THE STRUCTURE OF MATTER

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Contents

Voorwoord

Het college Structuur der Materie wordt in 2002 gegeven onder verantwoordelijkheid van Prof. Piet Mulders.

In het college wordt de materie om ons heen van groot tot klein behandeld waarbij gebruik gemaakt wordt van kennis opgedaan in quantummechanica (college Quantummechanica I), statistische fysica (college Statistische Fysica I) en relativiteitstheorie (college Relativiteitstheorie). Naast deze aantekeningen wordt het boek van Brehm and Mullin aangeraden als naslagwerk. Soms wordt gebruik gemaakt van (delen van) andere boeken. In een geintegreerd werkcollege worden opgaven gemaakt die betrekking hebben op de stof. Voor specifieke onderdelen van dit college, Atoomfysica, Elementaire deeltjesfysica, Vaste stoffysica, Biofysische onderwerpen en Astrofysica zijn vervolgcolleges gepland die aansluiten op de behandelde stof in het basiscollege Structuur der Materie. Electronisch zijn deze aantekeningen en verdere informatie verkrijgbaar via de http://www.nat.vu.nl/sdm/ website

Piet Mulders
Wim Ubachs
Maart 2002

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Chapter 1

The Structure of Matter

1.1 Introduction

In these lectures we study matter. On the one hand this includes unraveling matter for its constituents, and the search for the forces between these constituents. But it also includes understanding the beauty and principles underlying the complexity. Often these are symmetry principles. Depending on the domains of distances, velocities and energies one is considering one needs to employ quantum mechanics and/or special relativity.

In quantum mechanics a special role is played by *Planck's constant* h, usually given divided by 2π,

$$\begin{aligned} \hbar \;\equiv\; h/2\pi &= 1.054\ 571\ 596\ (82) \times 10^{-34}\ \text{J s} \\ &= 6.582\ 118\ 89\ (26) \times 10^{-22}\ \text{MeV s}. \end{aligned} \tag{1.1}$$

We already have choosen here two different, often used units for energy, the Joule (J) and the electronvolt (eV). The first is the formal MKS unit to be used ($1\ \text{J} = 1\ \text{kg}\,\text{m}^2\,\text{s}^{-2}$), but in many applications in condensed matter, atomic and molecular physics and subatomic physics one uses the eV, or powers thereof[1]. One eV is the energy obtained or needed when an elementary charge,

$$e = 1.602\ 176\ 462\ (63) \times 10^{-19}\ \text{C}, \tag{1.2}$$

is displaced over a potential difference of 1 V. Quantum effects become unimportant in the limit that the product of energy $\times$ time or equivalently momentum $\times$ distance or angular momentum is much larger than $\hbar$. More precisely formulated, when the action $A \gg \hbar$. Then one is in the *classical* domain.

In special relativity a special role is played by *the velocity of light* c,

$$c \;=\; 299\ 792\ 458\ \text{m s}^{-1}. \tag{1.3}$$

In the limit that $v \ll c$ one reaches the *non-relativistic* domain. Schematically one has

Classical Mechanics	$A \gg \hbar$	**Special Relativity**
$v \ll c$		$v \sim c$
Quantum Mechanics	$A \sim \hbar$	**Quantum Field Theory**

[1] k = kilo = 10^3; M = mega = 10^6; G = giga = 10^9; T = tera = 10^{12}; m = milli = 10^{-3}; μ = micro = 10^{-6}; n = nano = 10^{-9}, p = pico = 10^{-12}, f = femto = 10^{-15}.

1.2 Units

The choice of an appropriate set of units is often important, because physical sizes and magnitudes only acquire a meaning when they are considered in relation to each other. This is true specifically for the domain of atomic and molecular physics, nuclear physics and high energy physics, where the typical numbers are difficult to conceive on a macroscopic scale. They are governed by a few fundamental units and constants, which have been discussed in the previous section, namely $\hbar$ and c. In fact one can work with less units by making use of fundamental constants such as $\hbar$ and c. For instance, the quantity c is nowadays used to define the meter. We could as well have set $c = 1$. This would mean that one of the two units, meter or second, is eliminated, e.g. because l/c has the dimension of time, one has 1 m $= 0.33 \times 10^{-8}$ s or eliminating the second one would use that ct has dimension of length and hence 1 s $= 3 \times 10^8$ m. Using both $\hbar$ and c, all length, time and energy or mass units then can be expressed in one unit and powers thereof, for which one can use energy, as shown in the next table. The power of E determines what is referred to as the canonical dimension d of the quantity.

quantity	constructed quantity	dimension	d
time t	$t/\hbar$	(energy)$^{-1}$	-1
length l	$l/(\hbar c)$	(energy)$^{-1}$	-1
momentum p	pc	(energy)^{1}	1
angular momentum ℓ	$\ell/\hbar$	(energy)^{0}	0
energy E	E	(energy)^{1}	1
mass m	mc^2	(energy)^{1}	1
area A	$A/(\hbar c)^2$	(energy)$^{-2}$	-2
force F	$F\,\hbar c$	(energy)^{2}	2
G	$G/(\hbar c^5)$	(energy)$^{-2}$	-2
velocity v	v/c	(energy)^{0}	0

The most appropriate energy unit depends on the domain of applications, e.g. the eV for atomic physics the MeV or GeV for nuclear physics and the GeV or TeV for high energy physics. To convert to other units of length or time we use appropriate combinations of $\hbar$ and c, e.g. for lengths

$$\hbar c \ = \ 0.197\ 326\ 960\ 2\ (77)\ \text{GeV fm} \tag{1.4}$$

This quantity can of course be used to eliminate the meter if one puts $\hbar = c = 1$,

$$1\ \text{fm} \ = \ 10^{-15}\ \text{m} \ \approx \ 5.068\ \text{GeV}^{-1}. \tag{1.5}$$

Remembering only two numbers, e.g. $c \approx 3 \times 10^8$ m/s and $\hbar c \approx 200$ MeV fm ≈ 200 eV nm, it is possible to do the conversions. Often, this can also be used to give reasonable orders of magnitudes. Depending on the specific situation, of course masses come in that one needs to know or look up. Two important masses are that of the electron $m_e c^2 = 0.510\,988\,902\,(21)$ MeV and that of the proton $m_p c^2 \approx 0.938\,271\,998\,(38)$ GeV. Furthermore one encounters the strength of the various interactions. In some cases like the electromagnetic and strong interactions, these can be written as dimensionless quantities, e.g. for electromagnetism the *fine structure constant*

$$\alpha = \frac{e^2}{4\pi\,\epsilon_0\,\hbar c} = 1/137.035\,999\,76\,(50). \tag{1.6}$$

For weak interactions and gravity one has quantities with a dimension, e.g. for gravity Newton's constant,

$$\frac{G}{\hbar c^5} = 6.707\,(10) \times 10^{-39}\ \mathrm{GeV}^{-2}. \tag{1.7}$$

Having many particles, the concept of temperature becomes relevant. A relation with energy is established via the average energy of a particle being of the order of kT, with the Boltzmann constant given by

$$k = 1.380\,650\,3(24) \times 10^{-23}\ \mathrm{J/K} = 8.617\,342(15) \times 10^{-5}\ \mathrm{eV/K}. \tag{1.8}$$

1.3 Physics and mathematics

In order to illustrate the use of units and mathematics, consider as an example the radial Schrödinger equation for an electron in the hydrogen atom. Considering only the (central) electric potential between electron and a central charge Ze, one has the hamiltonian

$$H = -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} \underbrace{-\frac{Ze^2}{4\pi\epsilon_0\, r}}_{+V_c(r)}. \tag{1.9}$$

