, the above wave-function is still identical to our original wave-function at t = 0.

The probability density of our particle as a function of times is written

$$|\psi(x,t)|^2\propto\sigma^{-1}(t)\exp\left[-\frac{\left(x-x_0-v_gt\right)^2}{2\sigma^2(t)}\right].$$

Hence, the probability distribution is a Gaussian, of characteristic width $\sigma(t)$ (increasing in time), which peaks at $x=x_0+v_gt$. Now, the most likely position of our particle obviously coincides with the peak of the distribution function. Thus, the particle's most likely position is given by

$$x=x_0+v_gt.$$

It can be seen that the particle effectively moves at the uniform velocity

$$v_g=\frac{d\omega}{dk},$$

which is known as the **group-velocity**. In other words, a plane-wave travels at the phase-velocity, $v_p=\omega/k$, whereas a wave-packet travels at the group-velocity, $v_g=d\omega/dtv_g=d\omega/dt$. From the dispersion relation for particle waves the group velocity is

$$v_g=\frac{d(\hbar\omega)}{d(\hbar k)}=\frac{dE}{dp}=\frac{p}{m}.$$

which is identical to the classical particle velocity. Hence, the dispersion relation turns out to be consistent with classical physics, after all, as soon as we realize that particles must be identified with **wave-packets** rather than plane-waves.

Note that the width of our wave-packet grows as time progresses: the characteristic time for a wave-packet of original width $\Delta x \Delta x$ to double in spatial extent is

$$t_2 \sim \frac{m(\Delta x)^2}{\hbar}.$$

So, if an electron is originally localized in a region of atomic scale (i.e., $\Delta x \sim 10^{-10}\text{ m }$) then the doubling time is only about 10^{-16}s. Clearly, particle wave-packets (for freely moving particles) spread very rapidly.

The rate of spreading of a wave-packet is ultimately governed by the second derivative of $\omega(k)$ with respect to k, $\frac{\partial^2\omega}{\partial k^2}$. This is why the relationship between ω and k is generally known as a **dispersion relation**, because it governs how wave-packets disperse as time progresses.

If we consider light-waves, then ω is a *linear* function of k and the second derivative of ω with respect to k is zero. This implies that there is no dispersion of wave-packets, wave-packets propagate without changing shape. This is of course true for any other wave for which $\omega(k) \propto k$. Another property of linear dispersion relations is that the phase-velocity, $v_p = \omega/k$, and the group-velocity, $v_g = d\omega/dk$ are identical. Thus a light pulse propagates at the same speed of a plane light-wave; both propagate through a vacuum at the characteristic speed $c = 3 \times 10^8\text{ m/s}$.

Of course, the dispersion relation for particle waves is *not* linear in k (for example for free particles is quadratic). Hence, particle plane-waves and particle wave-packets propagate at different velocities, and particle wave-packets also gradually disperse as time progresses.

6.3: Evolution of Operators and Expectation Values

The Schrödinger equation describes how the state of a system evolves. Since via experiments we have access to observables and their outcomes, it is interesting to find a differential equation that directly gives the evolution of expectation values.

Heisenberg Equation

We start from the definition of expectation value and take its derivative wrt time

$$\begin{aligned}\frac{d\langle\hat{A}\rangle}{dt} &= \frac{d}{dt}\int d^3x\psi(x,t)^*\hat{A}[\psi(x,t)]\\ &= \int d^3x\frac{\partial\psi(x,t)^*}{\partial t}\hat{A}\psi(x,t) + \int d^3x\psi(x,t)^*\frac{\partial\hat{A}}{\partial t}\psi(x,t) + \int d^3x\psi(x,t)^*\hat{A}\frac{\partial\psi(x,t)}{\partial t}\end{aligned}$$

We then use the Schrödinger equation:

$$\frac{\partial\psi(x,t)}{\partial t} = -\frac{i}{\hbar}\mathcal{H}\psi(x,t), \qquad \frac{\partial\psi^*(x,t)}{\partial t} = \frac{i}{\hbar}(\mathcal{H}\psi(x,t))^*$$

and the fact $(\mathcal{H}\psi(x,t))^* = \psi(x,t)^*\mathcal{H}^* = \psi(x,t)^*\mathcal{H}$ (since the Hamiltonian is *hermitian* $\mathcal{H}^* = \mathcal{H}$). With this, we have

$$\begin{aligned}\frac{d\langle\hat{A}\rangle}{dt} &= \frac{i}{\hbar}\int d^3x\psi(x,t)^*\mathcal{H}\hat{A}\psi(x,t) + \int d^3x\psi(x,t)^*\frac{\partial\hat{A}}{\partial t}\psi(x,t) - \frac{i}{\hbar}\int d^3x\psi(x,t)^*\hat{A}\mathcal{H}\psi(x,t)\\ &= \frac{i}{\hbar}\int d^3x\psi(x,t)^*[\mathcal{H}\hat{A} - \hat{A}\mathcal{H}]\psi(x,t) + \int d^3x\psi(x,t)^*\frac{\partial\hat{A}}{\partial t}\psi(x,t)\end{aligned}$$

We now rewrite $[\mathcal{H}\hat{A} - \hat{A}\mathcal{H}] = [\mathcal{H}, \hat{A}]$ as a commutator and the integrals as expectation values:

$$\boxed{\frac{d\langle\hat{A}\rangle}{dt} = \frac{i}{\hbar}\langle[\mathcal{H}, \hat{A}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle}$$

This is an equivalent formulation of the system’s evolution (equivalent to the Schrödinger equation).

Observation

Notice that if the observable itself is time independent, then the equation reduces to $\frac{d\langle\hat{A}\rangle}{dt} = \frac{i}{\hbar}\langle[\mathcal{H}, \hat{A}]\rangle$. Then if the observable $\hat{A}$ commutes with the Hamiltonian, we have no evolution at all of the expectation value. An observable that commutes with the Hamiltonian is a constant of the motion. For example, we see again why energy is a constant of the motion (as seen before).

Notice that since we can take the expectation value with respect to any wavefunction, the equation above must hold also for the operators themselves. Then we have:

$$\boxed{\frac{d\hat{A}}{dt} = \frac{i}{\hbar}[\mathcal{H}, \hat{A}] + \frac{\partial\hat{A}}{\partial t}}$$

This is an equivalent formulation of the system’s evolution (equivalent to the Schrödinger equation).

Observation

Notice that if the operator A is time independent and it commutes with the Hamiltonian $\mathcal{H}$ then the operator is conserved, it is a constant of the motion (not only its expectation value).

Consider for example the angular momentum operator $\hat{L}^2$ for a central potential system (i.e. with potential that only depends on the distance, $V(r)$). We have seen when solving the 3D time-independent equation that $\left[\mathcal{H}, \hat{L}^2\right] = 0$. Thus the angular momentum is a constant of the motion.

Ehrenfest's Theorem

We now apply this result to calculate the evolution of the expectation values for position and momentum.

$$\frac{d\langle\hat{x}\rangle}{dt}=\frac{i}{\hbar}\langle[\mathcal{H},\hat{x}]\rangle=\frac{i}{\hbar}\left\langle\left[\frac{\hat{p}^2}{2m}+V(x),\hat{x}\right]\right\rangle$$

Now we know that $[V(x),\hat{x}]=0$ and we already calculated $\left[\hat{p}^2,\hat{x}\right]=-2i\hbar\hat{p}$. So we have:

$$\boxed{\frac{d\langle\hat{x}\rangle}{dt}=\frac{1}{m}\langle\hat{p}\rangle} \tag{6.3.1}$$

Notice that this is the same equation that links the classical position with momentum (remember $p/m=v$ velocity). Now we turn to the equation for the momentum:

$$\frac{d\langle\hat{p}\rangle}{dt}=\frac{i}{\hbar}\langle[\mathcal{H},\hat{p}]\rangle=\frac{i}{\hbar}\left\langle\left[\frac{\hat{p}^2}{2m}+V(x),\hat{p}\right]\right\rangle$$

Here of course $\left[\frac{\hat{p}^2}{2m},\hat{p}\right]=0$, so we only need to calculate $[V(x),\hat{p}]$. We substitute the explicit expression for the momentum:

$$\begin{aligned}[V(x),\hat{p}]f(x)&=V(x)\left[-i\hbar\frac{\partial f(x)}{\partial x}\right]-\left[-i\hbar\frac{\partial(V(x)f(x))}{\partial x}\right]\\&=-V(x)i\hbar\frac{\partial f(x)}{\partial x}+i\hbar\frac{\partial V(x)}{\partial x}f(x)+i\hbar\frac{\partial f(x)}{\partial x}V(x)=i\hbar\frac{\partial V(x)}{\partial x}f(x)\end{aligned}$$

Then,

$$\boxed{\frac{d\langle\hat{p}\rangle}{dt}=-\left\langle\frac{\partial V(x)}{\partial x}\right\rangle} \tag{6.3.2}$$

Observation

Notice that in both Equations 6.3.1 and 6.3.2, $\hbar$ canceled out. Moreover, both equations only involves real variables (as in classical mechanics).

Observation

Usually, the derivative of a potential function is a force, so we can write $-\frac{\partial V(x)}{\partial x}=F(x)$. If we could approximate $\langle F(x)\rangle\approx F(\langle x\rangle)$, then both two Equations 6.3.1 and 6.3.2 are rewritten:

$$\frac{d\langle\hat{x}\rangle}{dt}=\frac{1}{m}\langle\hat{p}\rangle\quad\frac{d\langle\hat{p}\rangle}{dt}=F(\langle x\rangle)$$

These are two equations in the expectation values only. Then we could just make the substitutions $\langle\hat{p}\rangle\rightarrow p$ and $\langle\hat{x}\rangle\rightarrow x$ (i.e. identify the expectation values of QM operators with the corresponding classical variables). We obtain in this way the usual classical equation of motions. This is **Ehrenfest's theorem**.

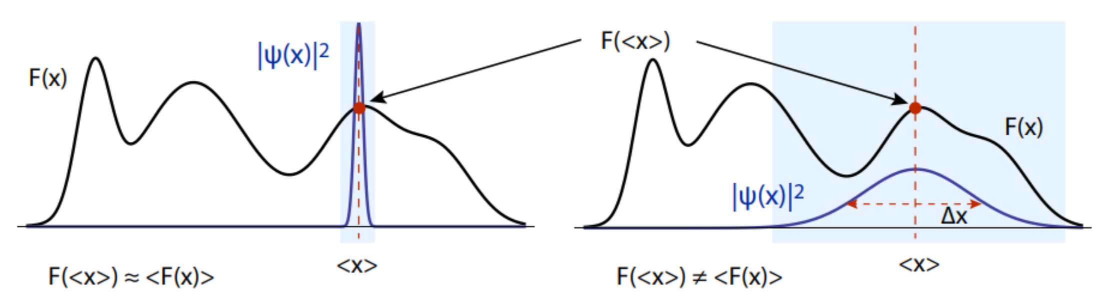


Figure 6.3.1: Localized (left) and spread-out (right) wavefunction. In the plot the absolute value square of the wavefunction is shown in blue (corresponding to the position probability density) for a system approaching the classical limit (left) or showing more quantum behavior. The force acting on the system is shown in black (same in the two plots). The shaded areas indicate the region over which $|\psi(x)|^2$ is non-negligible, thus giving an idea of the region over which the force is averaged. The wavefunctions give the same average position $\langle x\rangle$. However, while for the left one $F(\langle x\rangle) \approx \langle F(x)\rangle$, for the right wavefunction $F(\langle x\rangle) \neq \langle F(x)\rangle$(CC BY-NC-ND; Paola Cappellaro)

When is the approximation above valid? We want $\left\langle\frac{\partial V(x)}{\partial x}\right\rangle \approx \frac{\partial V(\langle x\rangle)}{\partial\langle x\rangle}$. This means that the wavefunction is localized enough such that the width of the position probability distribution is small compared to the typical length scale over which the potential varies. When this condition is satisfied, then the expectation values of quantum-mechanical probability observable will follow a classical trajectory.

Assume for example $\psi(x)$ is an eigenstate of the position operator $\psi(x)=\delta(x-\bar{x})$. Then $\langle\hat{x}\rangle=\int dx\, x \delta(x-\bar{x})^2=\bar{x}$ and

$$\left\langle\frac{\partial V(x)}{\partial x}\right\rangle=\int \frac{\partial V(x)}{\partial x} \delta(x-\langle x\rangle) dx=\frac{\partial V(\langle x\rangle)}{\partial\langle x\rangle}$$

If instead the wavefunction is a packet centered around $\langle x\rangle$ but with a finite width Δx (i.e. a Gaussian function) we no longer have an equality but only an approximation if $\Delta x \ll L=\left|\frac{1}{V} \frac{\partial V(x)}{\partial x}\right|^{-1}$ (or localized wavefunction).

6.4: Fermi’s Golden Rule

We consider now a system with an Hamiltonian $\mathcal{H}_0$, of which we know the eigenvalues and eigenfunctions:

$$\mathcal{H}_0 u_k(x) = E_k u_k(x) = \hbar\omega_k u_k(x)$$

Here I just expressed the energy eigenvalues in terms of the frequencies $\omega_k = E_k/\hbar$. Then, a general state will evolve as:

$$\psi(x,t) = \sum_k c_k(0) e^{-i\omega_k t} u_k(x)$$

If the system is in its equilibrium state, we expect it to be stationary, thus the wavefunction will be one of the eigenfunctions of the Hamiltonian. For example, if we consider an atom or a nucleus, we usually expect to find it in its ground state (the state with the lowest energy). We consider this to be the initial state of the system:

$$\psi(x,0) = u_i(x)$$

where i stands for *initial*). Now we assume that a perturbation is applied to the system. For example, we could have a laser illuminating the atom, or a neutron scattering with the nucleus. This perturbation introduces an extra potential $\hat{V}$ in the system’s Hamiltonian (a priori $\hat{V}$ can be a function of both position and time $\hat{V}(x,t)$, but we will consider the simpler case of time-independent potential $\hat{V}(x)$). Now the hamiltonian reads:

$$\mathcal{H} = \mathcal{H}_0 + \hat{V}(x)$$

What we should do, is to find the eigenvalues $\left\{E_h^v\right\}$ and eigenfunctions $\{v_h(x)\}$ of this new Hamiltonian and express $u_i(x)$ in this new basis and see how it evolves:

$$u_i(x) = \sum_h d_h(0) v_h \quad \rightarrow \quad \psi'(x,t) = \sum_h d_h(0) e^{-iE_h^v t/\hbar} v_h(x).$$

Most of the time however, the new Hamiltonian is a complex one, and we cannot calculate its eigenvalues and eigenfunctions. Then we follow another strategy.

Consider the examples above (atom+laser or nucleus+neutron): What we want to calculate is the probability of making a transition from an atom/nucleus energy level to another energy level, as induced by the interaction. Since $\mathcal{H}_0$ is the original Hamiltonian describing the system, it makes sense to always describe the state in terms of its energy levels (i.e. in terms of its eigenfunctions). Then, we *guess* a solution for the state of the form:

$$\psi'(x,t) = \sum_k c_k(t) e^{-i\omega_k t} u_k(x)$$

This is very similar to the expression for $\psi(x,t)$ above, except that now the coefficient c_k are time dependent. The time-dependency derives from the fact that we added an extra potential interaction to the Hamiltonian.