As should be familiar from elementary quantum mechanics, this hamiltonian and the angular momentum operators ℓ^2 and ℓ_z commute. Thus one can use the eigenfunctions of the latter two operators, the spherical harmonics $Y_\ell^m(\theta,\varphi)$ and find that the 3-dimensional problem after writing

$$\psi(\boldsymbol{r}) = \frac{u_{E\ell}(r)}{r}\, Y_\ell^m(\theta,\varphi), \tag{1.10}$$

reduces to the one-dimensional radial Schrödinger equation[2]

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \underbrace{\frac{\hbar^2\,\ell(\ell+1)}{2m\,r^2} + V_c(r)}_{V_{\mathrm{eff}}(r)} - E\right] u_{E\ell}(r) = 0, \tag{1.11}$$

with boundary condition $u_{E\ell}(0) = 0$ or more precisely, $u_{E\ell}(r) \stackrel{r\to 0}{\longrightarrow} r^{\ell+1}$. First of all it is useful to make this into a dimensionless differential equation for which we then can use our knowledge of mathematics. Define $\rho = r/a_0$ with for the time being a_0 still unspecified. Multiplying the radial Schrödinger equation with $2m\,a_0^2/\hbar^2$ we get

$$\left[-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \frac{e^2}{4\pi\epsilon_0}\frac{2m\,a_0}{\hbar^2}\frac{Z}{\rho} - \frac{2m\,a_0^2\,E}{\hbar^2}\right] u_{E\ell}(\rho) = 0. \tag{1.12}$$

From this dimensionless equation we find that the coefficient multiplying $1/\rho$ is a number. Since we haven't yet specified a_0, this is a good place to do so and one defines the *Bohr radius*

$$a_0 \equiv \frac{4\pi\epsilon_0\,\hbar^2}{m\,e^2}. \tag{1.13}$$

[2]Note that one often encounters the radial wave function $R_{n\ell}(r) = u_{n\ell}(r)/r$. The advantaage of working with $u_{n\ell}$ is that it satisfies precisely the one-dimensional Schrödinger equation (with a boundary condition).

The stuff in the last term in the equation multiplying E must be of the form 1/energy. One defines the *Rydberg energy*

$$R_\infty = \frac{\hbar^2}{2m\,a_0^2} = \frac{1}{2}\,\frac{e^2}{4\pi\epsilon_0\,a_0} = \frac{m\,e^4}{32\pi^2\epsilon_0^2\,\hbar^2}. \tag{1.14}$$

One then obtains the dimensionless equation

$$\left[-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \frac{2Z}{\rho} - \epsilon\right] u_{\epsilon\ell}(\rho) = 0 \tag{1.15}$$

with $\rho = r/a_0$ and $\epsilon = E/R_\infty$.

Before solving this equation let us look at the magnitude of the numbers with which the energies and distances in the problem are compared. We have

$$a_0 \equiv \frac{4\pi\epsilon_0\,\hbar^2}{m\,e^2} = \frac{4\pi\epsilon_0\,\hbar c}{e^2}\,\frac{\hbar c}{mc^2} = \frac{1}{\alpha}\,\frac{\hbar c}{mc^2} \approx 0.53 \times 10^{-10}\text{ m}, \tag{1.16}$$

$$R_\infty = \frac{\hbar^2}{2m\,a_0^2} = \frac{1}{2}\,\alpha\left(\frac{\hbar c}{a_0}\right) = \frac{1}{2}\,\alpha^2\,mc^2 \approx 13.6\text{ eV}. \tag{1.17}$$

One thing to be noticed is that the defining expressions for a_0 and R_∞ involve the electromagnetic charge $e/\sqrt{\epsilon_0}$ and Planck's constant $\hbar$, but it does not involve c. The hydrogen atom invokes quantum mechanics, but not relativity! To evaluate the expressions using our unit-analysis one of course can introduce c afterwards in making estimates. Secondly the nonrelativistic nature of the hydrogen atom is confirmed in the characteristic energy scale being R_∞. From Eq. 1.17 we see using $\alpha = 1/137$ that it is of the order $10^{-4} - 10^{-5}$ of the restenergy of the electron, i.e. very tiny!

Next, we can turn to an algebraic manipulation program or a mathematical handbook to look for the solutions of our dimensionless differential equation (see appendix B.1 on Laguerre polynomials). We see from this treatment that (using $p \rightarrow n-\ell-1$, $a \rightarrow 2\ell+1$ and $x \rightarrow 2Z\rho/n$) the solutions for hydrogen are

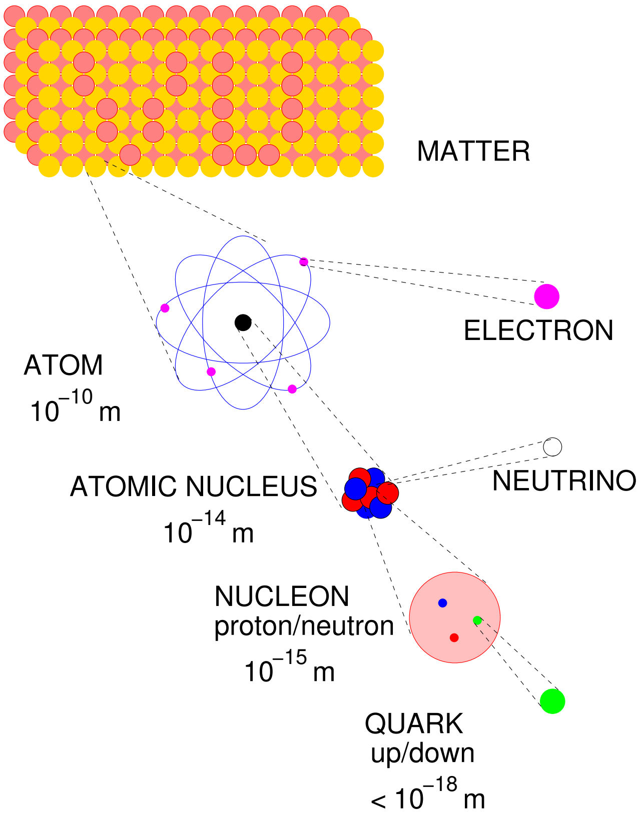
$$u_{n\ell}(\rho) = \left(\frac{2Z}{n\,a_0}\right)^{1/2}\sqrt{\frac{(n-\ell-1)!}{2n\,(n+\ell)!}}\;e^{-Z\rho/n}\left(\frac{2Z\rho}{n}\right)^{\ell+1} L^{2\ell+1}_{n-\ell-1}\left(\frac{2Z\rho}{n}\right) \tag{1.18}$$

with eigenvalues (energies)

$$E_{n\ell} = -\frac{Z^2}{n^2}\,R_\infty, \tag{1.19}$$

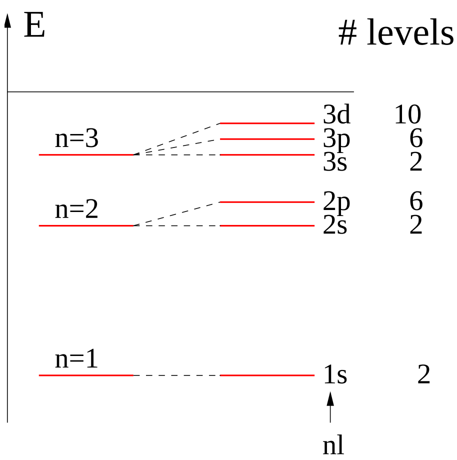
labeled by a principal quantum number number n, choosen such that the energy only depends on n. For a given ℓ one has $n \le \ell + 1$. Actually $n_r = n - \ell - 1$ is the number of nodes in the wave function.

1.4 The constituents of matter

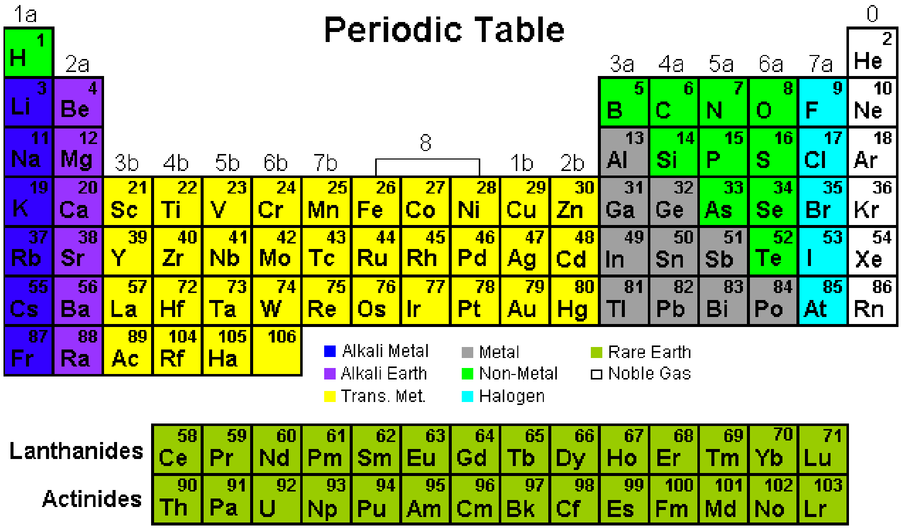


The structure of matter.

The basic units of the matter around us are the atoms. They are found as the building blocks of molecules or solids, bound in a variety of ways discussed in the sections on molecular physics and condensed matter physics. The atoms are composed of the atomic nucleus with a positive charge $+Ze$, which is a multiple of the elementary charge e. The *atomic number* Z characterizes the atom, $Z = 1$ for Hydrogen (H), $Z = 2$ for Helium (He), etc. In the atom the charge of the nucleus is neutralized by Z electrons, bound to the nucleus via the electromagnetic force. The atoms can be organized in the Periodic Table. Its structure is determined by the consecutive filling of the energetically lowest available electron orbits and the *Pauli exclusion principle*, which prohibits for particles with half-integer spin such as the electron (spin 1/2, i.e. two spin states) that identical particles occupy the same orbit.



Typical order of energy levels available for consecutive filling of electronic orbits in an atom. The ℓ-degeneracy of the levels in Hydrogen is lifted because of the electrons screening the nuclear charge, to be discussed in more detail later. The order determines the structure of the period table of the elements. For instance the electronic structure of Carbon (C) with $Z = 12$ is $(1s)^2\,(2s)^2\,(2p)^2$, the electronic structure of iron (Fe) with $Z = 26$ is $(1s)^2\,(2s)^2\,(2p)^6\,(3s)^2\,(3p)^6\,(4s)^2\,(3d)^6$. The order relevant for the periodic table is: 1s, 2s, 2p, 3s, 3p, [4s, 3d], 4p, [5s, 4d], 5p, [6s, 4f, 5d], 6p, [7s, 5f, 6d]. Levels enclosed with brackets have very similar energies.



The mass of an atom is in essence determined by the atomic nucleus, consisting of Z protons, each with a positive charge $+e$ and N neutrons being neutral. Protons and neutrons (together called *nucleons*) have similar masses,

$$m_p = 1.672\,621\,58(13) \times 10^{-27}\ \text{kg} = 938.271\,998(38)\ \text{MeV/c}^2, \tag{1.20}$$
$$m_n = 1.674\,927\,2(14) \times 10^{-27}\ \text{kg} = 939.565\,33(40)\ \text{MeV/c}^2. \tag{1.21}$$

The size of the atomic nucleus is tiny, of the order of 10 fm $= 10^{-14}$ m, as compared to the size of the atom, which is of the order of 1 Å$=$ 0.1 nm $= 10^{-10}$ m. The atomic size is determined by the configuration of the light electrons,

$$m_e = 9.109\,381\,88(72) \times 10^{-31}\ \text{kg} = 0.510\,998\,902(21)\ \text{MeV/c}^2 \tag{1.22}$$

(about 1836 times smaller than the proton), orbiting the nucleus. Electrons can be freed from an atom or additional electrons can be bound, leaving positive or negative *ions*, leading to ionic bounds. Electrons can also be shared by atoms in *covalent* bounds.

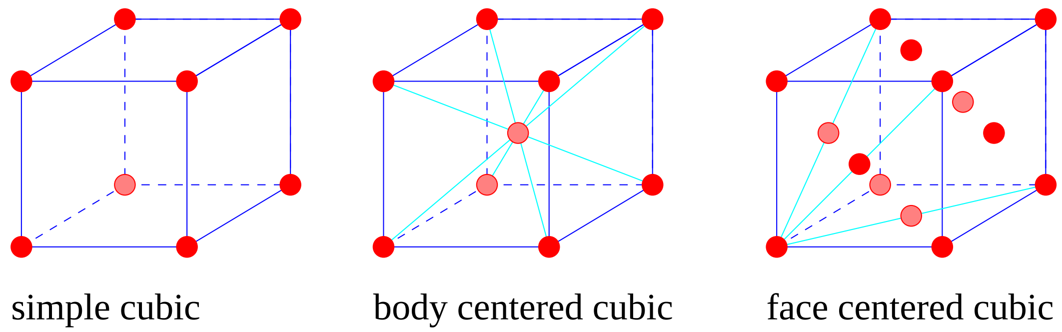
For the mass of the atom one has introduced as standard the *atomic mass unit* (u). It is defined as 1/12 of the mass of the ^{12}C atom,

$$1\ \text{u} = 1.660\,538\,73(13) \times 10^{-27}\ \text{kg} = 931.494\,013(37)\ \text{MeV/c}^2. \tag{1.23}$$

Via this unit one also defines *Avogadro's number*, N_{av},

$$N_{av} = (1\ \text{gr})/(1\ \text{u}) = 6.022\,141\,99(47) \times 10^{23}. \tag{1.24}$$

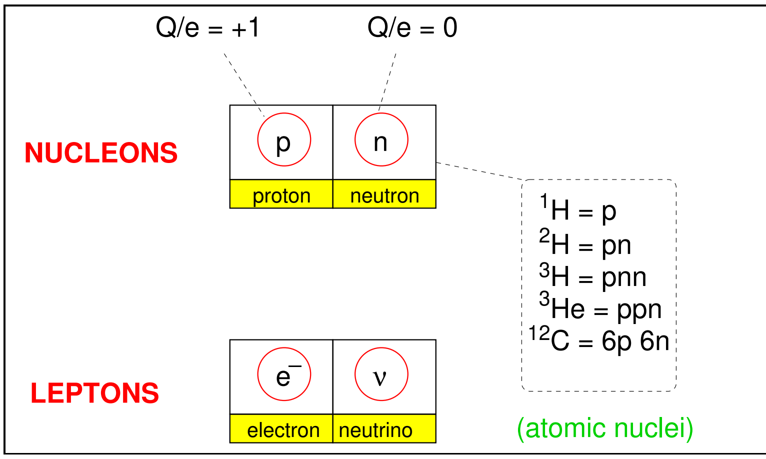
This is typically the number of atoms in a macroscopic sample. Without any mutual interactions, this would lead for the electrons typically to N_{av}-fold degenerate levels as compared to a single atom. In solids, the lifting of this degeneracy because of the e-e interactions and the interactions of electrons with neigboring atoms leads to the band structure. In particular in regularly layered structures such as cristals a wonderful world of phenomena occurs of which superconductivity is one of the most well-known ones. Depending on the occupation of these bands, the band gaps, the presence of impurities in the material and the temperature, completely different behavior emerges, e.g. in the conductivity (conductors, semiconductors and isolators).