Let us now insert this guess into the Schrödinger equation, $i\hbar\frac{\partial\psi'}{\partial t} = \mathcal{H}_0\psi' + \hat{V}\psi'$:

$$i\hbar\sum_k \left[\dot{c}_k(t) e^{-i\omega_k t} u_k(x) - i\omega c_k(t) e^{-i\omega_k t} u_k(x)\right] = \sum_k c_k(t) e^{-i\omega_k t}\left(\mathcal{H}_0 u_k(x) + \hat{V}\left[u_k(x)\right]\right)$$

(where $\dot{c}$ is the time derivative). Using the eigenvalue equation to simplify the RHS we find

$$\sum_k \left[i\hbar\dot{c}_k(t) e^{-i\omega_k t} u_k(x) + \hbar\omega c_k(t) e^{-i\omega_k t} u_k(x)\right] = \sum_k \left[c_k(t) e^{-i\omega_k t}\hbar\omega_k u_k(x) + c_k(t) e^{-i\omega_k t}\hat{V}\left[u_k(x)\right]\right]$$

$$\sum_k i\hbar\dot{c}_k(t) e^{-i\omega_k t} u_k(x) = \sum_k c_k(t) e^{-i\omega_k t}\hat{V}\left[u_k(x)\right]$$

Now let us take the inner product of each side with $u_h(x)$:

$$\sum_k i\hbar\dot{c}_k(t) e^{-i\omega_k t}\int_{-\infty}^{\infty} u_h^*(x) u_k(x) dx = \sum_k c_k(t) e^{-i\omega_k t}\int_{-\infty}^{\infty} u_h^*(x)\hat{V}\left[u_k(x)\right] dx$$

In the LHS we find that $\int_{-\infty}^{\infty} u_h^*(x) u_k(x) dx = 0$ for $h \neq k$ and it is 1 for $h = k$ (the eigenfunctions are orthonormal). Then in the sum over k the only term that survives is the one $k = h$:

$$\sum_k i\hbar \dot{c}_k(t) e^{-i\omega_k t} \int_{-\infty}^{\infty} u_h^*(x) u_k(x) dx = i\hbar \dot{c}_h(t) e^{-i\omega_h t}$$

On the RHS we do not have any simplification. To shorten the notation however, we call V_{hk} the integral:

$$V_{hk} = \int_{-\infty}^{\infty} u_h^*(x) \hat{V} \left[u_k(x) \right] dx$$

The equation then simplifies to:

$$\dot{c}_h(t) = -\frac{i}{\hbar} \sum_k c_k(t) e^{i(\omega_h - \omega_k)t} V_{hk}$$

This is a differential equation for the coefficients $c_h(t)$. We can express the same relation using an integral equation:

$$c_h(t) = -\frac{i}{\hbar} \sum_k \int_0^t c_k\left(t'\right) e^{i(\omega_h - \omega_k)t'} V_{hk} dt' + c_h(0)$$

We now make an important **approximation**. We said at the beginning that the potential $\hat{V}$ is a perturbation, thus we assume that its effects are small (or the changes happen slowly). Then we can approximate $c_k\left(t'\right)$ in the integral with its value at time 0, $c_k(t = 0)$:

$$c_h(t) = -\frac{i}{\hbar} \sum_k c_k(0) \int_0^t e^{i(\omega_h - \omega_k)t'} V_{hk} dt' + c_h(0)$$

[Notice: for a better approximation, an iterative procedure can be used which replaces $c_k\left(t'\right)$ with its first order solution, then second etc.].

Now let's go back to the initial scenario, in which we assumed that the system was initially at rest, in a stationary state $\psi(x, 0) = u_i(x)$. This means that $c_k(0) = 0$ for all $k \neq i$. The equation then reduces to:

$$c_h(t) = -\frac{i}{\hbar} \int_0^t e^{i(\omega_h - \omega_i)t'} V_{hi} dt'$$

or, by calling $\Delta\omega_h = \omega_h - \omega_i$,

$$c_h(t) = -\frac{i}{\hbar} V_{hi} \int_0^t e^{i\Delta\omega_h t'} dt' = -\frac{V_{hi}}{\hbar \Delta\omega_h} \left(1 - e^{i\Delta\omega_h t}\right)$$

What we are really interested in is the probability of making a transition from the initial state $u_i(x)$ to another state $u_h(x) : P(i \rightarrow h) = \left|c_h(t)\right|^2$. This transition is caused by the extra potential $\hat{V}$ but we assume that both initial and final states are eigenfunctions of the original Hamiltonian $\mathcal{H}_0$ (notice however that the final state will be a superposition of all possible states to which the system can transition to).

We obtain

$$P(i \rightarrow h) = \frac{4\left|V_{hi}\right|^2}{\hbar^2 \Delta\omega_h^2} \sin\left(\frac{\Delta\omega_h t}{2}\right)^2$$

The function $\frac{\sin z}{z}$ is called a sinc function (see Figure 6.4.1). Take $\frac{\sin(\Delta\omega t/2)}{\Delta\omega/2}$. In the limit $t \rightarrow \infty$ (i.e. assuming we are describing the state of the system after the new potential has had a long time to change the state of the quantum system) the sinc function becomes very narrow, until when we can approximate it with a delta function. The exact limit of the function gives us:

$$P(i \rightarrow h) = \frac{2\pi \left|V_{hi}\right|^2 t}{\hbar^2} \delta\left(\Delta\omega_h\right)$$

We can then find the transition rate from $i \rightarrow h$ as the probability of transition per unit time, $W_{ih} = \frac{dP(i \rightarrow h)}{dt}$:

$$\boxed{W_{ih}=\frac{2\pi}{\hbar^2}\left|V_{hi}\right|^2\delta\left(\Delta\omega_h\right)}$$

This is the so-called **Fermi’s Golden Rule**, describing the transition rate between states.

Obs.

This transition rate describes the transition from u_i to a single level u_h with a given energy $E_h=\hbar\omega_h$. In many cases the final state is an unbound state, which, as we saw, can take on a continuous of possible energy available. Then, instead of the point-like delta function, we consider the transition to a set of states with energies in a small interval $E\rightarrow E+dE$. The transition rate is then proportional to the number of states that can be found with this energy. The number of state is given by $dn=\rho(E)dE$, where $\rho(E)$ is called the density of states (we will see how to calculate this in a later lecture). Then, Fermi’s Golden rule is more generally expressed as:

$$\boxed{W_{ih}=\frac{2\pi}{\hbar}\left|V_{hi}\right|^2\rho\left(E_h\right)\Big|_{E_h=E_i}}$$

[Note, before making the substitution $\delta(\Delta\omega)\rightarrow\rho(E)$ we need to write $\delta(\Delta\omega)=\hbar\delta(\hbar\Delta\omega)=\hbar\delta\left(E_h-E_i\right)\rightarrow\hbar\rho\left(E_h\right)|_{E_h=E_i}$. This is why in the final formulation for the Golden rule we only have a factor $\hbar$ and not its square.]

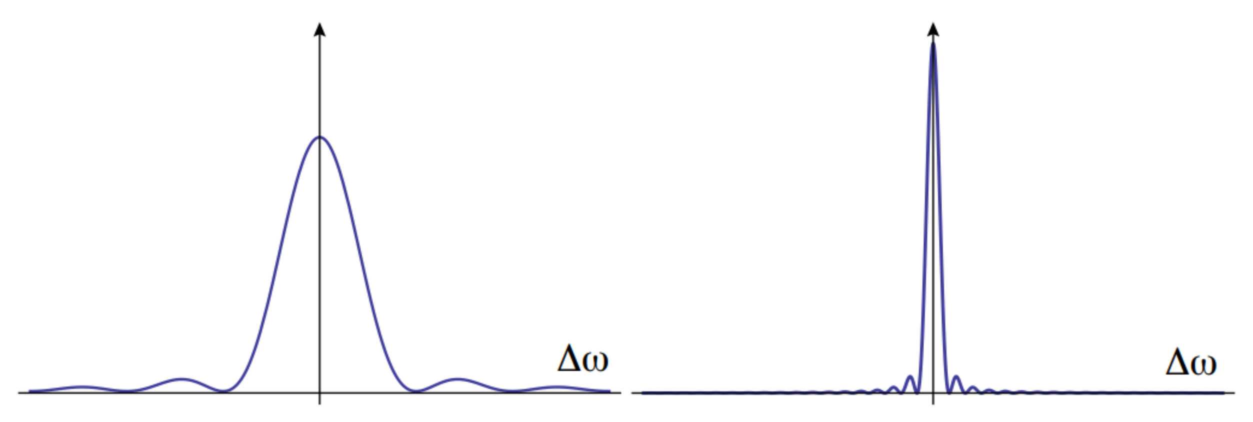


Figure 6.4.1: Sinc function $\frac{\sin(\Delta\omega t/2)}{\Delta\omega/2}$. Left: Sinc function at short times. Right: Sinc function at longer times, the function becoming narrower and closer to a Dirac delta function (CC BY-NC-ND; Paola Cappellaro)

CHAPTER OVERVIEW

7: Radioactive Decay II

Radioactive decay is the process in which an unstable nucleus spontaneously loses energy by emitting ionizing particles and radiation. This decay, or loss of energy, results in an atom of one type, called the **parent** nuclide, transforming to an atom of a different type, named the **daughter** nuclide.

The three principal modes of decay are called the alpha, beta and gamma decays. We already introduced the general principles of radioactive decay in Section 1.3 and we studied more in depth alpha decay in Section 3.3. In this chapter we consider the other two type of radioactive decay, beta and gamma decay, making use of our knowledge of quantum mechanics and nuclear structure.

Thumbnail: Beta particle emission of a nucleus.(Public Domain; Inductiveload via Wikipedia)

7.1: Gamma Decay

Gamma decay is the third type of radioactive decay. Unlike the two other types of decay, it does not involve a change in the element. It is just a simple decay from an excited to a lower (ground) state. In the process of course some energy is released that is carried away by a photon. Similar processes occur in atomic physics, however there the energy changes are usually much smaller, and photons that emerge are in the visible spectrum or x-rays.

The nuclear reaction describing gamma decay can be written as

$$ {}^{A}_{Z}X^{*} \rightarrow {}^{A}_{Z}X + \gamma $$

where * indicates an excited state.

We have said that the photon carries aways some energy. It also carries away momentum, angular momentum and parity (but no mass or charge) and all these quantities need to be conserved. We can thus write an equation for the energy and momentum carried away by the gamma-photon.

From special relativity we know that the energy of the photon (a massless particle) is

$$ E=\sqrt{m^2c^4+p^2c^2} \rightarrow \quad E=pc $$

(while for massive particles in the non-relativistic limit $v \ll c$ we have $E \approx mc^2+\frac{p^2}{2m}$.) In quantum mechanics we have seen that the momentum of a wave (and a photon is well described by a wave) is $p=\hbar k$ with k the wave number. Then we have

$$ \boxed{E=\hbar kc=\hbar\omega_k} $$

This is the energy for photons which also defines the frequency $\omega_k=kc$ (compare this to the energy for massive particles, $E=\frac{\hbar^2k^2}{2m}$).

Gamma photons are particularly energetic because they derive from nuclear transitions (that have much higher energies than e.g. atomic transitions involving electronic levels). The energies involved range from $E \sim .1 \div 10\mathrm{MeV}$, giving $k \sim 10^{-1} \div 10^{-3}\mathrm{fm}^{-1}$. Than the wavelengths are $\lambda=\frac{2\pi}{k} \sim 100 \div 10^4\mathrm{fm}$, much longer than the typical nuclear dimensions.

Gamma ray spectroscopy is a basic tool of nuclear physics, for its ease of observation (since it's not absorbed in air), accurate energy determination and information on the spin and parity of the excited states. Also, it is the most important radiation used in nuclear medicine.

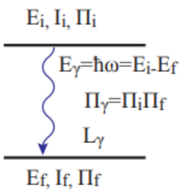


Figure 7.1.1: Schematics of gamma decay (CC BY-NC-ND; Paola Cappellaro)

Classical Theory of Radiation

From the theory of electrodynamics it is known that an accelerating charge radiates. The power radiated is given by the integral of the energy flux (as given by the Poynting vector) over all solid angles. This gives the radiated power as:

$$ \boxed{P=\frac{2}{3}\frac{e^2|a|^2}{c^3}} $$

where a is the acceleration. This is the so-called Larmor formula for a non-relativistic accelerated charge.

Example 7.1.1

As an important example we consider an electric dipole. An electric dipole can be considered as an oscillating charge, over a range r_0, such that the electric dipole is given by $d(t) = qr(t)$. Then the equation of motion is

$$r(t) = r_0 \cos(\omega t)$$

and the acceleration

$$a = \ddot{r} = -r_0\omega^2 \cos(\omega t)$$

Averaged over a period $T = 2\pi/\omega$, this is

$$\langle a^2 \rangle = \frac{\omega}{2\pi}\int_0^T dt a(t) = \frac{1}{2}r_0^2\omega^4$$

Finally we obtain the radiative power for an electric dipole:

$$P_{E1} = \frac{1}{3}\frac{e^2\omega^4}{c^3}|\vec{r}_0|^2$$

Electromagnetic Multipoles

In order to determine the classical e.m. radiation we need to evaluate the charge distribution that gives rise to it. The electrostatic potential of a charge distribution $\rho_e(r)$ is given by the integral:

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0}\int_{Vol'}\frac{\rho_e\left(\overrightarrow{r'}\right)}{\left|\vec{r}-\overrightarrow{r'}\right|}$$

When treating radiation we are only interested in the potential outside the charge and we can assume the charge (e.g. a particle!) to be well localized ($r' \ll r$). Then we can expand $\frac{1}{\left|\vec{r}-\vec{r}'\right|}$ in power series. First, we express explicitly the **norm**

$$\left|\vec{r}-\vec{r}'\right| = \sqrt{r^2+r'^2-2rr'\cos\vartheta} = r\sqrt{1+\left(\frac{r'}{r}\right)^2-2\frac{r'}{r}\cos\vartheta}\,.$$

We set

$$R = \frac{r'}{r}$$

and

$$\epsilon = R^2 - 2R\cos\vartheta.$$

This is a small quantity, given the assumption $r' \ll r$. Then we can expand:

$$\frac{1}{\left|\vec{r}-\vec{r}'\right|} = \frac{1}{r}\frac{1}{\sqrt{1+\epsilon}} = \frac{1}{r}\left(1-\frac{1}{2}\epsilon+\frac{3}{8}\epsilon^2-\frac{5}{16}\epsilon^3+\dots\right)$$

Replacing ϵ with its expression we have:

$$\begin{aligned}\frac{1}{r}\frac{1}{\sqrt{1+\epsilon}} &= \frac{1}{r}\left(1-\frac{1}{2}(R^2-2R\cos\vartheta)+\frac{3}{8}\left(R^2-2R\cos\vartheta\right)^2-\frac{5}{16}\left(R^2-2R\cos\vartheta\right)^3+\dots\right)\\ &\qquad =\frac{1}{r}\left(1+\left[-\frac{1}{2}R^2+R\cos\vartheta\right]+\left[\frac{3}{8}R^4-\frac{3}{2}R^3\cos\vartheta+\frac{3}{2}R^2\cos^2\vartheta\right]\right.\\ &\qquad\left.+\left[-\frac{5R^6}{16}+\frac{15}{8}R^5\cos(\vartheta)-\frac{15}{4}R^4\cos^2(\vartheta)+\frac{5}{2}R^3\cos^3(\vartheta)\right]+\dots\right)\\ &=\frac{1}{r}\left(1+R\cos\vartheta+R^2\left(\frac{3\cos^2\vartheta}{2}-\frac{1}{2}\right)+R^3\left(\frac{5\cos^3(\vartheta)}{2}-\frac{3\cos(\vartheta)}{2}\right)+\dots\right)\end{aligned}$$

We recognized in the coefficients to the powers of R the Legendre Polynomials $P_l(\cos\vartheta)$ (with l the power of R^l, and note that for powers > 3 we should have included higher terms in the original ϵ expansion):

$$\frac{1}{r}\frac{1}{\sqrt{1+\epsilon}}=\frac{1}{r}\sum_{l=0}^{\infty}R^lP_l(\cos\vartheta)=\frac{1}{r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^lP_l(\cos\vartheta)$$

With this result we can as well calculate the potential:

$$V(\vec{r})=\frac{1}{4\pi\epsilon_0}\frac{1}{r}\int_{Vol'}\rho\left(\vec{r}'\right)\frac{1}{r}\sum_{l=0}^{\infty}\left(\frac{r'}{r}\right)^lP_l(\cos\vartheta)d\vec{r}'$$

The various terms in the expansion are the multipoles. The few lowest ones are :

$$\begin{array}{ll}\frac{1}{4\pi\epsilon_0}\frac{1}{r}\int_{Vol'}\rho\left(\vec{r}'\right)d\overrightarrow{r'}=\frac{Q}{4\pi\epsilon_0 r} & \text{Monopole}\\ \frac{1}{4\pi\epsilon_0}\frac{1}{r^2}\int_{Vol'}\rho\left(\vec{r}'\right)r'P_1(\cos\vartheta)d\overrightarrow{r'}=\frac{1}{4\pi\epsilon_0}\frac{1}{r^2}\int_{Vol'}\rho\left(\vec{r}'\right)r'\cos\vartheta d\overrightarrow{r'}=\frac{\hat{r}\cdot\vec{d}}{4\pi\epsilon_0 r^2} & \text{Dipole}\\ \frac{1}{4\pi\epsilon_0}\frac{1}{r^3}\int_{Vol'}\rho\left(\vec{r}'\right)r'^2P_2(\cos\vartheta)d\overrightarrow{r'}=\frac{1}{4\pi\epsilon_0}\frac{1}{r^3}\int_{Vol'}\rho\left(\vec{r}'\right)r'^2\left(\frac{3}{2}\cos^2\vartheta-\frac{1}{2}\right)d\overrightarrow{r'} & \text{Quadrupole}\end{array}$$

This type of expansion can be carried out as well for the magnetostatic potential and for the electromagnetic, time-dependent field.

At large distances, the lowest orders in this expansion are the only important ones. Thus, instead of considering the total radiation from a charge distribution, we can approximate it by considering the radiation arising from the first few multipoles: i.e. radiation from the electric dipole, the magnetic dipole, the electric quadrupole etc.

Each of these radiation terms have a peculiar angular dependence. This will be reflected in the quantum mechanical treatment by a specific angular momentum value of the radiation field associated with the multipole. In turns, this will give rise to selection rules determined by the addition rules of angular momentum of the particles and radiation involved in the radiative process.

Quantum mechanical theory

In quantum mechanics, gamma decay is expressed as a transition from an excited to a ground state of a nucleus. Then we can study the transition rate of such a decay via Fermi's Golden rule

$$W=\frac{2\pi}{\hbar}\left|\left\langle\psi_f|\hat{V}|\psi_i\right\rangle\right|^2\rho\left(E_f\right)$$

There are two important ingredients in this formula, the density of states $\rho\left(E_f\right)$ and the interaction potential $\hat{V}$.

Density of states

The density of states is defined as the number of available states per energy: $\rho\left(E_f\right)=\frac{dN_s}{dE_f}$, where N_s is the number of states. We have seen at various time the concept of degeneracy: as eigenvalues of an operator can be degenerate, there might be more than one eigenfunction sharing the same eigenvalues. In the case of the Hamiltonian, when there are degeneracies it means that more than one state share the same energy.

By considering the nucleus+radiation to be enclosed in a cavity of volume L^3, we have for the emitted photon a wavefunction represented by the solution of a particle in a 3D box that we saw in a Problem Set.

As for the 1D case, we have a quantization of the momentum (and hence of the wave-number k) in order to fit the wavefunction in the box. Here we just have a quantization in all 3 directions:

$$k_x=\frac{2\pi}{L}n_x,\quad k_y=\frac{2\pi}{L}n_y,\quad k_z=\frac{2\pi}{L}n_z$$

(with n integers). Then, going to spherical coordinates, we can count the number of states in a spherical shell between n and $n+dn$ to be $dN_s=4\pi n^2dn$. Expressing this in terms of k, we have $dN_s=4\pi k^2dk\frac{L^3}{(2\pi)^3}$. If we consider just a small solid angle $d\Omega$ instead of 4π we have then the number of state $dN_s=\frac{L^3}{(2\pi)^3}k^2dkd\Omega$. Since $E=\hbar kc=\hbar\omega$, we finally obtain the density of states:

$$\rho(E)=\frac{dN_s}{dE}=\frac{L^3}{(2\pi)^3}k^2\frac{dk}{dE}d\Omega=\frac{L^3}{(2\pi)^3}\frac{k^2}{\hbar c}d\Omega=\frac{\omega^2}{\hbar c^3}\frac{L^3}{(2\pi)^3}d\Omega$$

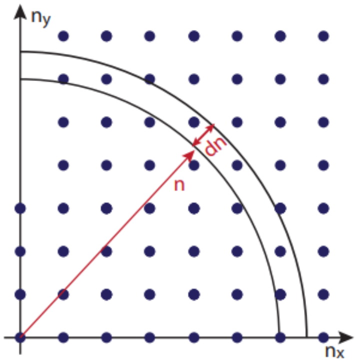


Figure 7.1.2: Density of states: counting the states 2D (CC BY-NC-ND; Paola Cappellaro)

The vector potential

Next we consider the potential causing the transition. The interaction of a particle with the e.m. field can be expressed in terms of the vector potential $\hat{\vec{A}}$ of the e.m. field as:

$$\hat{V}=\frac{e}{mc}\hat{\vec{A}}\cdot\hat{\vec{p}}$$

where $\hat{\vec{p}}$ is the particle's momentum. The vector potential $\hat{\vec{A}}$ in QM is an operator that can *create* or *annihilate* photons,

$$\hat{\vec{A}}=\sum_k\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}\left(\hat{a}_k e^{i\vec{k}\cdot\vec{r}}+\hat{a}_k^\dagger e^{-i\vec{k}\cdot\vec{r}}\right)\vec{\epsilon}_k$$

where $\hat{a}_k$ $\left(\hat{a}_k^\dagger\right)$ annihilates (creates) one photon of momentum $\vec{k}$. Also, $\vec{\epsilon}_k$ is the polarization of the e.m. field. Since gamma decay (and many other atomic and nuclear processes) is able to create photons (or absorb them) it makes sense that the operator describing the e.m. field would be able to describe the creation and annihilation of photons. The second characteristic of this operator are the terms $\propto e^{-i\vec{k}\cdot\vec{r}}$ which describe a plane wave, as expected for e.m. waves, with momentum $\hbar k$ and frequency ck.

Dipole transition for gamma decay

To calculate the transition rate from the Fermi's Golden rule,

$$W=\frac{2\pi}{\hbar}\left|\left\langle\psi_f|\hat{V}|\psi_i\right\rangle\right|^2\rho\left(E_f\right),$$

we are really only interested in the matrix element $\left\langle\psi_f|\hat{V}|\psi_i\right\rangle$, where the initial state does not have any photon, and the final has one photon of momentum $\hbar k$ and energy $\hbar\omega=\hbar kc$.. Then, the only element in the sum above for the vector potential that gives a non-zero contribution will be the term $\propto\hat{a}_k^\dagger$, with the appropriate $\vec{k}$ momentum:

$$V_{if} = \frac{e}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}\vec{\epsilon}_k\cdot\left\langle\hat{\vec{p}}e^{-i\vec{k}\cdot\vec{r}}\right\rangle$$

This can be simplified as follow. Remember that $\left[\hat{\vec{p}}^2,\hat{\vec{r}}\right] = -2i\hbar\hat{\vec{p}}$. Thus we can write, $\hat{\vec{p}} = \frac{i}{2\hbar}\left[\hat{\vec{p}}^2,\hat{\vec{r}}\right] = \frac{im}{\hbar}\left[\frac{\hat{\vec{p}}^2}{2m},\hat{\vec{r}}\right] = \frac{im}{\hbar}\left[\frac{\hat{\vec{p}}^2}{2m}+V_{nuc}(\hat{\vec{r}}),\hat{\vec{r}}\right]$. We introduced the nuclear Hamiltonian $\mathcal{H}_{nuc} = \frac{\hat{\vec{p}}^2}{2m}+V_{nuc}(\hat{\vec{r}})$: thus we have $\hat{\vec{p}} = \frac{im}{\hbar}\left[\mathcal{H}_{nuc},\hat{\vec{r}}\right]$. Taking the expectation value

$$\left\langle\psi_f|\hat{\vec{p}}|\psi_i\right\rangle = \frac{im}{\hbar}\left(\left\langle\psi_f\left|\mathcal{H}_{nuc}\hat{\vec{r}}\right|\psi_i\right\rangle - \left\langle\psi_f\left|\hat{\vec{r}}\mathcal{H}_{nuc}\right|\psi_i\right\rangle\right)$$

and remembering that $|\psi_{i,f}\rangle$ are eigenstates of the Hamiltonian, we have

$$\left\langle\psi_f|\hat{\vec{p}}|\psi_i\right\rangle = \frac{im}{\hbar}(E_f-E_i)\left\langle\psi_f|\hat{\vec{r}}|\psi_i\right\rangle = im\omega_k\left\langle\psi_f|\hat{\vec{r}}|\psi_i\right\rangle,$$

where we used the fact that $(E_f-E_i)=\hbar\omega_k$ by conservation of energy. Thus we obtain

$$V_{if} = \frac{e}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}im\omega\vec{\epsilon}_k\cdot\left\langle\hat{\vec{r}}e^{-i\vec{k}\cdot\vec{r}}\right\rangle = i\sqrt{\frac{2\pi\hbar e^2\omega_k}{V}}\vec{\epsilon}_k\cdot\left\langle\hat{\vec{r}}e^{-i\vec{k}\cdot\vec{r}}\right\rangle$$

We have seen that the wavelengths of gamma photons are much larger than the nuclear size. Then $\vec{k}\cdot\vec{r}\ll 1$ and we can make an expansion in series : $e^{-\vec{k}\cdot\vec{r}} \sim \sum_l \frac{1}{l!}(-i\vec{k}\cdot\vec{r})^l = \sum_l \frac{1}{l!}(-ikr\cos\vartheta)^l$. This series is very similar in meaning to the multipole series we saw for the classical case.

For example, for *l* = 0 we obtain:

$$V_{if} = \sqrt{\frac{2\pi\hbar e^2\omega_k}{V}}\langle\hat{\vec{r}}\rangle\cdot\vec{\epsilon}_k$$

which is the dipolar approximation, since it can be written also using the electric dipole operator $e\hat{\vec{r}}$.

The angle between the polarization of the e.m. field and the position $\hat{\vec{r}}$ is $\langle\hat{\vec{r}}\rangle\cdot\vec{\epsilon} = \langle\hat{\vec{r}}\rangle\sin\vartheta$

The transition rate for the dipole radiation, $W\equiv\lambda(E1)$ is then:

$$\lambda(E1) = \frac{2\pi}{\hbar}\left|\left\langle\psi_f|\hat{V}|\psi_i\right\rangle\right|^2\rho(E_f) = \frac{\omega^3}{2\pi c^3\hbar}|\langle\hat{\vec{r}}\rangle|^2\sin^2\vartheta d\Omega$$

and integrating over all possible direction of emission ($\int_0^{2\pi}d\varphi\int_0^{\pi}\left(\sin^2\vartheta\right)\sin\vartheta d\vartheta = 2\pi\frac{4}{3}$):

$$\lambda(E1) = \frac{4}{3}\frac{e^2\omega^3}{\hbar c^3}|\langle\hat{\vec{r}}\rangle|^2$$

Multiplying the transition rate (or photons emitted per unit time) by the energy of the photons emitted we obtain the radiated power, $P = W\hbar\omega$:

$$P = \frac{4}{3}\frac{e^2\omega^4}{c^3}|\langle\hat{\vec{r}}\rangle|^2$$

Notice the similarity of this formula with the classical case:

$$P_{E1} = \frac{1}{3}\frac{e^2\omega^4}{c^3}|\vec{r}_0|^2$$

We can estimate the transition rate by using a typical energy $E=\hbar\omega$ for the photon emitted (equal to a typical energy difference between excited and ground state nuclear levels) and the expectation value for the dipole ($|\langle\hat{\vec{r}}\rangle|\sim R_{nuc}\approx r_0A^{1/3}$). Then, the transition rate is evaluated to be

$$\lambda(E1)=\frac{e^2}{\hbar c}\frac{E^3}{(\hbar c)^3}r_0^2A^{2/3}=1.0\times 10^{14}A^{2/3}E^3$$

(with E in MeV). For example, for A = 64 and E = 1MeV the rate is $\lambda\approx 1.6\times 10^{15}s^{-1}$ or $\tau=10^{-15}$ (femtoseconds!) for E = 0.1MeV τ is on the order of picoseconds.

Obs.

Because of the large energies involved, very fast processes are expected in the nuclear decay from excited states, in accordance with Fermi's Golden rule and the energy/time uncertainty relation.

Extension to Multipoles

We obtained above the transition rate for the electric dipole, i.e. when the interaction between the nucleus and the e.m. field is described by an electric dipole and the emitted radiation has the character of electric dipole radiation. This type of radiation can only carry out of the nucleus one quantum of angular momentum (i.e. $\Delta l=\pm 1$, between excited and ground state). In general, excited levels differ by more than 1 l, thus the radiation emitted need to be a higher multipole radiation in order to conserve angular momentum.

Electric Multipoles

We can go back to the expansion of the radiation interaction in multipoles:

$$\hat{V}\sim\sum_l\frac{1}{l!}(i\hat{\vec{k}}\cdot\hat{\vec{r}})^l$$

Then the transition rate becomes:

$$\lambda(El)=\frac{8\pi(l+1)}{l[(2l+1)!!]^2}\frac{e^2}{\hbar c}\left(\frac{E}{\hbar c}\right)^{2l+1}\left(\frac{3}{l+3}\right)^2c\langle|\hat{\vec{r}}|\rangle^{2l}$$

Notice the strong dependence on the l quantum number. Setting again $|\langle\hat{\vec{r}}\rangle|\sim r_0A^{1/3}$ we also have a strong dependence on the mass number.

Thus, we have the following estimates for the rates of different electric multipoles:

- $\lambda(E1)=1.0\times 10^{14}A^{2/3}E^3$
- $\lambda(E2)=7.3\times 10^{7}A^{4/3}E^5$
- $\lambda(E3)=34A^2E^7$
- $\lambda(E4)=1.1\times 10^{-5}A^{8/3}E^9$

Magnetic Multipoles

The e.m. potential can also contain magnetic interactions, leading to magnetic transitions. The transition rates can be calculated from a similar formula:

$$\lambda(Ml)=\frac{8\pi(l+1)}{l[(2l+1)!!]^2}\frac{e^2}{\hbar c}\frac{E^{2l+1}}{\hbar c}\left(\frac{3}{l+3}\right)^2c\langle|\hat{\vec{r}}|\rangle^{2l-2}\left[\frac{\hbar}{m_pc}\left(\mu_p-\frac{1}{l+1}\right)\right]$$

where μ_p is the magnetic moment of the proton (and m_p its mass).

Estimates for the transition rates can be found by setting $\mu_p-\frac{1}{l+1}\approx 10$:

- $\lambda(M1)=5.6\times 10^{13}E^3$
- $\lambda(M2)=3.5\times 10^{7}A^{2/3}E^5$
- $\lambda(M3)=16A^{4/3}E^7$
- $\lambda(M4)=4.5\times 10^{-6}A^2E^9$

Selection Rules

The angular momentum must be conserved during the decay. Thus the difference in angular momentum between the initial (excited) state and the final state is carried away by the photon emitted. Another conserved quantity is the total parity of the system.

Parity change

The parity of the gamma photon is determined by its character, either magnetic or electric multipole. We have

$$\Pi_\gamma(El) = (-1)^l \quad \text{Electric multipole}$$

$$\Pi_\gamma(Ml) = (-1)^{l-1} \quad \text{Magnetic multipole}$$

Then if we have a parity change from the initial to the final state $\Pi_i \rightarrow \Pi_f$ this is accounted for by the emitted photon as:

$$\Pi_\gamma = \Pi_i \Pi_f$$

This of course limits the type of multipole transitions that are allowed given an initial and final state.

$$\Delta\Pi = \text{no} \rightarrow \text{ Even Electric, Odd Magnetic}$$

$$\Delta\Pi = \text{ yes } \rightarrow \text{ Odd Electric, Even Magnetic}$$

Angular momentum

From the conservation of the angular momentum:

$$\hat{\vec{I}}_i = \hat{\vec{I}}_f + \hat{\vec{L}}_\gamma$$

the allowed values for the angular momentum quantum number of the photon, l, are restricted to

$$l_\gamma = |I_i - I_f|, \ldots, I_i + I_f$$

Once the allowed l have been found from the above relationship, the character (magnetic or electric) of the multipole is found by looking at the parity.

In general then, the most important transition will be the one with the lowest allowed l, Π. Higher multipoles are also possible, but they are going to lead to much slower processes.