The cubic lattices are fairly common lattices. Shown are the simple cubic (sc), body-centered cubic (bcc; in addition 1 atom in the middle of each cube) and face-center cubic (fcc; in the middle of each side also an atom) structures. It turns out that fcc has the most dense packing, but density is not the only factor in determining the lattice structure of a material. Filling the sides of a simple cubic lattices with atoms of a different kind, resembles an fcc structure, but is of course just a simple cubic structure, because the lattice structure is determined by translations leaving the structure invariant.

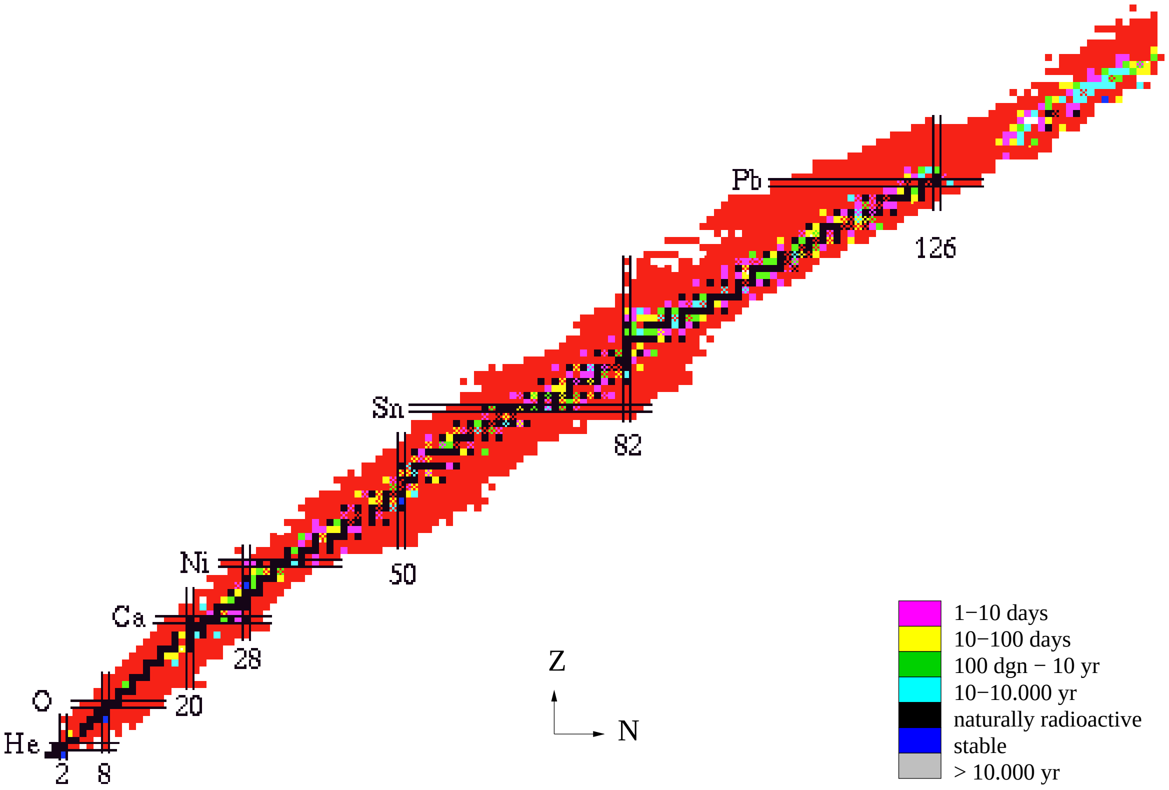
The richness of phenomena ranging from *plasmas* (a hot but usually neutral collection of free atomic nuclei and electrons) in stars or fusion reactors, the cristalline structure of matter extending to macroscopic sizes, superconductivity, macromolecules like DNA and all interactions with light are described with electromagnetic interactions. For this one has a well-developed theoretical framework. Quantum electrodynamics (QED) is a fully relativistic quantummechanical description for the interactions between charges via exchange of *photons* (the light quanta). QED is the basis for obtaining the full (quantum-mechanical) Hamiltonian used in the Schrödinger equation to calculate the wave functions of the electrons. Several techniques, ranging from smart approximations to extensive computer calculations are employed to obtain an effective inter-atomic potential that is used in molecular physics and chemistry. QED also underlies the Maxwell equations. These can be used to describe classically the interactions of charges with electric ($\boldsymbol{E}$) and magnetic ($\boldsymbol{B}$) fields or at a semiclassical level the interactions of charges/atoms with light (quantum optics).

As mentioned already, atoms are characterized by the atomic number Z corresponding to the number of protons in the nucleus. Often there is more than one possibility for the



Constituents of matter (as known in 1935) relevant for length scales above 1 fm.

Island of stability for nuclei.



number of neutrons (N). Nuclei with different number of neutrons for a given Z are called different *isotopes* for the same element. Nuclei are denoted by the atomic symbol (H, He, etc.) and in order to distinguish the isotopes one adds as a left superscript the total number of nucleons $A = Z + N$. One has for Hydrogen ^{1}H = p, ^{2}H = pn (nucleus is called *deuteron*, atom is called *deuterium*) and ^{3}H = pnn (nucleus is called *triton*, atom is called *tritium*). The isotope ^{1}H is most abundant. The ^{2}H abundance is only 0.015 %. The third isotope ^{3}H is not stable. For Helium one has two isotopes, ^{3}He and ^{4}He (α-particle), the latter being the most abundant one. The elements Hydrogen and Helium also make up the bulk of the (at least visible) matter in the universe, roughly in the order 12 : 1 (atoms) or 3 : 1 (mass).

Characteristic binding and excitation energies in nuclei are at the MeV level (compare this with the eV-level for atoms), which for emission and absorption of photons means wavelengths as small as 10^{-12} m. Protons and neutrons in atomic nuclei are bound via a completely different force than that in atoms, namely the *strong force*. To understand the main features of nuclear structure one employs a (nonrelativistic) quantummechanical description with in the Hamiltonian an (effective) potential of which the longest range part is coming from the exchange of pions with masses $m_\pi \approx 140$ MeV, leading to a Yukawa-like tail of the form $V(r) \propto \exp(-r/\lambda\!\!\!^{-}_\pi)/r$ where $\lambda\!\!\!^{-}_\pi$ is the Compton wavelength $\hbar/m_\pi c \approx 1.4$ fm, which is also the characteristic size of nuclei.

As seen in the Z versus N plot for nuclei, stable nuclei lie mostly on or just above the $Z = N$ diagonal and there are many unstable nuclei with vastly different lifetimes. For the magic numbers indicated in the figure, nuclei are particularly stable. An important decay mode for heavy nuclei is the emission of α-particles. The α-decay is a nice example of quantummechanical tunneling through a potential barrier. A second decay is β-decay in which a neutron changes into a proton under emission of an electron and a neutrino,

$$n \longrightarrow p + e^- + \bar{\nu}_e. \tag{1.25}$$

It is this decay that is also responsible for the instability of ^{3}H, decaying via $^3\mathrm{H} \longrightarrow {}^3\mathrm{He} + e^- + \bar{\nu}_e$. β-decay is the manifestation of yet another force, the *weak force*.

In processes like β-decay, but also in interactions of photons or electrons with atoms, conservation laws plays an important role. The most important conservation laws are the conservation of energy, momentum, and angular momentum. For energy and momentum the sum of all energies and the (component-wise) sum of all momenta in initial and final state is the same. For angular momentum the conservation law applies to the total angular momentum of the initial and final state. This is made up from the spins and the orbital angular momenta in a multi-particle or composite system.

Consider β-decay as an example. For protons, neutrons and electrons, the spin is 1/2 (two spin states). This implies that

$$\boldsymbol{J} = \sum_i \boldsymbol{\ell}_i + \sum_i s_i \Longrightarrow \begin{cases} \text{integer J for even number of constituents} \\ \text{half-integer J for odd number of constituents} \end{cases} \tag{1.26}$$

This led e.g. Pauli to postulate the existence of a neutral spin 1/2 particle, the *neutrino*, in β-decay (Eq. 1.25). Indeed, the neutrino was found and turned out to have spin 1/2 (although with only a lefthanded state having $m_s = -1/2$, antiparallel to the momentum).