Multipolarity	Angular Momentum l	Parity Π	Multipolarity	Angular Momentum l	Parity Π
M1	1	+	E1	1	-
M2	2	-	E2	2	+
M3	3	+	E3	3	-
M4	4	-	E4	4	+
M5	5	+	E5	5	-

Table 7.1.1: Angular momentum and parity of the gamma multipoles (CC BY-NC-ND; Paola Cappellaro)

Dominant Decay Modes

In general we have the following predictions of which transitions will happen:

1. The lowest permitted multipole dominates
2. Electric multipoles are more probable than the same magnetic multipole by a factor $\sim 10^2$ (however, which one is going to happen depends on the parity)

$$\frac{\lambda(El)}{\lambda(Ml)} \approx 10^2$$

3. Emission from the multipole $l + 1$ is 10^{-5} times less probable than the l-multipole emission.

$$\frac{\lambda(E, l+1)}{\lambda(El)} \approx 10^{-5}, \quad \frac{\lambda(M, l+1)}{\lambda(Ml)} \approx 10^{-5}$$

4. Combining 2 and 3, we have:

$$\frac{\lambda(E, l+1)}{\lambda(M l)} \approx 10^{-3}, \quad \frac{\lambda(M, l+1)}{\lambda(E l)} \approx 10^{-7}$$

Thus E2 competes with M1 while that’s not the case for M2 vs. E1

Internal conversion

What happen if no allowed transitions can be found? This is the case for even-even nuclides, where the decay from the 0^{+} excited state must happen without a change in angular momentum. However, the photon always carries some angular momentum, thus gamma emission is impossible.

Then another process happens, called **internal conversion**:

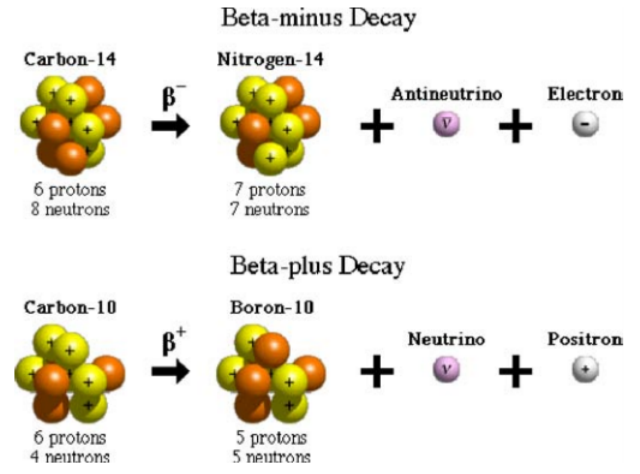
$$\overset{A}{Z} X^{*} \rightarrow_{Z}^{A} X+e^{-}$$

where ${}_{Z}^{A}X$ is a ionized state and e^{-} is one of the atomic electrons.

Besides the case of even-even nuclei, internal conversion is in general a competing process of gamma decay (see Krane for more details).

7.2: Beta Decay

The beta decay is a radioactive decay in which a proton in a nucleus is converted into a neutron (or vice-versa). In the process the nucleus emits a beta particle (either an electron or a positron) and quasi-massless particle, the **neutrino**.



Courtesy of Thomas Jefferson National Accelerator Facility - Office of Science Education. Used with permission.

Figure 7.2.1: Beta decay schematics (CC BY-NC-ND; Paola Cappellaro)

Recall the mass chain and Beta decay plots of Fig. 7. When studying the binding energy from the SEMF we saw that at fixed A there was a minimum in the nuclear mass for a particular value of Z. In order to reach that minimum, unstable nuclides undergo beta decay to transform excess protons in neutrons (and vice-versa).

Reactions and Phenomenology

The beta-decay reaction is written as:

$$ {}^{\mathrm{A}}_{\mathrm{Z}}\mathrm{X}_{\mathrm{N}} \longrightarrow {}^{\mathrm{A}}_{\mathrm{Z}_1^+}\mathrm{X}'_{\mathrm{N}-1} + \mathrm{e}^- + \bar{\nu} $$

This is the β^- decay. (or negative beta decay) The underlying reaction is:

$$ \mathrm{n} \rightarrow \mathrm{p} + \mathrm{e}^- + \bar{\nu} $$

which converts a proton into a neutron with the emission of an electron and an anti-neutrino. There are two other types of reactions, the β^+ reaction,

$$ {}^{\mathrm{A}}_{\mathrm{Z}}\mathrm{X}_{\mathrm{N}} \longrightarrow {}^{\mathrm{A}}_{\mathrm{Z}-1}\mathrm{X}'_{\mathrm{N}_1^+} + \mathrm{e}^+ + \nu $$

with this underlying reaction

$$ \mathrm{p} \longrightarrow \mathrm{n} + \mathrm{e}^+ + \nu $$

which sees the emission of a positron (the electron anti-particle) and a neutrino; and the electron capture:

$$ {}^{A}_{Z}X_N + e^- \rightarrow {}^{A}_{Z-1}X'_{N+1} + \nu $$

with this underlying reaction

$$ \mathrm{p} + \mathrm{e}^- \rightarrow \mathrm{n}^+ \nu $$

a process that competes with, or substitutes, the positron emission.

Example 7.2.1

$$ {}^{64}_{29}\text{Cu}\begin{array}{l}\nearrow \\ \searrow\end{array} \begin{array}{ll} {}^{64}\text{Zn}+e^-+\bar{\nu}, & Q_\beta=0.57MeV \\ {}^{64}_{28}\text{Ni}+e^++\nu, & Q_\beta=0.66\text{MeV}\end{array} $$

The neutrino and beta particle ($\beta^\pm$) share the energy.

Since the neutrinos are very difficult to detect (as we will see they are almost massless and interact very *weakly* with matter), the electrons/positrons are the particles detected in beta-decay and they present a characteristic energy spectrum (see Fig. 45). The difference between the spectrum of the $\beta^\pm$ particles is due to the Coulomb repulsion or attraction from the nucleus. Notice that the neutrinos also carry away angular momentum. They are spin-1/2 particles, with no charge (hence the name) and very small mass. For many years it was actually believed to have zero mass. However it has been confirmed that it does have a mass in 1998.

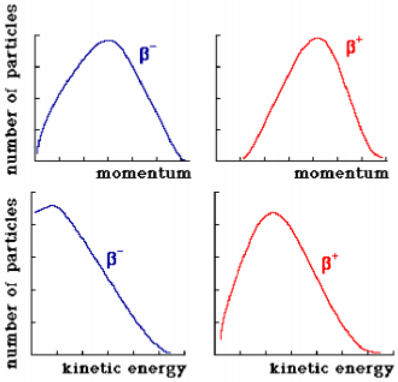


Figure \(\PageIndex{2}\): : Beta decay spectra: Distribution of momentum (top plots) and kinetic energy (bottom) for β^- (left) and β^+ (right) decay. © Neil Spooner. All rights reserved. This content is excluded from the Creative Commons license. For more information, see http://ocw.mit.edu/fairuse.

Conservation Laws

As the neutrino is hard to detect, initially the beta decay seemed to violate energy conservation. Introducing an extra particle in the process allows one to respect conservation of energy. Besides energy, there are other conserved quantities:

- **Energy:** The Q value of a beta decay is given by the usual formula:

$$Q_{\beta^-}=\left[m_N\left({}^AX\right)-m_N\left({}^{A}_{Z+1}X'\right)-m_e\right]c^2.$$

Using the atomic masses and neglecting the electron's binding energies as usual we have

$$\begin{aligned} Q_{\beta^-} &=\left\{\left[m_A\left({}^AX\right)-Zm_e\right]-\left[m_A\left({}^{A}_{Z+1}X'\right)-(Z+1)m_e\right]-m_e\right\}c^2 \\ &=\left[m_A\left({}^AX\right)-m_A\left({}^{A}_{Z+1}X'\right)\right]c^2. \end{aligned}$$

The kinetic energy (equal to the Q) is shared by the neutrino and the electron (we neglect any recoil of the massive nucleus). Then, the emerging electron (remember, the only particle that we can really observe) does not have a fixed energy, as it was for example for the gamma photon. But it will exhibit a spectrum of energy (which is the number of electron at a given energy) as well as a distribution of momenta. We will see how we can reproduce these plots by analyzing the QM theory of beta decay.

- **Momentum:** The momentum is also shared between the electron and the neutrino. Thus the observed electron momentum ranges from zero to a maximum possible momentum transfer.
- **Angular momentum** (both the electron and the neutrino have spin 1/2)
- **Parity?** It turns out that parity is not conserved in this decay. This hints to the fact that the interaction responsible violates parity conservation (so it cannot be the same interactions we already studies, e.m. and strong interactions)
- **Charge** (thus the creation of a proton is for example always accompanied by the creation of an electron)

- **Lepton number:** we do not conserve the total number of particles (we create beta and neutrinos). However the number of massive, heavy particles (or baryons, composed of 3 quarks) is conserved. Also the lepton number is conserved. Leptons are fundamental particles (including the electron, muon and tau, as well as the three types of neutrinos associated with these 3). The lepton number is +1 for these particles and -1 for their antiparticles. Then an electron is always accompanied by the creation of an antineutrino, e.g., to conserve the lepton number (initially zero).

Fermi’s Theory of Beta Decay

The properties of beta decay can be understood by studying its quantum-mechanical description via Fermi’s Golden rule, as done for gamma decay.

$$W=\frac{2\pi}{\hbar}\left|\left\langle\psi_f|\hat{V}|\psi_i\right\rangle\right|^2\rho\left(E_f\right)$$

In gamma decay process we have seen how the e.m. field is described as an operator that can create (or destroy) photons. Nobody objected to the fact that we can create this massless particles. After all, we are familiar with charged particles that produce (create) an e.m. field. However in QM photons are also particles, and by analogy we can have also creation of other types of particles, such as the electron and the neutrino.

For the beta decay we need another type of interaction that is able to create massive particles (the electron and neutrino). The interaction cannot be given by the e.m. field; moreover, in the light of the possibilities of creating and annihilating particles, we also need to find a new description for the particles themselves that allows these processes. All of this is obtained by **quantum field theory** and the second quantization. Quantum field theory gives a unification of e.m. and weak force (electro-weak interaction) with one coupling constant e. The interaction responsible for the creation of the electron and neutrino in the beta decay is called the **weak interaction** and its one of the four fundamental interactions (together with gravitation, electromagnetism and the strong interaction that keeps nucleons and quarks together). One characteristic of this interaction is parity violation.

Matrix element

The weak interaction can be written in terms of the particle field wavefunctions:

$$V_{int}=g\Psi_e^\dagger\Psi_{\bar{\nu}}^\dagger$$

where $\Psi_a\left(\Psi_a^\dagger\right)$ annihilates (creates) the particle a, and g is the coupling constant that determines how strong the interaction is. Remember that the analogous operator for the e.m. field was $\propto a_k^\dagger$ (creating one photon of momentum k).

Then the matrix element

$$V_{if}=\langle\psi_f\left|\mathcal{H}_{int}\right|\psi_i\rangle$$

can be written as:

$$V_{if}=g\int d^3\vec{x}\Psi_p^*(\vec{x})\left[\Psi_e^*(\vec{x})\Psi_{\bar{\nu}}^*(\vec{x})\right]\Psi_n(\vec{x})$$

(Here $\dagger\rightarrow *$ since we have scalar operators).

To first approximation the electron and neutrino can be taken as plane waves:

$$V_{if}=g\int d^3\vec{x}\Psi_p^*(\vec{x})\frac{e^{i\vec{k}_e\cdot\vec{x}}}{\sqrt{V}}\frac{e^{i\vec{k}_\nu\cdot\vec{x}}}{\sqrt{V}}\Psi_n(\vec{x})$$

and since $kR\ll 1$ we can approximate this with

$$V_{if}=\frac{g}{V}\int d^3\vec{x}\Psi_p^*(\vec{x})\Psi_n(\vec{x})$$

We then write this matrix element as

$$V_{if}=\frac{g}{V}M_{np}$$

where M_{np} is a very complicated function of the nuclear spin and angular momentum states. In addition, we will use in the Fermi's Golden Rule the expression

$$|M_{np}|^2 \rightarrow |M_{np}|^2 F(Z_0, Q_\beta)$$

where the Fermi function $F(Z_0, Q_\beta)$ accounts for the Coulomb interaction between the nucleus and the electron that we had neglected in the previous expression (where we only considered the weak interaction).

Density of states

In studying the gamma decay we calculated the density of states, as required by the Fermi's Golden Rule. Here we need to do the same, but the problem is complicated by the fact that there are two types of particles (electron and neutrino) as products of the reaction and both can be in a continuum of possible states. Then the number of states in a small *energy volume* is the product of the electron and neutrino's states:

$$d^2N_s = dN_e dN_\nu.$$

The two particles share the Q energy:

$$Q_\beta = T_e + T_\nu.$$

For simplicity we assume that the mass of the neutrino is zero (it's much smaller than the electron mass and of the kinetic mass of the neutrino itself). Then we can take the relativistic expression

$$T_\nu = cp_\nu,$$

while for the electron

$$E^2 = p^2c^2 + m^2c^4 \quad \rightarrow \quad E = T_e + m_ec^2 \quad \text{with } T_e = \sqrt{p_e^2c^2 + m_e^2c^4} - m_ec^2$$

and we then write the kinetic energy of the neutrino as a function of the electron's,

$$T_\nu = Q_\beta - T_e.$$

The number of states for the electron can be calculated from the quantized momentum, under the assumption that the electron state is a free particle $\left(\psi \sim e^{i\vec{k}\cdot\vec{r}}\right)$ in a region of volume $V = L^3$:

$$dN_e = \left(\frac{L}{2\pi}\right)^3 4\pi k_e^2 dk_e = \frac{4\pi V}{(2\pi\hbar)^3} p_e^2 dp_e$$

and the same for the neutrino,

$$dN_\nu = \frac{4\pi V}{(2\pi\hbar)^3} p_\nu^2 dp_\nu$$

where we used the relationship between momentum and wavenumber: $\vec{p} = \hbar\vec{k}$.

At a given momentum/energy value for the electron, we can write the density of states as

$$\rho(p_e)\,dp_e = dN_e \frac{dN_\nu}{dT_\nu} = 16\pi^2 \frac{V^2}{(2\pi\hbar)^6} p_e^2 dp_e p_\nu^2 \frac{dp_\nu}{dT_\nu} = \frac{V^2}{4\pi^4\hbar^6c^3}[Q - T_e]^2 p_e^2 dp_e$$

where we used : $\frac{dT_\nu}{dp_\nu} = c$ and $p_\nu = (Q_\beta - T_e)/c$.

The density of states is then

$$\rho(p_e)\,dp_e = \frac{V^2}{4\pi^4\hbar^6c^3}[Q - T_e]^2 p_e^2 dp_e = \frac{V^2}{4\pi^4\hbar^6c^3}\left[Q - \left(\sqrt{p_e^2c^2 + m_e^2c^4} - m_ec^2\right)\right]^2 p_e^2 dp_e$$

or rewriting this expression in terms of the electron kinetic energy:

$$\rho(T_e) = \frac{V^2}{4\pi^4\hbar^6c^3}[Q - T_e]^2 p_e^2 \frac{dp_e}{dT_e} = \frac{V^2}{4c^6\pi^4\hbar^6}[Q - T_e]^2 \sqrt{T_e^2 + 2T_em_ec^2}\,\left(T_e + m_ec^2\right)$$

$\left(\text{as } p_e dp_e = \left(T_e + m_e c^2\right)/c^2 dT_e\right)$

Knowing the density of states, we can calculate how many electrons are emitted in the beta decay *with a given energy*. This will be proportional to the rate of emission calculated from the Fermi Golden Rule, times the density of states:

$$N(p) = CF(Z,Q)|V_{fi}|^2 \frac{p^2}{c^2}[Q-T]^2 = CF(Z,Q)|V_{fi}|^2 \frac{p^2}{c^2}\left[Q - \left(\sqrt{p_e^2 c^2 + m_e^2 c^4} - m_e c^2\right)\right]^2$$

and

$$N\left(T_e\right) = \frac{C}{c^5} F(Z,Q)|V_{fi}|^2 \left[Q - T_e\right]^2 \sqrt{T_e^2 + 2T_e m_e c^2}\left(T_e + m_e c^2\right)$$

These distributions are nothing else than the *spectrum* of the emitted beta particles (electron or positron). In these expression we collected in the constant C various parameters deriving from the Fermi Golden Rule and density of states calculations, since we want to highlight only the dependence on the energy and momentum. Also, we introduced a new function, F(Z, Q), called the Fermi function, that takes into account the *shape* of the nuclear wavefunction and in particular it describes the Coulomb attraction or repulsion of the electron or positron from the nucleus. Thus, F(Z, Q) is different, depending on the type of decay. These distributions were plotted in Fig. 45. Notice that these distributions (as well as the decay rate below) are the product of three terms:

- the Statistical factor (arising from the density of states calculation), $\frac{p^2}{c^2}[Q-T]^2$
- the Fermi function (accounting for the Coulomb interaction), F(Z, Q)
- and the Transition amplitude from the Fermi Golden Rule, $|V_{fi}|^2$

These three terms reflect the three ingredients that determine the spectrum and decay rate of in beta decay processes.

Decay rate

The decay rate is obtained from Fermi’s Golden rule:

$$W = \frac{2\pi}{\hbar}|V_{if}|^2 \rho(E)$$

where ρ(E) is the total density of states. ρ(E) (and thus the decay rate) is obtained by summing over all possible states of the beta particle, as counted by the density of states. Thus, in practice, we need to integrate the density of states over all possible momentum of the outgoing electron/positron. Upon integration over p_e we obtain:

$$\rho(E) = \frac{V^2}{4\pi^4\hbar^6 c^3}\int_0^{p_e^{max}} dp_e \left[Q - T_e\right]^2 p_e^2 \approx \frac{V^2}{4\pi^4\hbar^6 c^3}\frac{\left(Q - mc^2\right)^5}{30c^3}$$

(where we took $T_e \approx pc$ in the relativistic limit for high electron speed).

We can finally write the decay rate as:

$$\begin{aligned} W = \frac{2\pi}{\hbar}|V_{if}|^2 \rho(E) &= \frac{2\pi}{\hbar}\frac{g}{V}^2 |M_{np}|^2 F\left(Z, Q_\beta\right)\frac{V^2}{4\pi^4\hbar^6 c^3}\frac{\left(Q - mc^2\right)^5}{30c^3} \\ &= G_F^2 |M_{np}|^2 F\left(Z, Q_\beta\right)\frac{\left(Q - mc^2\right)^5}{60\pi^3\hbar(\hbar c)^6} \end{aligned}$$

where we introduced the constant

$$G_F = \frac{1}{\sqrt{2\pi^3}}\frac{g m_e^2 c}{\hbar^3}$$

which gives the strength of the weak interaction. Comparing to the strength of the electromagnetic interaction, as given by the fine constant $\alpha = \frac{e^2}{\hbar c} \sim \frac{1}{137}$, the weak is interaction is much smaller, with a constant $\sim 10^{-6}$.

We can also write the differential decay rate $\frac{dW}{dp_e}$:

$$\frac{dW}{dp_e} = \frac{2\pi}{\hbar}|V_{if}|^2 \rho\left(p_e\right) \propto F(Z,Q)\left[Q - T_e\right]^2 p_e^2$$

The square root of this quantity is then a linear function in the neutrino kinetic energy, $Q-T_e$:

$$\sqrt{\frac{dW}{dp_e}\frac{1}{p_e^2F(Z,Q)}}\propto Q-T_e$$

This is the Fermi-Kurie relation. Usually, the Fermi-Kurie plot is used to infer by linear regression the maximum electron energy (or Q) by finding the straight line intercept.

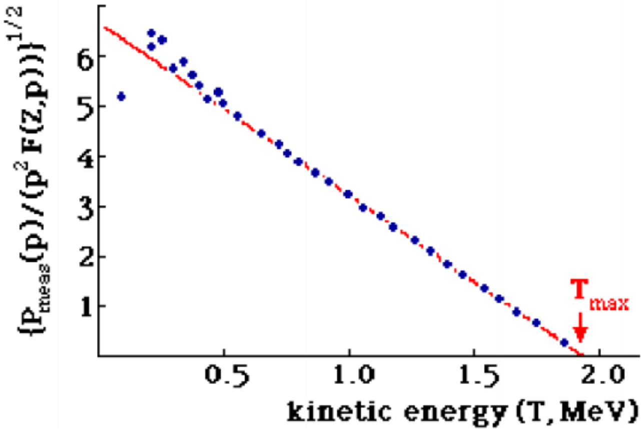


Figure 7.2.3: Example of Fermi-Kurie plot (see also Krane, Fig. 9.4, 9.5) (CC BY-NC-ND; Paola Cappellaro)

CHAPTER OVERVIEW

8: Applications of Nuclear Science

We have now a clearer picture of the nuclear structure and of the radioactive decays, as well as the formalism –based on quantum mechanics and quantum field theory– that describes their dynamics. We can turn to the study of some applications of these ideas.

First, we will study how radiation interacts with matter. This is fundamental both in order to know what are the effects of radiation emitted during nuclear processes on the materials around (and the people) and in order to devise detectors that can measure these radiations. At the same time the knowledge of how radiation interacts with matter leads to many important applications in e.g. nuclear medicine, for imaging and therapy, in materials science, for imaging and diagnostic, in agriculture, archeology etc. Most of you might have already studied these applications in 22.01 and also analyzed the processes that give rise to the interactions. Thus we will be here only have a quick review, focusing mostly on the physical processes.

Then we will study two nuclear reactions (fission and fusion) that can be used as sources of energy (or in the case of fusion, that holds that promise).

8.1: Interaction of Radiation with Matter

Cross Section

Classically, the cross section is the area on which a colliding projectile can impact. Thus for example the cross section of a spherical target of radius r is just given by πr^2. The cross section has then units of an area. Let's consider for example a nucleus with mass number A. The radius of the nucleus is then $R \approx R_0 A^{1/3} = 1.25 A^{1/3}\text{fm}$ and the classical cross section would be $\sigma = \pi R_0^2 A^{2/3} \approx 5 A^{2/3}\text{fm}^2$. For a typical heavy nucleus, such as gold, A = 197, we have $\sigma \approx 100\text{fm}^2 = 1 \text{ barn } (\text{ symbol b}, 1b = 10^{-28} \text{ m}^2 = 10^{-24} \text{ cm}^2 = 100\text{fm}^2 \ )$.

When scattering a particle off a target however, what becomes important is not the head-on collision (as between balls) but the interaction between the particle and the target (e.g. Coulomb, nuclear interaction, weak interaction etc.). For macroscopic objects the details of these interactions are lumped together and hidden. For single particles this is not the case, and for example we can as well have a collision even if the distance between projectile and target is larger than the target radius. Thus the cross section takes on a different meaning and it is now defined as the effective area or more precisely as a measure of the probability of a collision. Even in the classical analogy, it is easy to see why the cross section has this statistical meaning, since in a collision there is a certain (probabilistic) distribution of the impact distance. The cross section also describes the probability of a given (nuclear) reaction to occur, a reaction that can be generally written as:

$$a + X \rightarrow X' + b \quad \text{ or } \quad X(a, b)X'$$

where X is an heavy target and a a small projectile (such as a neutron, proton, alpha...) while X' and b are the reaction products (again with b being nucleons or light nucleus, or in some cases a gamma ray).

Then let I_a be the current of incoming particles, hitting on an heavy (hence stationary) target. The heavy product X' will also be almost stationary and only b will escape the material and be measured. Thus we will observe the b products arriving at a detector at a rate R_b. If there are n target nuclei per unit area, the cross section can then be written as

$$\sigma = \frac{R_b}{I_a n}$$

This quantity do not always agree with the estimated cross section based on the nucleus radius. For example, proton scattering x-section can be higher than neutrons, because of the Coulomb interaction. Neutrinos x-section then will be even smaller, because they only interact via the weak interaction.

Differential Cross Section

The outgoing particles (b) are scattered in all directions. However most of the time the detector only occupies a small region of space. Thus we can only measure the rate R_b at a particular location, identified by the angles ϑ, φ. What we are actually measuring is the rate of scattered particles in the small solid angle $d\Omega$, $r(\vartheta, \varphi)$, and the relevant cross section is the differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{r(\vartheta, \varphi)}{4\pi I_a n}$$

From this quantity, the total cross section, defined above, can be calculated as

$$\sigma = \int_{4\pi} \frac{d\sigma}{d\Omega} d\Omega = \int_0^\pi \sin\vartheta d\vartheta \int_0^{2\pi} d\varphi \frac{d\sigma}{d\Omega}$$

(Notice that having added the factor 4π gives $\sigma = 4\pi \frac{d\sigma}{d\Omega}$ for constant $\frac{d\sigma}{d\Omega}$).

Doubly differential cross section

When one is also interested in the energy of the outgoing particles E_b, because this can give information e.g. on the structure of the target or on the characteristic of the projectile-target interaction, the quantity that is measured is the cross section as a function of energy. This can be simply

$$\frac{d\sigma}{dE_b}$$

if the detector is energy-sensitive but collect particles in any direction, or the **doubly differential cross section**

$$\frac{d^2\sigma}{d\Omega dE_b}$$

Neutron Scattering and Absorption

When neutrons travel inside a material, they will undergo scattering (elastic and inelastic) as well as other reactions, while interacting with the nuclei via the strong, nuclear force. Given a beam of neutron with intensity I_0, when traveling through matter it will interact with the nuclei with a probability given by the total cross section σ_T. At high energies, reactions such as (n,p), (n, α) are possible, but at lower energy usually what happens is the capture of the neutron (n, γ) with the emission of energy in the form of gamma rays. Then, when crossing a small region of space dx the beam is reduced by an amount proportional to the number of nuclei in that region:

$$dI = -I_0\sigma_T n dx \quad \rightarrow \quad I(x) = I_0 e^{-\sigma_T n x}$$

This formula, however, is too simplistic: on one side the cross section depends on the neutron energy (the cross section increases at lower velocity as $1/v$ and at higher energies, the cross section can present some resonances – some peaks) and neutrons will lose part of their energy while traveling, thus the actual cross section will depend on the position. On the other side, not all reactions are absorption reactions, many of them will ”produce” another neutron (i.e., they will only change the energy of the neutron or its direction, thus not attenuating the beam). We then need a better description of the fate of a neutron beam in matter. For example, when one neutron with energy $\sim 1\mathrm{MeV}$ enters the material, it is first slowed down by elastic and inelastic collisions and it is then finally absorbed.

We then want to know how many collisions are necessary to slow down a neutron and to calculate that, we first need to know how much energy does the neutron loose in one collision. Different materials can have different cross sections, however the energy exchange in collision is much higher the lightest the target. Consider an elastic collision with a nucleus of mass M. In the lab frame, the nucleus is initially at rest and the neutron has energy E_0 and momentum mv_0. After the scattering, the neutron energy is E_1, speed $\vec{v}_1$ at an angle φ with $\vec{v}_0$, while the nucleus recoil gives a momentum $M\vec{V}$ at an angle ψ (I will use the notation w for the

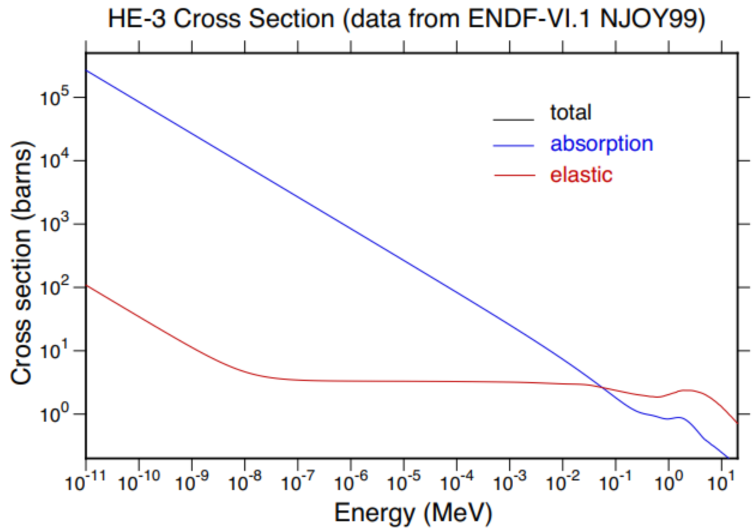


Figure 8.1.1: Cross section $\sigma(E)$ for the neutron-He3 reactions. The data and plot can be obtained online from http://t2.lanl.gov/data/ndviewer.html. (CC BY-NC-ND; Paola Cappellaro)

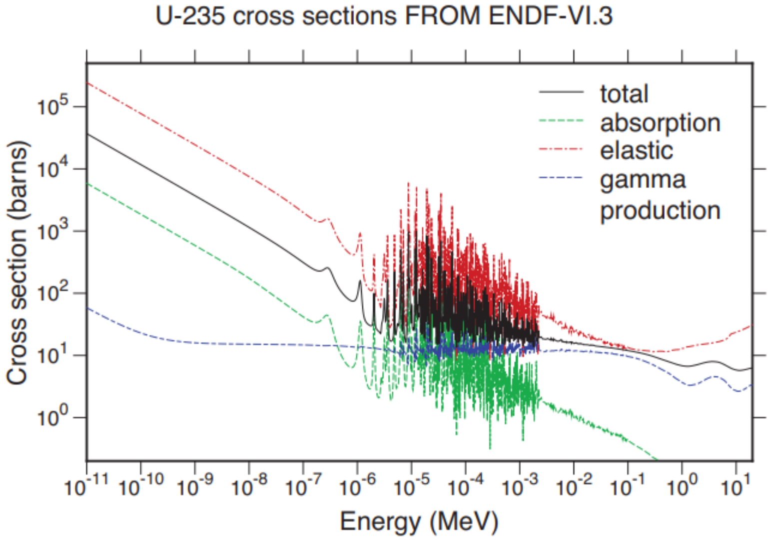


Figure 8.1.2: Cross section $\sigma(E)$ for the neutron-U235 reactions. Notice the $1/v$ dependence at higher energies and resonances at lower energies. (CC BY-NC-ND; Paola Cappellaro)

magnitude of a vector $\vec{w}, w=|\vec{w}|$). The collision is better analyzed in the center of mass frame, where the condition of elastic scattering implies that the relative velocities only change their direction but not their magnitude.

The center of mass velocity is defined as $\vec{v}_{CM}=\frac{m\vec{v}_0+M\dot{V}_0}{m+M}=\frac{m}{m+M}\vec{v}_0$. Relative velocities in the center of mass frame are defined as $\vec{u}=\vec{v}-\vec{v}_{CM}$. We can calculate the neutron (kinetic) energy after the collision from $E_1=\frac{1}{2}m|\vec{v}_1|^2$. An expression for $|\vec{v}_1|^2$ is obtained from the CM speed:

$$|\vec{v}_1|^2=|\vec{u}_1+\vec{v}_{CM}|^2=|\vec{u}_1|^2+|\vec{v}_{CM}|^2+2\vec{u}_1\cdot\vec{v}_{CM}=u_1^2+v_{CM}^2+2u_1v_{CM}\cos\vartheta$$

where we defined ϑ as the scattering angle in the center of mass frame (see Figure 8.1.3).

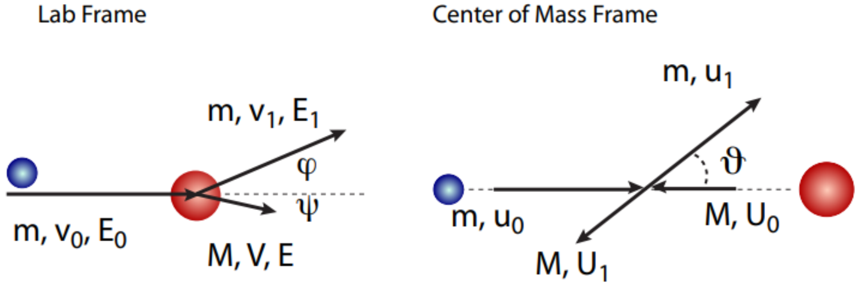


Figure 8.1.3: Neutron scattering from a nucleus. Left, lab frame. Right, center of mass frame (CC BY-NC-ND; Paola Cappellaro)

Given the assumption of elastic scattering, we have $|\vec{u}_1|=|\vec{u}_0|=u_0$, but $u_0=v_0-v_{CM}=v_0\left(1-\frac{m}{m+M}\right)=\frac{M}{m+M}v_0$.