Angular momentum is also very important in the study of transitions where photons are absorbed or emitted. Photons have spin 1 (although with only the two states with $m_s = \pm 1$, parallel or antiparallel to the momentum). It leads to the selection rule $\Delta J = 0,\ \pm 1$.

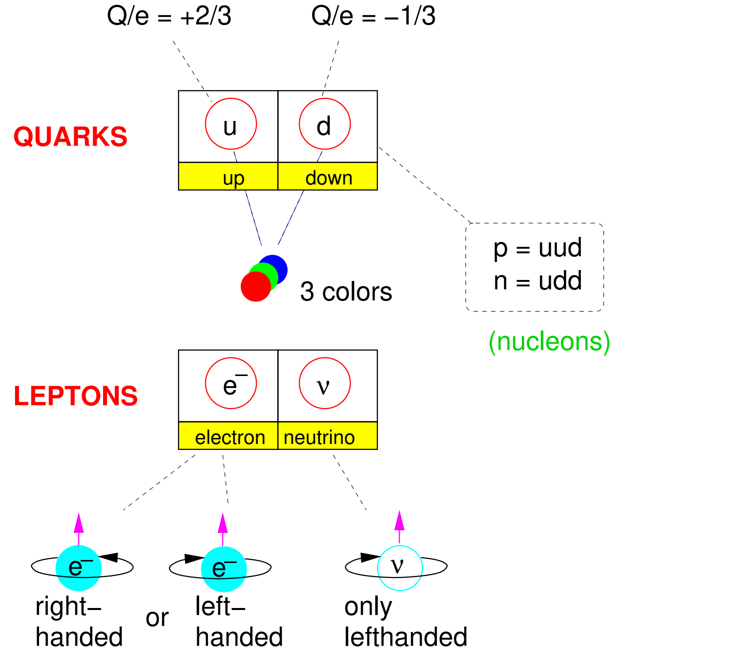
A last example we want to mention here is the Nitrogen atom. The nucleus ^{14}N contains 7 protons and 7 neutrons. Including the 7 electrons the total angular momentum is half-integer[3]. Indeed it turns out that for the atom $J = 1/2$. Before one knew of the existence of the neutron and β-decay, it seemed natural to think of the ^{14}N nucleus as 14 protons and 7 electrons. In that case the atom would have had an integer J, in disagreement with observation. This illustrates how simple combinatorial rules for angular momentum provide strong discriminatory power.

To our present knowledge e^- and ν_e are elementary particles without substructure. This is not true for the proton and neutron. They have a substructure, e.g. evident from the magnetic moments of the particles. Writing

$$\boldsymbol{\mu}_i = g_i \frac{e}{2m_i}\, \boldsymbol{s}_k, \tag{1.27}$$

one has $g_e = 2$, which was shown by Dirac to be (up to a very tiny correction) the natural value for an elementary spin 1/2 particle. One has $g_p = 5.586$ and $g_n = -3.826$. In particular the latter is a surprising result for a neutral particle. Proton and neutron turned out to be composed of two quark species, *up* (u) and *down* (d) quarks with fractional charges $Q_u = +2/3\,e$ and $Q_d = -1/3\,e$, having spin 1/2. In addition to these quantum numbers, the quarks carry one of 3 color charges. One of the strongest indications for the

[3]Note that if we talk about total angular momentum of a composite system, we refer standard to its rest-frame. In other frames one has to add orbital angular momentum

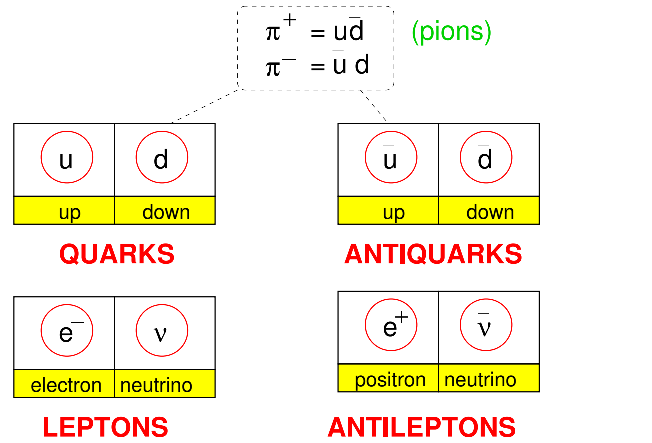


Quarks and leptons (of the first family); these quarks are the ones making up the protons and neutrons.

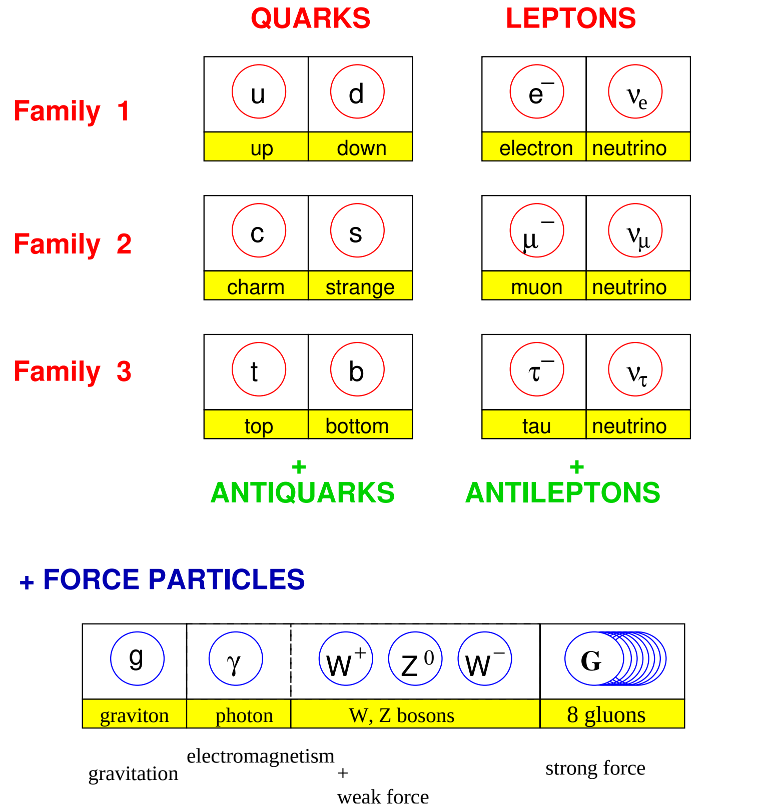
need of such an additional quantum number came from the existence of doubly-charged Δ^{++} particle which turned out to have spin $J = 3/2$. The natural explanation is a state consisting of three u-quarks, which all are in an s-orbital ($\ell = 0$). Without an additional quantum number this would be in contradiction with the Pauli principle, however. With the introduction of color everything is fine.

The color charge turned out to be more than just an additional quantum number. It is the source for the strong interactions. The interactions between color charges are mediated by gluons and the theory has been given the name Quantum Chromodynamics (QCD) because of the analogy with QED. The presence of 3 colors leads to a more complex underlying structure with eight noncommuting charge operators being 3×3 matrices (in analogy to the three noncommuting spin operators being 2×2 matrices). Coupling to each of these eight operators with the same strength one has *eight gluons*, whereas QED only has *one* photon. The gluons actually have a color charge themselves, leading to a linearly rising potential between color charges. This leads to the *confinement* of quarks in the nucleons. Only a color neutral configuration requiring 3 quarks has a finite energy. Further substructure than the quarks has not (yet) been found. Quarks are known to be smaller than 10^{-18} m (about 10^{-3} times the size of the nucleons). What has been seen is the possibility to excite the nucleon. The excitation energies are in the 100 MeV range, to be compared with the nuclear MeV-range and the atomic eV-range. Because of the confining potential, one does not have the situation that the mass (energy) of the composite system is less than that of the constituents, as is the case for molecules, atoms and nuclei. In fact the masses of the up and down quarks turn out to be in essence zero on the scale of the nucleon mass. The scales are set by the size, $R_N \sim 1$ fm and $\hbar c/R_N \sim 200$ MeV.