Finally, we can express everything in terms of v_0:

$$|\vec{v}_1|^2=\frac{M^2}{(m+M)^2}v_0^2+\frac{m^2}{(m+M)^2}v_0^2+2\frac{M}{(m+M)}v_0\frac{m}{(m+M)}v_0\cos\vartheta=v_0^2\frac{M^2+m^2+2mM\cos\vartheta}{(m+M)^2}$$

We now simplify this expression by making the approximation $M/m\approx A$, where A is the mass number of the nucleus.

In terms of the neutron energy, we finally have

$$E_1=E_0\frac{A^2+1+2A\cos\vartheta}{(A+1)^2},$$

This means that the final energy can be equal to E_0 (the initial one) if $\vartheta = 0$ – corresponding to no collision– and reaches a minimum value of $E_1 = E_0 \frac{(A-1)^2}{(A+1)^2} = \alpha E_0$ for $\vartheta = \pi$ (here $\alpha = \frac{(A-1)^2}{(A+1)^2}\Big)$.

Notice that from this expression it is clear that the neutron loose more energy in the impact with lighter nuclei, in particular all the energy in the impact with proton:

- If $A \gg 1, E_1 \approx E_0 \frac{A^2+2A\cos\vartheta}{A^2} \approx E_0$, that is, almost no energy is lost.
- If $A = 1, E_1 = E_0 \frac{2+2\cos\vartheta}{4} = E_0 \cos\left(\frac{\vartheta}{2}\right)^2$, and for $\vartheta = \pi$ all the energy is lost.

For low energy, the cross section is independent of ϑ thus we have a flat distribution of the outgoing energies: the probability to scatter in any direction is constant, thus $P(\cos\vartheta) = \frac{1}{2}$. What is the probability of a given energy E_1?

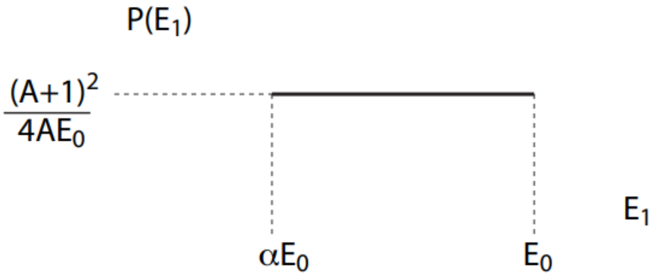


Figure 8.1.4: Probability distribution of the outgoing energy in neutron scattering from a nucleus. (CC BY-NC-ND; Paola Cappellaro)

We have $P\left(E_1\right) dE_1 = -P(\cos\vartheta) d(\cos\vartheta) = -\frac{1}{2}\sin\vartheta d\vartheta$. Then, since $\frac{dE}{d\vartheta} = -\frac{2E_0A}{(A+1)^2}\sin\vartheta$, the probability of a given scattering energy is constant, as expected, and equal to $P\left(E_1\right) = \frac{(A+1)^2}{4E_0A}$. Notice that the probability is different than zero only for $\alpha E_0 \leq E_1 \leq E_0$. The average scattering energy is then $\langle E_1\rangle = E_0 \frac{1+\alpha}{2}$ and the average energy lost in a scattering event is $\langle E_{\text{loss}}\rangle = E_0 \frac{1-\alpha}{2}$.

It still requires many collision to lose enough energy so that a final capture is probable. How many?

The average energy after one collision is $\langle E_1\rangle = E_0 \frac{1+\alpha}{2}$. After two collision it can be approximated by $\langle E_2\rangle \approx \langle E_1\rangle \frac{1+\alpha}{2} = E_0 \left(\frac{1+\alpha}{2}\right)^2$. Then, after n collision, we have $\langle E_n\rangle \approx E_0 \left(\frac{1+\alpha}{2}\right)^n = E_0 \left(\frac{\langle E_1\rangle}{E_0}\right)^n$. Thus, if we want to know how many collisions are needed to reach an average thermal energy $E_{th} = \langle E_n\rangle$ we need to calculate n:

$$\frac{E_{th}}{E_0} = \frac{\langle E_n\rangle}{E_0} \approx \left(\frac{\langle E_1\rangle}{E_0}\right)^n \quad \rightarrow \quad n\log\left(\frac{\langle E_1\rangle}{E_0}\right) = \log\left(\frac{E_{th}}{E_0}\right) \quad \rightarrow \quad n = \log\left(\frac{E_{th}}{E_0}\right) / \log\left(\frac{\langle E_1\rangle}{E_0}\right)$$

However, this calculation is not very precise, since the approximation we made, that we can calculate the average energy after the n^{th} scattering $\langle E_n\rangle$ considering only the average after the $(n-1)^{th}$ scattering is not a good one, since the energy distribution is not peaked around its average (but is quite flat). Consider instead the quantity $\log\left(\frac{E_{n-1}}{E_n}\right)$ and take the average over the possible final energy (note that this is the same as calculating for the first collision):

$$\left\langle \log\left(\frac{E_{n-1}}{E_n}\right)\right\rangle = \int_{\alpha E_{n-1}}^{E_{n-1}} \log\left(\frac{E_{n-1}}{E_n}\right) P\left(E_n\right) dE_n = \int_{\alpha E_{n-1}}^{E_{n-1}} \log\left(\frac{E_{n-1}}{E_n}\right) \frac{(A+1)^2}{4AE_{n-1}} dE_n = 1 + \frac{(A-1)^2}{2A} \log\left(\frac{A-1}{A+1}\right)$$

The expression $\xi = \left\langle \log\left(\frac{E_{n-1}}{E_n}\right)\right\rangle$ does not depend on the energy, but only on the moderating nucleus (it depends on A).

Then we have that $\left\langle \log\left(\frac{E_0}{E_n}\right)\right\rangle = \left\langle \log\left(\frac{E_{n-1}}{E_n}\right)^n\right\rangle$ or $\langle\log(E_n)\rangle = \log(E_0) - n\xi$, from which we can calculate the En En number of collisions needed to arrive at a certain energy:

$$n\left(E_0 \rightarrow E_{th}\right)=\frac{1}{\xi} \log \left(\frac{E_{th}}{E_0}\right)$$

with ξ the average logarithmic energy loss:

$$\xi=1+\frac{(A-1)^2}{2 A} \log \left(\frac{A-1}{A+1}\right)$$

For protons $\left({ }^1 \mathrm{H}\right), \xi=1$ and it takes 18 collision to moderate neutrons emitted in fission $(E=2 \mathrm{MeV})$ while 2200 collisions are needed in $238 \mathrm{U}$.

Material	A	α	ξ	n
H	1	0	1	18.2
$\mathrm{H}_2 0$	1&16	–	0.920	19.8
D	2	0.111	0.725	25.1
He	4	0.360	0.425	42.8
Be	9	0.640	0.207	88.1
C	12	0.716	0.158	115
U	238	0.983	0.0084	2172

Charged particle interaction

Charged particles (such as alpha particles and electrons/positrons) going through matter can interact both with the nuclei –via the nuclear interaction and the coulomb interaction– and with the electron cloud –via the Coulomb interaction. Although the effects of a collision with the light electron is going to affect the colliding particle much less than an impact with the heavy nucleus, the probability of such a collision is much higher. This can be intuitively understood by analyzing the effective *size* of the nucleus and the electronic cloud. While the nucleus have a radius of about 8fm, the atomic radius is on the order of angstroms $\left(\text{or } 10^5 \mathrm{fm}\right)$ Then the *area* offered to the incoming particle is on the order of $\pi(8 f m)^2 \sim 200 f m^2=2$ barns .

On the other side, the electronic cloud present an area of $\pi\left(10^5 f m\right)^2 \sim \pi 10^8$ barns to the incoming particle. Although the cross section of the reaction (or the probability of interaction between particles) is not the same as the area (as it is for classical particles) still these rough estimates give the correct order of magnitude for it.

Thus the interactions with the electrons in the atom dominate the overall charged particle/matter interaction. However the collision with the nucleus gives rise to a peculiar angular distribution, which is what lead to the discovery of the nucleus itself. We will thus study both types of scattering for light charged projectiles such as alpha particles and protons.

Alpha particles collision with the electronic cloud

Let us consider first the slowing down of alpha particles in matter. We first analyze the collision of one alpha particle with one electron.

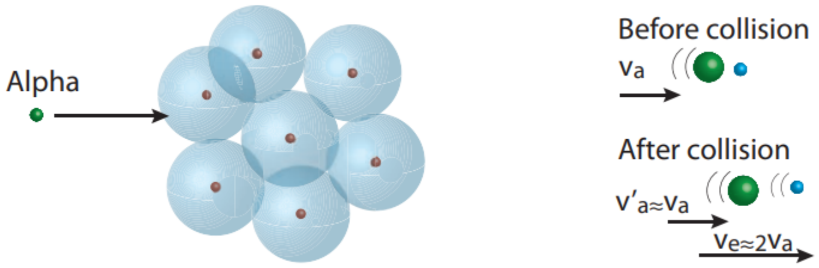


Figure 8.1.5: Left: Charged particles interact mostly with the electronic cloud. Right: Conservation of momentum and kinetic energy in the collision of a very heavy object with a very light one (CC BY-NC-ND; Paola Cappellaro)

If the collision is elastic, momentum and kinetic energy are conserved (here we consider a classical, non-relativistic collision)

$$m_\alpha v_\alpha=m_\alpha v_\alpha^{\prime}+m_e v_e, \quad m_\alpha v_\alpha^2=m_\alpha v_\alpha^{\prime 2}+m_e v_e^2$$

Solving for $v_a^{\prime}$ and v_e we find:

$$v'_\alpha = v_\alpha - 2v_\alpha \frac{m_e}{m_e + m_\alpha}, \quad v_e = 2v_\alpha \frac{m_\alpha}{m_e + m_\alpha}$$

Since $m_e/m_\alpha \ll 1$, we can approximate the electron velocity by $v_e \approx 2v_\alpha$. Then the change in energy for the alpha particle, given by the energy acquired by the electron, is

$$\Delta E = \frac{1}{2} m_e v_e^2 = \frac{1}{2} m_e (2v_\alpha)^2 = 4\frac{m_e}{m_\alpha} E_\alpha$$

thus the alpha particle looses a tiny fraction of its original energy due to the collision with a single electron:

$$\frac{\Delta E_\alpha}{E_\alpha} \sim \frac{m_e}{m_\alpha} \ll 1$$

The small fractional energy loss yields the characteristics of alpha slowing down:

1. Thousands of events (collisions) are needed to effectively slow down and stop the alpha particle
2. As the alpha particle momentum is barely perturbed by individual collisions, the particle travels in a straight line inside matter.
3. The *collisions* are due to Coulomb interaction, which is an infinite-range interaction. Then, the alpha particle interacts simultaneously with many electrons, yielding a continuous slowing down until the particle is stopped and a certain stopping range.
4. [The electrons which are the collision targets get ionized, thus they lead to a visible trail in the alpha particle path (e.g. in cloud chambers)

Definition: Stopping power

We calculated the energy lost by the alpha particle in the collision with one electron. A more important quantity is the average energy loss of the particle per unit path length, which is called the stopping power.

We consider an alpha particle traveling along the x direction and interacting with an electron at the origin of the x-axis and at a distance b from it. It is natural to assume cylindrical coordinates for this problem.

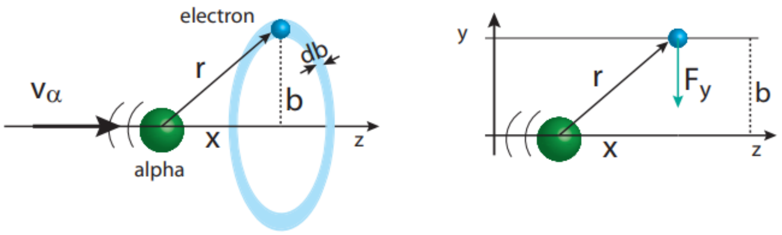


Figure 8.1.6: Geometry for the alpha/electron collision. Left: Impact parameter b and cylindrical coordinates (x, b). Right: Coulomb force parallel to the momentum change (in the y direction). (CC BY-NC-ND; Paola Cappellaro)

The change in momentum of the electron is given by the Coulomb force, integrated over the interaction time. The Coulomb interaction is given by $\vec{F} = \frac{eQ}{4\pi\epsilon_0}\frac{\hat{r}}{|\vec{r}|^2}$, where $\vec{r} = r\hat{r}$ is the vector joining the alpha to the electron. Only the component of the force in the “radial” (y) direction gives rise to a change in momentum (the longitudinal force when integrated has a zero net contribution), so we calculate $\vec{F}\cdot\hat{y} = |F|\hat{r}\cdot\hat{y}$. From the figure above we have $\hat{r}\cdot\hat{y} = \frac{b}{(x^2+b^2)^{1/2}}$ and finally the force $F_y = \frac{eQ}{4\pi\epsilon_0}\frac{b}{(x^2+b^2)^{3/2}}$. The change in momentum is then

$$\Delta p_{=} \int_0^\infty F_y dt = \int_{-\infty}^{\infty} \frac{dx}{v_\alpha} \frac{e^2 Z_\alpha}{4\pi\epsilon_0} \frac{b}{(x^2+b^2)^{3/2}}$$

where we used the relation $\frac{dx}{dt} = v_\alpha$ between the alpha particle velocity (which is constant with time under our assumptions) and $Q = Z_\alpha e = 2e$. By considering the electron initially at rest we have

$$\Delta p = p_e = \frac{e^2 Z}{4\pi\epsilon_0 v b} \int \frac{d\xi}{(1+\xi^2)^{3/2}} = 2\frac{e^2 Z_\alpha}{4\pi\epsilon_0 v_\alpha b}$$

where we used $\xi = x/b$. Then, the energy lost by the alpha particle due to one electron is

$$\Delta E = \frac{p_e^2}{2m} = 2\frac{e^4 Z_\alpha^2}{(4\pi\epsilon_0)^2 m_e v^2 b^2}$$

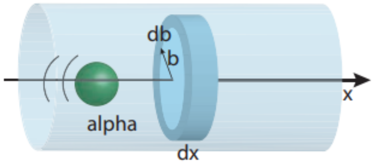


Figure 8.1.7: To find the stopping power we integrate over all impact parameters b, in a small thickness dx. (CC BY-NC-ND; Paola Cappellaro)

We now sum over all electrons in the material. The number of electrons in an infinitesimal cylinder is $dN_e = n_e 2\pi b db dx$, where n_e is the electron's number density (which can be e.g. calculate from $n_e = \frac{N_A Z\rho}{A}$, with N$_A$ Avogadro's number and ρ the mass density of the material).

Then

$$-dE = 2\pi dx \int n_e \Delta E b db \rightarrow \frac{dE}{dx} = -2\pi \int n_e \Delta E(b) b db = -\frac{4\pi e^4 Z_\alpha^2 n_e}{(4\pi\epsilon_0)^2 m_e v_\alpha^2}\int \frac{db}{b}$$

The integral should be evaluated between 0 and ∞. However this is not mathematically possible (since it diverges) and it is also physically unsound. We expect in fact to have a distance of closest approach such that the maximum energy exchange (as in the hard-on collision studied previously) is achieved. We had obtained $E_e = 2m_e v_\alpha^2$. Then we set this energy equal to the electron's Coulomb potential energy: $E_e \approx \frac{1}{4\pi\epsilon_0}\frac{e^2}{b_{\min}}$ from which we obtain

$$b_{\min} \sim \frac{1}{4\pi\epsilon_0}\frac{e^2}{2m_e v_\alpha^2}$$

The maximum b is given by approximately the Bohr radius (or the atom's radius). This can be calculated by setting $\frac{1}{4\pi\epsilon_0}\frac{e^2}{b_{\max}} \sim E_I$ where E_I is the mean excitation energy of the atomic electrons. Then what we are stating is that the maximum impact parameter is the one at which the minimum energy exchange happen, and this minimum energy is the minimum energy required to excite (knock off) an electron out of the atom. Although the mean excitation energy of the atomic electrons is a concept related to the ionization energy (which is on the order of 4 − 15eV) here E_I is taken as an empirical parameter, which has been found to be well approximated by $E_I \sim 10Z$eV (with Z the atomic number of the target). Finally we have

$$\frac{b_{\max}}{b_{\min}} = \frac{2m_e v_\alpha^2}{Z_\alpha E_I}$$

and the stopping power is

$$-\frac{dE}{dx} = \frac{4\pi e^4 Z_\alpha^2 n_e}{(4\pi\epsilon_0)^2 m_e v_\alpha^2}\ln\left(\frac{b_{\max}}{b_{\min}}\right) = \frac{4\pi e^4 Z_\alpha^2 n_e}{(4\pi\epsilon_0)^2 m_e v_\alpha^2}\ln\Lambda$$

with Λ called the Coulomb logarithm.