The quarks and leptons all turned out to have corresponding antiparticles, of which the positron (e^+) was the first to be discovered. Antiparticles have opposite electric and color charges, but identical masses as compared to the particles. Three quarks can form color neutral combinations (*baryons*) but also a quark and an antiquark can form a color



Quarks and leptons (of the first family) and their antiparticles. Particles and antiparticles can annihilate, e.g. e^+e^- can be transformed into other particles, e.g. a few photons. The opposite process is the *creation* of a particle-antiparticle pair.



The particle content of the Standard Model, quarks, leptons belonging to three families and the force particles, responsible for the different interactions.

neutral particle, called *mesons*. The lightest of these are the *pions*. Mesons of course must have integer spin, e.g. the pions have spin 0.

While the exchange of gluons produces the binding force of the quarks (and antiquarks) in baryons (qqq) or mesons ($q\bar{q}$), it is the exchange of mesons that produces the long-range (effective) interaction responsible for the nuclear binding. Via the formation of quark-antiquark pairs, e.g. by colliding electrons and positrons,

$$e^+ + e^- \longrightarrow q + \bar{q}, \tag{1.28}$$

one has found that other quark *flavors* exist besides up and down. There exist two other families of quarks and leptons. Besides these new fermions, which in essence differ only from the first family by mass, one has found 3 heavy bosons, the Z^0 and $W^\pm$-particles, which are responsible for the weak force, e.g. in β-decay.

The 3 families of quarks and leptons, their antiparticles and the force-carrying particles form the content of the socalled *Standard Model* of elementary particles. Presently one degree of freedom, mostly referred to as *Higgs particle* remains to be uncovered. It will be interesting to see if this degree of freedom is actually a particle or if it is the effect of some underlying structure.

Exercises

Exercise 1.1

(a) The (quantum mechanical) size of the hydrogen atom is of the order of the Bohr radius a_0. Re-express this quantity in terms of the electron Compton wavelength $\lambda\!\!\!^{-}_e = \hbar/m_e c$ and the fine structure constant α. Similarly express the (relativistic) classical radius of the electron, $r_e = e^2/4\pi\epsilon_0\, m_e c^2$ in the Compton wavelength and the fine structure constant.

(b) Calculate the Compton wavelength of the electron and the quantities under (a) using the value of $\hbar c$, α and $m_e c^2$. This demonstrates how a careful use of units can save a lot of work. One does not need to know $\hbar$, c, ϵ_0, m_e, e, but only appropriate combinations.

(c) Estimate the maximal magnitude of the angular momentum if the electron would be a rotating sphere with the radius being the classical radius under (a).

(d) Use the value of the gravitational constant $G/\hbar c^5$ to construct a mass M_p (Planck mass) and a corresponding length r_p and give the value of the latter.

(e) Consider photons with wavelength of 500 nm. Calculate the frequency in Hz, the energy in J and in eV and the wavenumber in cm^{-1} (Recall the relations $\lambda = c/\nu$, $E = h\nu$). Calculate the Rydberg energy in cm^{-1}.

Exercise 1.2

For the Hydrogen atom we have seen that for the radial wave functions $u_{n\ell}(r)$ one has to look for eigenvalues of

$$H_r = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2\,\ell(\ell+1)}{2m\,r^2} - \frac{Z\,e^2}{4\pi\,\epsilon_0\,r},$$

which can be rewritten as

$$H_r = E_0\left[-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \frac{2}{\rho}\right],$$

where $\rho = r/r_0$ (choice of 2 in numerator of $2/\rho$ is convention) and

$$E_0 = \frac{Z^2\,e^4\,m}{32\pi^2\,\epsilon_0^2\,\hbar^2}, \qquad r_0 = \frac{4\pi\,\epsilon_0\,\hbar^2}{Z\,e^2\,m}.$$

Construct in a similar way the characteristic energy and length scales for the case of the harmonic oscillator,

$$H_r = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2\,\ell(\ell+1)}{2m\,r^2} + \frac{1}{2}\,m\omega^2\,r^2$$

and a linear potential

$$H_r = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2\,\ell(\ell+1)}{2m\,r^2} + T_0\,r.$$

Exercise 1.3

Calculate the maximal packing fraction for sc, bcc and fcc lattices. What is the maximal radius for atoms that would fit into the holes of maximally packed lattices.

Exercise 1.4

Find an elegant way to calculate the Bohr and nuclear magnetons,

$$\mu_e = \frac{e\hbar}{2m_e} = 5.788 \times 10^{-5}\ \text{eV/T},$$
$$\mu_p = \frac{e\hbar}{2m_p} = 3.152 \times 10^{-8}\ \text{eV/T},$$

in electronvolt per Tesla (eV/T). As a hint, what is the unit V/T?

Exercise 1.5

Not only on the basis of spin the presence of electrons in a nucleus can be excluded. A second argument comes from the kinetic energy of electrons confined to nuclear distances. Estimate this (relativistic!) energy using the uncertainty relation to get the momentum of the electron in a nucleus of say $R_A \sim 2$ fm. What about the energy of nucleons in a nucleus?

Chapter 2

Atoms

2.1 Introduction

Historical Perspective

Some important developments that predate our present view of atoms were the Periodic Table of elements, for which a concept was developed by D.I. Mendeleev in 1869. The ordering was based on the chemical behavior of the elements. The table was not yet complete. We also mention the work of A. Avogadro, who had conceived the idea that gasses consist of discrete particles and established the law that equal volumes of gas at equal pressure and temperature contain the *same* number of particles. The first determination of Avogadro's number was performed by J.B. Perrin. The experiments of J.J. Thomson on cathode rays were important, leading to the discovery of the electron in 1897. From the deflection by an electric field one finds the ratio e/m_e. In his famous oil-drop experiment in 1906, R.A. Millikan unravelled the two values and determined the value of the *elementary* charge e.

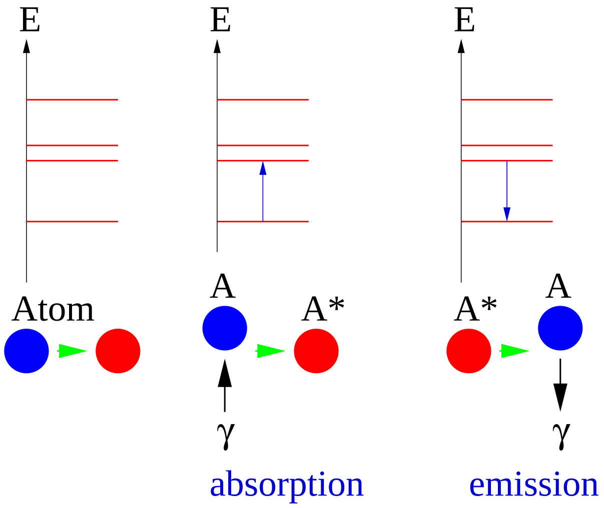
Based on the previous concepts Thomson developed a model for the atom consisting of electrons as negatively charged particles of low mass and some substance that should carry positie charge and nearly all the mass within the atom. The atoms were thought to consist of a mixture of A positive particles and A electrons. In this model the atomic number Z did not yet play a role. After his studies into radioactivity E. Rutherford in the first decade of the 20th century performed scattering experiments with α particles to investigate the structure of the atom. Conclusions drawn from the angular distribution of the scattered particles were that the atom was in essence empty with a heavy positively charged nucleus at the center carrying all the mass of the atom within a size of few fm and electrons around this extending up to distances of a few $\mathring{A}$.

There are, however, a number of shortcomings to this planetary model of an atom bound by classical electromagnetic forces, such as

- The problem of stability of the electrons. Electrons are accelerated in their orbits but they do not loose energy.
- The model does not give any indication for the size of the atom.
- The model does not give an explanation for the characteristic spectroscopy of the atom.

Spectroscopy

Investigation of atomic spectra started in early 19th century with the discovery of dark lines in the spectrum of light from the Sun by among others J. von Fraunhofer. Moreover heating elements gave rise to emission of discrete lines. Kirchhoff explained the difference between absorption and emission spectra and showed that the spectrum was characteristic for the elements. This made it possible to identify new elements, e.g. Helium was first discovered on the Sun before it was found on Earth.



Absorption or emission of lightquanta with energies $\hbar\omega = h\nu = hc/\lambda = E_2 - E_1$, corresponding to the difference of two energy levels for the electrons in an atom. The atom A is after absorption left in an excited state A^*. Characteristic quantities of the photon are the radial frequency ω or the frequency $\nu = 2\pi\,\omega$ and the wavelength λ.

Balmer was the first to recognize a regularity in a series of lines in the Hydrogen atom in 1885, in 1890 generalized by J. Rydberg. He found

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n^2} - \frac{1}{m^2}\right), \tag{2.1}$$

for integer n and m, from which one can deduce the energy spectrum of the Hydrogen atom. The constant $R_H = (\mu/m_e)R_\infty$ (where μ is the electron's reduced mass in Hydrogen, which will be discussed below) is named after Rydberg.

The series of lines $m \to n = 1$ are called the *Lyman* series, the lines $m \to n = 2$, the *Balmer* series and the $m \to n = 3$ the *Paschen* series. The limiting (shortest) wavelength of the Lyman series is at 91.1 nm in the ultraviolet, that of the Balmer series at 364.5 nm in the visible light, while all higher series have the limits in the infrared and beyond.

The Bohr model of the atom

The model of N. Bohr of the atom imposes quantization in an ad hoc way by requiring $L = n\,\hbar$ with n being integer. For the electron in the atom one obtains after using the condition that the central force to bind the electron is provided by the Coulomb attraction,

$$\frac{mv^2}{r} = \frac{Z\,e^2}{4\pi\epsilon_0\,r^2}, \tag{2.2}$$

Using the condition on L to eliminate v one immediately finds:

$$r_n = \frac{n^2}{Z}\,\frac{4\pi\epsilon_0\,\hbar^2}{m\,e^2}, \tag{2.3}$$

$$E_n = \frac{Z^2}{n^2}\,\frac{m\,e^4}{32\pi\epsilon_0^2\hbar^2}, \tag{2.4}$$

which turns out to give the correct (quantized) energy levels and also a good estimate of the radii (see next section). At the classical level the Sommerfeld model of the atom even includes quantization conditions for treating elliptical orbits.

2.2 The Schrödinger equation for the hydrogen atom

The starting point for the quantummechanical treatment of the hydrogen atom is the hamiltonian

$$H = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \frac{Ze^2}{4\pi\epsilon_0\, r}. \tag{2.5}$$

We will discuss the solution of this hamiltonian and its refinements, first recalling the various steps

Transformation to the center of mass

In fact one starts with the hamiltonian for the nucleus of the hydrogen atom, a proton, and the electron,

$$H = -\frac{\hbar^2}{2m_p}\boldsymbol{\nabla}_p^2 - \frac{\hbar^2}{2m_e}\boldsymbol{\nabla}_e^2 - \frac{Ze^2}{4\pi\epsilon_0\, |\boldsymbol{r}_e - \boldsymbol{r}_p|}. \tag{2.6}$$

This can using total mass $M = m_e + m_p$ and reduced mass $\mu = m_e m_p/M$ be rewritten in terms of the center of mass and relative coordinates,

$$M\boldsymbol{R} = m_p\boldsymbol{r}_p + m_e\boldsymbol{r}_e, \tag{2.7}$$

$$\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_p, \tag{2.8}$$

and dito momenta

$$\boldsymbol{P} = \boldsymbol{p}_e + \boldsymbol{p}_p = -i\hbar\boldsymbol{\nabla}_R, \tag{2.9}$$

$$\frac{\boldsymbol{p}}{\mu} = \frac{\boldsymbol{p}_e}{m_e} - \frac{\boldsymbol{p}_p}{m_p} = -i\hbar\boldsymbol{\nabla}_r. \tag{2.10}$$

One obtains

$$H = \underbrace{-\frac{\hbar^2}{2M}\boldsymbol{\nabla}_R^2}_{H_{\rm cm}} \underbrace{-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}_r^2 - \frac{Ze^2}{4\pi\epsilon_0\, r}}_{H_{\rm rel}}. \tag{2.11}$$

The hamiltonian is separable, the eigenfunction $\psi_E(\boldsymbol{R},\boldsymbol{r})$ is the product of the solutions $\psi_{E_{\rm cm}}(\boldsymbol{R})$ of $H_{\rm cm}$ and $\psi_{E_{\rm rel}}(\boldsymbol{r})$ of $H_{\rm rel}$, while the eigenvalue is the sum of the eigenvalues. In particular one knows that $\psi_{E_{\rm cm}}(\boldsymbol{R}) = \exp\left(i\,\boldsymbol{P}\cdot\boldsymbol{R}\right)$ with $E_{\rm cm} = \boldsymbol{P}^2/2M$, leaving a one-particle problem in the relative coordinate $\boldsymbol{r}$ for a particle with reduced mass μ.

Time dependence

The hamiltonian determines the time dependence of the wave function,

$$-i\hbar\,\frac{\partial}{\partial t}\,\psi(\boldsymbol{r},t) = H\,\psi(\boldsymbol{r},t). \tag{2.12}$$

For a hamiltonian that does not contain explicit t-dependence, one can separate the time dependence. One has $\psi(\boldsymbol{r},t) = \psi_E(\boldsymbol{r})\, e^{-iEt/\hbar}$ for the time-independent eigenfunctions $\psi_E(\boldsymbol{r})$ of H with eigenvalues E,

$$H\,\psi_E(\boldsymbol{r}) = E\,\psi_E(\boldsymbol{r}). \tag{2.13}$$

Spherical coordinates

Introducing polar coordinates it is straightforward to write

$$\boldsymbol{\nabla}^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\boldsymbol{\ell}^2}{r^2}. \tag{2.14}$$

where $\boldsymbol{\ell} = \boldsymbol{r}\times\boldsymbol{p}$ are the three angular momentum operators. The hamiltonian actually commutes with all three angular momentum operators, $[H,\boldsymbol{\ell}] = 0$. Since ℓ_x, ℓ_y and ℓ_z do not commute with one another, one makes a choice to find a set of commuting operators (hence, with a common set of eigenfunctions). An appropriate set is H, $\boldsymbol{\ell}^2$ and ℓ_z. The eigenfunctions of the latter two determine the angular dependence of the eigenfunctions of the hamiltonian (see appendix on spherical harmonics),

$$\psi_{E\ell m}(\boldsymbol{r}) = \frac{u_{E\ell}(r)}{r}\,Y_\ell^m(\theta,\varphi), \tag{2.15}$$

where $u_{E\ell}(r)$ satisfies the radial Schrödinger equation,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \underbrace{\frac{\hbar^2\,\ell(\ell+1)}{2m\,r^2} - \frac{Ze^2}{4\pi\epsilon_0\,r}}_{V_{\rm eff}(r)} - E\right]u_{E\ell}(r) = 0, \tag{2.16}$$

with boundary condition $u_{E\ell}(0) = 0$. The solutions are

$$u_{n\ell}(\rho) = \left(\frac{2Z}{n\,a_0}\right)^{1/2}\sqrt{\frac{(n-\ell-1)!}{2n\,(n+\ell)!}}\;e^{-Z\rho/n}\left(\frac{2Z\rho}{n}\right)^{\ell+1}L_{n-\ell-1}^{2\ell+1}\left(\frac{2Z\rho}{n}\right) \tag{2.17}$$

with eigenvalues (energies)

$$E_{n\ell} = -\frac{Z^2}{n^2}\,R_\infty, \tag{2.18}$$

where $\rho = r/a_0$ and

$$a_0 \equiv \frac{4\pi\epsilon_0\,\hbar^2}{m\,e^2} = 0.529\times 10^{-10}\ \text{m}. \tag{2.19}$$