Since the stopping power, or energy lost per unit length, is given by the energy lost in one collision (or ΔE) times the number of collision (given by the number of electron per unit volume times the probability of one electron collision, given by the cross section) we have the relation:

$$-\frac{dE}{dx} = \sigma_c n_e \Delta E$$

from which we can obtain the cross section itself. Since $\Delta E = 2m_e v^2$, we have

$$\sigma_c = \frac{2\pi e^4 Z_\alpha^2}{(4\pi\epsilon_0)^2 m_e^2 v_\alpha^4}\ln\Lambda$$

This can also be rewritten in terms of more general constants. We define the classical electron radius as

$$r_e = \frac{1}{4\pi\epsilon_0}\frac{e^2}{m_e c^2} \sim 2.8\mathrm{fm},$$

which is the distance at which the Coulomb energy is equal to the rest mass. Although this is not close to the real size of an electron (as for example we would expect the electron radius –if it could be well defined– to be much smaller than the nucleus radius) it gives the correct order of magnitude of the effective area in the collision by charged particles. Also we write $\beta = \frac{v}{c}$, so that

$$\sigma_c = 2\pi r_e^2 \frac{Z_\alpha^2}{\beta^4} \ln\Lambda$$

Since β is usually quite small for alpha particles, the cross section can be quite large. For example for a typical alpha energy of $E_\alpha = 4\mathrm{MeV}$, and its rest mass $m_\alpha c^2 \sim 4000\mathrm{MeV}$, we have $\frac{v^2}{c^2} \sim 2\times 10^{-3}$. The Coulomb logarithm is on the order of $\ln\Lambda \sim 5-15$, while $2\pi r_e^2 \sim \frac{1}{2}$ barn. Then the cross section is $\sigma_c \sim \frac{1}{2} 4\cdot 10^6/4\cdot 10 b = 5\times 10^6 b$.

Definition: Stopping length

This is defined by

$$1/l_\alpha = -\frac{1}{E}\frac{dE}{dx}.$$

Then we can write an exponential decay for the energy as a function of distance traveled inside a material: $E(x) = E_0 \exp(-x/l_\alpha)$. Thus the stopping length also gives the distance at which the energy has been reduced by $1/e (\approx 63\%)$.

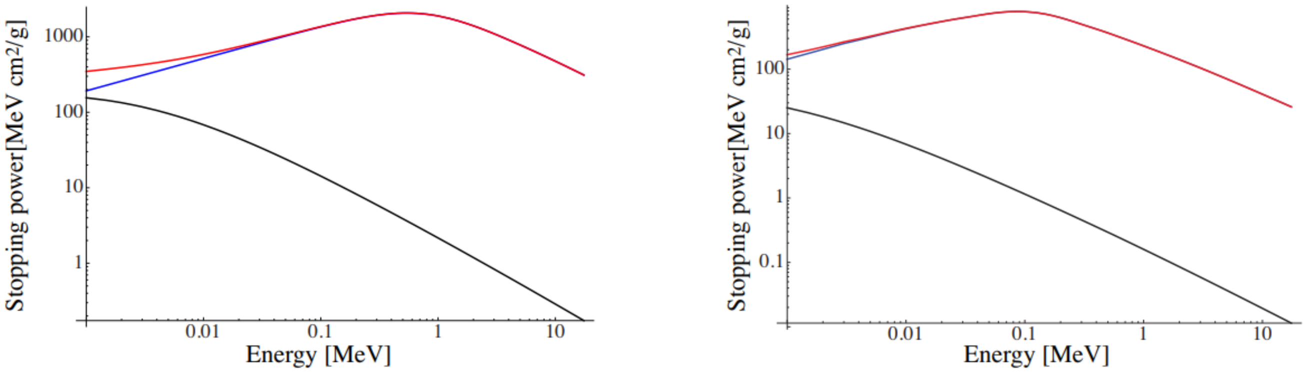


Figure 8.1.8: Stopping power for alpha particles (left) and protons (right) in graphite. x-axis: Energy in MeV. y-axis: Stopping power (MeV cm^2/g). The red curve is the total stopping power, given by the Coulomb stopping power from collision with the electrons (blue) and the Rutherford stopping power (black) from collision with the nuclei. The data is taken from NIST. (CC BY-NC-ND; Paola Cappellaro)

In terms of the cross section the stopping length is:

$$1/l_\alpha = 4\frac{m_2}{m_\alpha}\sigma_c Z n,$$

where n, the atomic number density can be expressed in terms of the mass density and the Avogadro number, $n = \frac{\rho}{A} N_A$.

Example 8.1.1

Stopping length for lead: $1/l_\alpha = 4\times 10^4\ \mathrm{cm}^{-1}$ or $l_\alpha = 2.5\times 10^{-5}$ cm . The range of the particle in the material is however many stopping lengths (on the order of 10), thus the range in lead is around 2.5μm.

Definition: Range

The range is more precisely defined as the distance a particle travels before coming to rest. Then, the range for a particle of initial kinetic energy E_α is defined as

$$R\left(E_\alpha\right)=\int_{r\left(E_\alpha\right)}^{r(E=0)} d x=-\int_0^{E_\alpha}\left(\frac{d E}{d x}\right)^{-1} d E$$

Notice that these is a strong dependence of the stopping power on the mass density of the material (a linear dependence) such that heavier materials are better at stopping charged particles.

However, for alpha particles, it doesn't take a lot to be stopped. For example, they are stopped in 5 mm of air.

Definition: Bragg curve

The Bragg curve describes the Stopping power as a function of the distance traveled inside matter. As the stopping power (and the cross section) increase at lower energies, toward the end of the trajectory there is an increase in energy lost per unit length. This gives rise to a characteristic *Bragg peak* in the curve. This feature is exploited for example for radiation therapy, since it allows a more precise spatial delivery of the dose at the desired location.

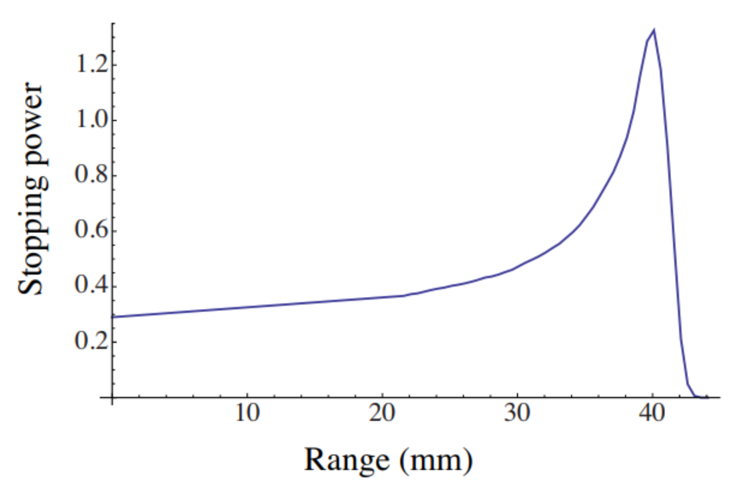


Figure 8.1.9: Bragg curve for protons (distance in mm) (CC BY-NC-ND; Paola Cappellaro)

B. Rutherford - Coulomb scattering

Elastic Coulomb scattering is called Rutherford scattering because of the experiments carried out in Rutherford lab in 1911-1913 that lead to the discovery of the nucleus. The experiments involved scattering alpha particles off a thin layer of gold and observing the scattering angle (as a function of the gold layer thickness).

The interaction is given as before by the Coulomb interaction, but this time between the alpha and the protons in the nucleus. Thus we have some difference with respect to the previous case. First, the interaction is repulsive (as both particle have positive charges). Then more importantly, the projectile is now the smaller particle, thus loosing considerable energy and momentum in the interaction.

What we want to calculate in this interaction is the differential cross section $\frac{d\sigma}{d\Omega}$. The differential (infinitesimal) cross section can be calculated (in a classical picture) by considering the impact parameter b and the small annular region between b and $b+db$:

$$d\sigma=2\pi b db$$

Then the differential cross-section, calculated from the solid angle $d\Omega=d\varphi\sin\vartheta d\vartheta\rightarrow 2\pi\sin\vartheta d\vartheta$ (given the symmetry about φ), is:

$$\frac{d\sigma}{d\Omega}=\frac{2\pi b db}{2\pi \sin\vartheta d\vartheta}=\frac{b}{\sin\vartheta}\frac{db}{d\vartheta}$$

What we need is then a relationship between the impact parameter and the scattered angle ϑ (see figure).

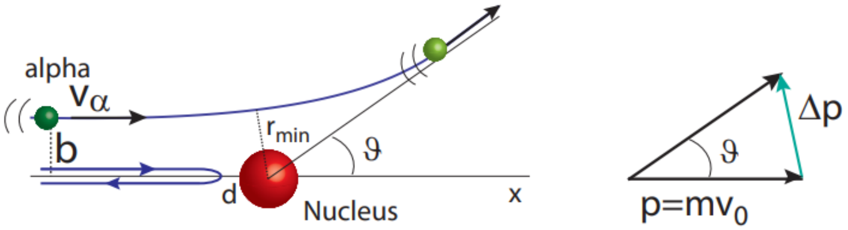


Figure 8.1.10: Rutherford scattering and momentum change (CC BY-NC-ND; Paola Cappellaro)

In order to find b(ϑ) we study the variation of energy, momentum and angular momentum. Conservation of energy states that:

$$\frac{1}{2}mv_0^2=\frac{1}{2}mv^2+\frac{zZe^2}{4\pi\epsilon_0 r}$$

which gives the minimum distance (or distance of closest approach) for zero impact parameter b = 0, that happens when the particle stops and gets deflected back: $\frac{1}{2}mv_0^2=\frac{zZe^2}{4\pi\epsilon_0 d}$.

The momentum changes due to the Coulomb force, as seen in the case of interaction with electrons. Here however the nucleus almost does not acquire any momentum at all, so that only the momentum direction is changed, but not its absolute value: initially the momentum is $p_0=mv_0$ along the incoming (x) direction, and at the end of the interaction it is still mv_0 but along the ϑ direction. Then the change in momentum is $\Delta p=2p_0\sin\frac{\vartheta}{2}=2mv_0\sin\frac{\vartheta}{2}$ (see Fig. above). This momentum difference is along the direction $\delta\hat{p}$, which is at an angle $\frac{\pi-\vartheta}{2}$ with x. We then switch to a reference frame where $\vec{r}=\{r,\gamma\}$, with r the distance $|\vec{r}|$ and γ the angle between the particle position and $\delta\hat{p}$.

The momentum change is brought about by the force in that direction:

$$\Delta p=\int_0^\infty \vec{F}\cdot\delta\hat{p}dt=\frac{zZe^2}{4\pi\epsilon_0}\int_0^\infty \frac{\hat{r}\cdot\delta\hat{p}}{|r^2|}dt=\frac{zZe^2}{4\pi\epsilon_0}\int_0^\infty \frac{\cos\gamma}{r^2}dt$$

Notice that at t = 0, $\gamma=-\frac{\pi-\vartheta}{2}$ (as $\vec{r}$ is almost aligned with x) and at t = ∞, $\gamma=\frac{\pi-\vartheta}{2}$ (Fig). How does γ changes with time?

The angular momentum conservation (which is always satisfied in central potential) provides the answer. At t = 0, the angular momentum is simply $L=mv_0b$. At any later time, we have $L=m\vec{r}\times\vec{v}$. In the coordinate system $\vec{r}=\{r,\gamma\}$ the velocity has a radial and an angular component:

$$\vec{v}=\dot{r}\hat{r}+r\dot{\gamma}\vec{\gamma}$$

and only this last one contributes to the angular momentum (the other being parallel):

$$L=mr^2\frac{d\gamma}{dt}\quad\rightarrow\quad\frac{1}{r^2}=\frac{\dot{\gamma}}{v_0b}$$

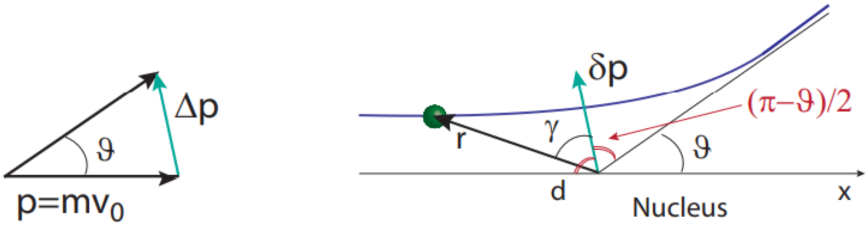


Figure 8.1.11: Momentum change and coordinate system ($\{r,\gamma\}$) for Rutherford scattering. (CC BY-NC-ND; Paola Cappellaro)

Inserting into the integral we have :

$$\Delta p=\frac{zZe^2}{4\pi\epsilon_0}\int_0^\infty\frac{\cos\gamma\dot{\gamma}}{v_0 b}dt=\frac{zZe^2}{4\pi\epsilon_0}\int_{\frac{\pi-\vartheta}{2}}^{\frac{\pi+\vartheta}{2}}\frac{\cos\gamma}{v_0 b}d\gamma=\frac{zZe^2}{4\pi\epsilon_0 v_0 b}2\cos\frac{\vartheta}{2}$$

By equating the two expressions for Δp, we have the desired relationship between b and ϑ:

$$2mv_0\sin\frac{\vartheta}{2}=\frac{zZe^2}{4\pi\epsilon_0 v_0 b}2\cos\frac{\vartheta}{2}\quad\rightarrow\quad b=\frac{zZe^2}{4\pi\epsilon_0 m v_0^2}\cot\frac{\vartheta}{2}$$

Finally the cross section is:

$$\frac{d\sigma}{d\Omega}=\left(\frac{zZe^2}{4\pi\epsilon_0}\right)^2(4T_a)^{-2}\sin^{-4}\left(\frac{\vartheta}{2}\right)$$

(where $T_a=\frac{1}{2}mv_0$ is the incident –alpha– particle kinetic energy). In particular, the Z^2, T^{-2} and $\sin^{-4}$ dependence are in excellent agreement with the experiments. The last dependence is characteristic of single scattering events and observing particles at large angles (although less probable) confirm the presence of a massive nucleus. Consider gold foil of thickness $\zeta=2\mu\mathrm{m}$ and an incident beam of 8MeV alpha particles. The impact parameter that gives a scattering angle of 90 degrees or more is $b\leq\frac{d}{2}=14\mathrm{fm}$. Then the fraction of particles with that impact parameter is $\propto\pi b^2$, thus we have $\zeta n\pi b^2\approx 7.5\times 10^{-5}$ particles scattering at an angle $\geq 90^\circ$ (with n the target density). Although this is a small number, it is quite large compared to the scattering from a uniformly dense target.

C. Electron stopping in matter

Electrons interact with matter mainly due to the Coulomb interaction. However, there are differences in the interaction effects with respect to heavier particles. The differences between the alpha particle and electron behavior in matter is due to their very different mass:

1. Electron-electron collisions change the momentum of the incoming electron, thus deflecting it. Then the path of the electron is not straight anymore.
2. The stopping power is much less, so that e.g. the range is 1cm in lead. (remember that the ratio of the energy lost to the initial energy for alpha particles was small, since it was proportional to the ratio of masses -electron to alpha. Here the masses ratio is 1, and we expect a large change in energy).
3. Electrons have more often a relativistic speed. For example, electrons emitted in the beta decay travel at relativistic speed.
4. There is a second mechanism for deceleration. Since the electrons can undergo rapid changes of velocity due to the collision, it is constantly accelerating (or decelerating) and thus it radiates. This radiation is called **Bremsstrahlung**, or braking radiation (in German).

The stopping power due to the Coulomb interaction can be calculated in a very similar way to what done for the alpha particle. We obtain:

$$-\frac{dE}{dx}=4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{Z\rho N_A}{A}\frac{1}{m_e c^2\beta^2}\ln\Lambda^\prime$$

Here $\Lambda^\prime$ is now a different ratio than the one obtained for the alpha particles, but with a similar meaning: $\Lambda^\prime=\sqrt{\frac{T}{2m_e v^2}}\frac{(T+mc^2)}{E_I}$, where again we can recognize the ratio of the electron energy (determining the minimum distance) and the mean excitation energy E_I (which sets the maximum distance) as well as a correction due to relativistic effects.

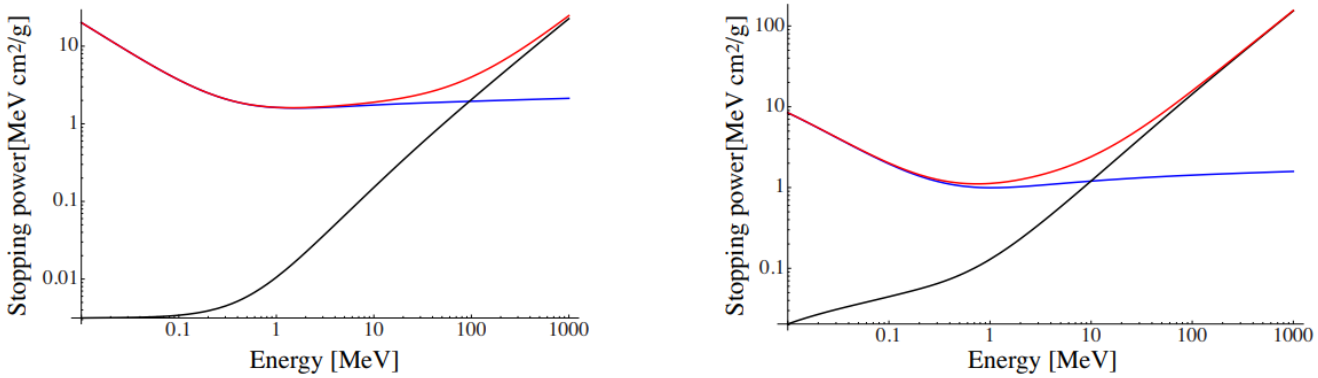


Figure 8.1.12: Stopping power for electrons in graphite (left) and Lead (right). x-axis: Energy in MeV. y-axis: Stopping power (MeV cm^2/g). The red curve is the total stopping power, given by the Coulomb stopping power (blue) and the radiative stopping power (black). Note the different contributions of the two types of processes for the two nuclides: the Bremsstrahlung is much higher for heavier elements such as Lead. The data is taken from NIST. (CC BY-NC-ND; Paola Cappellaro)

A quantum mechanical calculation gives some corrections (for the alpha as well) that become important at relativistic energies (see Krane):

$$-\frac{dE}{dx}=4\pi\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{Z\rho N_A}{A}\frac{1}{m_ec^2\beta^2}\left[\ln\Lambda'+\text{relativistic corrections}\right]$$

To this stopping power, we must add the effects due to the “braking radiation”. Instead of calculating the exact contribution (see Krane), we just want to estimate the relative contribution of Bremsstrahlung to the Compton scattering. The ratio between the radiation stopping power and the coulomb stopping power is given by

$$-\left.\frac{dE}{dx}\right|_r\Big/-\left.\frac{dE}{dx}\right|_c=\frac{e^2}{\hbar c}\frac{Z}{f_c}\frac{T+m_ec^2}{m_ec^2}\approx\frac{T+m_ec^2}{m_ec^2}\frac{Z}{1600}$$

where $f_c\sim 10-12$ is a factor that takes into account relativistic corrections and remember $\frac{e^2}{\hbar c}\approx\frac{1}{137}$. Then the radiation stopping power is important only if $T\gg m_ec^2$ and for large Z. This expression is valid only for relativistic energies; below 1MeV the radiation losses are negligible. Then the total stopping power is given by the sum of the two contributions:

$$\frac{dE}{dx}=\left.\frac{dE}{dx}\right|_c+\left.\frac{dE}{dx}\right|_r$$

Since the electron do not have a linear path in the materials (but a random path with many collisions) it becomes more difficult to calculate ranges from first principles (in practice, we cannot just take $dt=dx/v$ as done in the calculations for alphas). The ranges are then calculated empirically from experiments in which the energy of monoenergetic electron beams is varied to calculate $R(E)$. NIST provides databases of stopping power and ranges for electrons (as well as for alpha particles and protons, see the STAR database at http://www.nist.gov/pml/data/star/index.cfm. Since the variation with the material characteristics (once normalized by the density) is not large, the range measured for one material can be used to estimate ranges for other materials.

8.1.4 Electromagnetic radiation

The interaction of the electromagnetic radiation with matter depends on the energy (thus frequency) of the e.m. radiation itself. We studied the origin of the gamma radiation, since it derives from nuclear reactions. However, it is interesting to also study the behavior of less energetic radiations in matter.

In order of increasing photon energy, the interaction of matter with e.m. radiation can be classified as:

Rayleigh Scattering	Photoelectric Absorption	Compton Scattering	Pair Production
$\hbar\omega < E_I$	$\hbar\omega \geq E_I$	$\hbar\omega \sim m_e c^2$	$\hbar\omega > 2m_e c^2$
$\sim$eV	$\sim$keV	$\sim$MeV	$\geq$MeV
Visible	X-rays	γ-rays	hard γ-rays

Here E_I is the ionization energy for the given target atom.

A classical picture is enough to give some scaling for the scattering cross section. We consider the effects of the interaction of the e.m. wave with an oscillating dipole (as created by an atomic electron).

The electron can be seen as being attached to the atom by a ”spring”, and oscillating around its rest position with frequency ω_0. When the e.m. is incident on the electron, it exerts an additional force. The force acting on the electron is $F=-eE(t)$, with $E(t)=E_0\sin(\omega t)$ the oscillating electric field. This oscillating driving force is in addition to the attraction of the electron to the atom $\sim -kx_e$, where k (given by the Coulomb interaction strength and related to the binding energy E_I) is linked to the electron’s oscillating frequency by $\omega_0^2=k/m_e$. The equation of motion for the electron is then

$$m_e\ddot{x}_e=-kx_e-eE(t) \quad\rightarrow\quad \ddot{x}_e+\omega_0^2x_e=-\frac{e}{m_e}E(t)$$

We seek a solution of the form $x_e(t)=A\sin(\omega t)$, then we have the equation

$$\left(-\omega^2+\omega_0^2\right)A=-\frac{e}{m_e}E_0 \quad\rightarrow\quad A=\frac{1}{\omega^2-\omega_0^2}\frac{e}{m_e}E_0$$

We have already seen that an accelerated charge (or an oscillating dipole) radiates, with a power

$$P=\frac{2}{3}\frac{e^2}{c^3}a^2$$

where the accelaration a is here $a=-\omega^2A\sin(\omega t)$, giving a mean square acceleration

$$\left\langle a^2\right\rangle=\left(\frac{\omega^2}{\omega_0^2-\omega^2}\frac{e}{m_e}E_0\right)^2\frac{1}{2}$$

The radiated power is then

$$P=\frac{1}{3}\left(\frac{e^2}{m_ec^2}\right)^2\frac{\omega^4}{\left(\omega_0^2-\omega^2\right)^2}cE_0^2$$

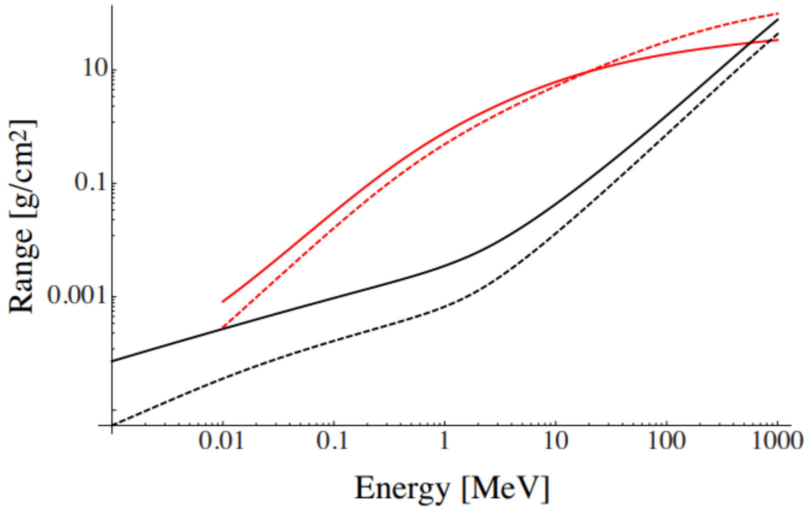


Figure 8.1.13: Range for alpha particles (black) and electrons (red) in Lead (solid curves) and air (dashed). x-axis: Energy in MeV. y-axis: Range (g/cm^2). Note the much longer range for electrons than for alpha particles. Only at very high energy, for lead, the range is shorter for electrons, thanks to the contribution from Bremsstrahlung. The data is taken from NIST. (CC BY-NC-ND; Paola Cappellaro)

The radiation intensity is given by $I_0=\frac{cE_0^2}{8\pi}$ (recall that the e.m. energy density is given by $u=\frac{1}{2}E^2$ and the intensity, or power per unit area, is then $I\sim cu$). Then we can express the radiated power as cross-section×radiation intensity:

$$P=\sigma I_0$$

This yields the cross section for the interaction of e.m. radiation with atoms :

$$\boxed{\sigma=\frac{8\pi}{3}\left(\frac{e^2}{m_ec^2}\right)^2\left(\frac{\omega^2}{\omega_0^2-\omega^2}\right)^2}$$

or in SI units:

$$\sigma=\frac{8\pi}{3}\left(\frac{e^2}{4\pi\epsilon_0m_ec^2}\right)^2\left(\frac{\omega^2}{\omega_0^2-\omega^2}\right)^2=4\pi r_e^2\frac{2}{3}\left(\frac{\omega^2}{\omega_0^2-\omega^2}\right)^2$$

where we used the classical electron radius r_e.

A. Rayleigh Scattering

We first consider the limit in which the e.m. radiation has very low energy: $\omega\ll\omega_0$. In this limit the electron is initially bound to the atom and the e.m. is not going to change that (and break the bound). We can simplify the frequency factor in the scattering cross-section by $\frac{\omega^2}{\omega_0^2-\omega^2}\approx\frac{\omega^2}{\omega_0^2}$, then we have:

$$\boxed{\sigma_R=\frac{8\pi}{3}\left(\frac{e^2}{4\pi\epsilon_0 m_e c^2}\right)^2\frac{\omega^4}{\omega_0^4}}$$

The Rayleigh scattering has a very strong dependence on the wavelength of the e.m. wave. This is what gives the blue color to the sky (and the red color to the sunsets).

B. Thomson Scattering

Thomson scattering is scattering of e.m. radiation that is energetic enough that the electron appears to be initially unbound from the atom (or a free electron) but not energetic enough to impart a relativistic speed to the electron. (If the electron is a free electron, the final frequency of the electron will be the e.m. frequency).

We are then considering the limit:

$$\hbar\omega_0 \ll \hbar\omega \ll m_e c^2$$

where the first inequalities tells us that the binding energy is much smaller than the e.m. energy (hence free electron) while the second tells us that the electron will not gain enough energy to become relativistic.

Then we can simplify the factor $\frac{\omega^2}{\omega_0^2-\omega^2}=\frac{1}{(\omega_0/\omega)^2-1}\approx -1$ and the cross section is simply

$$\boxed{\sigma_T=\frac{8\pi}{3}\left(\frac{e^2}{4\pi\epsilon_0 m_e c^2}\right)^2}$$

with $\sigma_T\sim\frac{2}{3}\text{ barn}$. Notice that contrasting with the Rayleigh scattering, Thomson scattering cross-section is completely independent of the frequency of the incident e.m. radiation (as long as this is in the given range). Both these two types of scattering are elastic scattering, meaning that the atom is left in the same state as it was initially (so conservation of energy is satisfied without any additional energy coming from the internal atomic energy). Even in Thomson scattering we neglect the recoil of the electron (as stated by the inequality $\hbar\omega \ll m_e c^2$). This means that the electron is not changed by this scattering event (the atom is not ionized) even if in its interaction with the e.m. field it behaves as a free electron.

Notice that the cross section is proportional to the classical electron radius square: $\sigma_T=\frac{8\pi}{3}r_e^2$.

C. Photoelectric Effect

At resonance $\omega\approx\omega_0$ the cross-section becomes (mathematically) infinite. The resonance condition means that the e.m. energy is equal to the ionization energy E_I of the electron. Thus, what it really happens is that the electron gets ejected from the atom. Then our simple model, from which we calculated the cross section, is no longer valid (hence the infinite cross section) and we need QM to fully calculate the cross-section. This is the photoelectric effect. Its cross section is strongly dependent on the atomic number (as $\sigma_{pe}\propto Z^5$).

D. Compton Scattering

Compton scattering is the scattering of highly energetic photons from electrons in atoms. In the process the electron acquire an energy high enough to become relativistic and escape the atom (that gets ionized). Thus the scattering is now inelastic (compared to the previous two scattering) and the scattering is an effective way for e.m. radiation to lose energy in matter. At lower energies, we would have the photoelectric effect, in which the photon is absorbed by the atom. The effect is important because it demonstrates that light cannot be explained purely as a wave phenomenon.

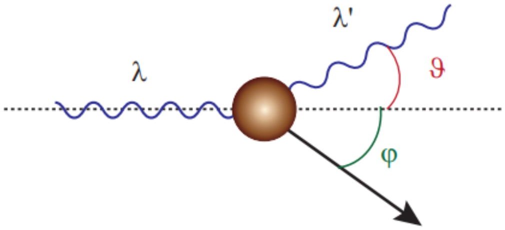


Figure 8.1.14: Photon/Electron collision in Compton scattering. (CC BY-NC-ND; Paola Cappellaro)

From conservation of energy and momentum, we can calculate the energy of the scattered photon.

$$E_\gamma + E_e = E'_\gamma + E'_e \quad \rightarrow \quad \hbar\omega + m_e c^2 = \hbar\omega' + \sqrt{|p|^2 c^2 + m^2 c^4}$$

$$\hbar\vec{k} = \hbar\vec{k}' + \vec{p} \quad \rightarrow \quad \begin{cases} \hbar k = \hbar k' \cos\vartheta + p\cos\varphi \\ \hbar k' \sin\vartheta = p\sin\varphi \end{cases}$$

From these equations we find $p^2 = \frac{(\omega'-\omega)}{c^2}\left[\hbar(\omega'-\omega) - 2mc^2\right]$ and $\cos\varphi = \sqrt{1 - \hbar^2 k'^2 \sin^2\vartheta / p^2}$. Solving for the change in the wavelength $\lambda = \frac{2\pi}{k}$ we find (with $\omega = kc$):

$$\boxed{\Delta\lambda = \frac{2\pi\hbar}{m_e c}(1-\cos\vartheta)}$$

or for the frequency:

$$\hbar\omega' = \hbar\omega\left[1 + \frac{\hbar\omega}{m_e c^2}(1-\cos\vartheta)\right]^{-1}$$

The cross section needs to be calculated from a full QM theory. The result is that

$$\boxed{\sigma_C \approx \sigma_T \frac{m_e c^2}{\hbar\omega}}$$

thus Compton scattering decreases at larger energies.

E. Pair Production

Pair production is the creation of an electron and a positron pair when a high-energy photon interacts in the vicinity of a nucleus. In order not to violate the conservation of momentum, the momentum of the initial photon must be absorbed by something. Thus, pair production cannot occur in empty space out of a single photon; the nucleus (or another photon) is needed to conserve both momentum and energy .

Photon-nucleus pair production can only occur if the photons have an energy exceeding twice the rest mass ($m_e c^2$) of an electron (1.022 MeV):

$$\hbar\omega = T_{e^-} + m_{e^-}c^2 + T_{e^+} + m_{e^+}c^2 \geq 2m_e c^2 = 1.022 MeV$$

Pair production becomes important after the Compton scattering falls off (since its cross-section is \propto 1 / \omega\)).

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