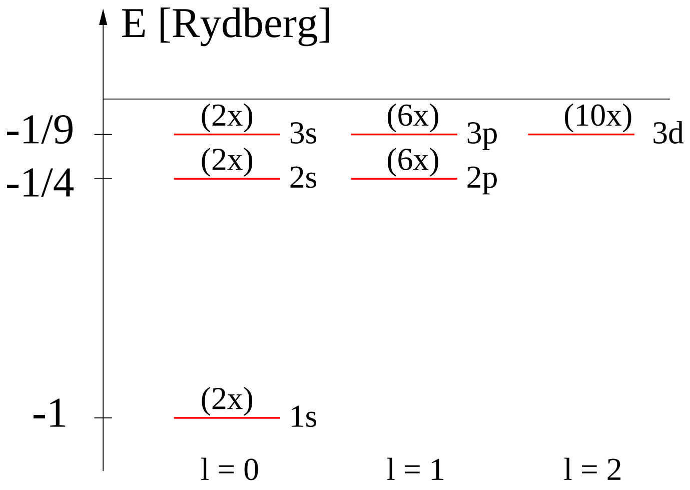
$$R_\infty \equiv \frac{\hbar^2}{2\mu\,a_0^2} = \frac{m\,e^4}{32\pi^2\epsilon_0^2\hbar^2} = 13.6\ \text{eV}. \tag{2.20}$$

Note that in fact one should be using the reduced mass instead of the electron mass. This means replacing everywhere $a_0 \to a_\mu$ and $R_\infty \to R_\mu$, e.g. $E_{n\ell} = -(Z^2/n^2)\,R_\mu$ and $\rho = r/a_\mu$, where

$$a_\mu \equiv \frac{4\pi\epsilon_0\,\hbar^2}{\mu\,e^2} = \frac{m_e}{\mu}\,a_0. \tag{2.21}$$

$$R_\mu = \frac{\hbar^2}{2\mu\,a_\mu^2} = \frac{\mu}{m_e}\,R_\infty. \tag{2.22}$$

This causes e.g. a small difference in the levels and hence the spectral lines of different isotopes, the socalled *isotope shift*. We note that also the *Hartree* is used as a reference energy, being equal to twice the Rydberg energy.



The spectrum of the hydrogen atom. For a given n one has degenerate ℓ-levels with $\ell = 0, 1, \ldots, n-1$. The degeneracy, including the electron spin, adds up to $2n^2$. The hamiltonian is invariant under inversion, hence its eigenstates are also parity eigenstates. The parity of ψ_{nlm} is given by $\Pi = (-)^\ell$.

Some explicit solutions are:

$$u_{10}(r) = 2\left(\frac{Z}{a_0}\right)^{1/2} e^{-Zr/a_0}\left(\frac{Zr}{a_0}\right), \tag{2.23}$$

$$u_{20}(r) = \frac{1}{\sqrt{2}}\left(\frac{Z}{a_0}\right)^{1/2} e^{-Zr/2a_0}\left(\frac{Zr}{a_0}\right)\left(1-\frac{1}{2}\frac{Zr}{a_0}\right) \tag{2.24}$$

$$u_{21}(r) = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{1/2} e^{-Zr/2a_0}\left(\frac{Zr}{a_0}\right)^2 \tag{2.25}$$

$$u_{30}(r) = \frac{2}{3\sqrt{3}}\left(\frac{Z}{a_0}\right)^{1/2} e^{-Zr/3a_0}\left(\frac{Zr}{a_0}\right)\left(1-\frac{2}{3}\frac{Zr}{a_0}+\frac{2}{27}\left(\frac{Zr}{a_0}\right)^2\right) \tag{2.26}$$

$$u_{31}(r) = \frac{8}{27\sqrt{6}}\left(\frac{Z}{a_0}\right)^{1/2} e^{-Zr/3a_0}\left(\frac{Zr}{a_0}\right)^2\left(1-\frac{1}{6}\frac{Zr}{a_0}\right) \tag{2.27}$$

$$u_{32}(r) = \frac{4}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{1/2} e^{-Zr/3a_0}\left(\frac{Zr}{a_0}\right)^3 \tag{2.28}$$

Useful integrals involving the solutions are expectation values like

$$\langle\frac{r^2}{a_0^2}\rangle = \frac{n^2}{2Z^2}\left[5n^2 - 3\,\ell(\ell+1)+1\right], \tag{2.29}$$

$$\langle\frac{r}{a_0}\rangle = \frac{1}{2Z}\left[3\,n^2 - \ell(\ell+1)\right], \tag{2.30}$$

$$\langle\frac{a_0}{r}\rangle = \frac{Z}{n^2}, \tag{2.31}$$

$$\langle\frac{a_0^2}{r^2}\rangle = \frac{2\,Z^2}{n^3(2\ell+1)}, \tag{2.32}$$

$$\langle\frac{a_0^3}{r^3}\rangle = \frac{2\,Z^3}{n^3\,\ell(\ell+1)(2\ell+1)}. \tag{2.33}$$

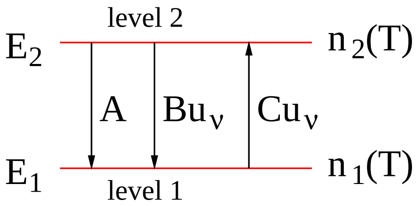
We note that the Bohr quantization condition not only gives the right characteristic size (a_0) and energy (R_∞) and the right power dependence on quantities like Z, but what is more surprising also the right power behavior of the quantum numbers (n, ℓ). Note e.g. that the Bohr model gives $r \propto n^2$ and (indeed) all the expectation values involving r^p have a polynomial behavior in (n, ℓ) of order $2p$.

The full hamiltonian for the Hydrogen atom has a number of additional terms, which give rise to splittings in the spectrum. These level splittings give rise to splitting of lines in emission and absorption spectra. Before discussing the fine structure and hyperfine structure we discuss radiative transitions.

2.3 Radiative transitions

Optical transitions in a two-level system

In an important paper in 1917, Einstein discussed the radiation balance in a two-level system. Involved are two levels with energies E_1 and E_2, such that $E_2 - E_1 = h\nu = \hbar\omega$, i.e. the transition corresponds to a photon energy corresponding with frequency ν or $\omega = 2\pi\,\nu$. We assume an energy density of the radiation field of u_ν and level populations n_1 and n_2, which may depend e.g. on the temperature T.



One has in the system

- spontaneous emission from level 2 to 1 (first arrow),
- stimulated emission from level 2 to 1 (second arrow),
- absorption from level 1 to 2 (third arrow).

The Einstein coefficients A, B and C are the proportionality constants that determine the change in the population according to

$$\frac{dn_2}{dt} = C\,u_\nu\,n_1 - (A + B\,u_\nu)\,n_2, \tag{2.34}$$

$$\frac{dn_1}{dt} = -\frac{dn_2}{dt} \tag{2.35}$$

with the constraint $n_1 + n_2 =$ constant. In the stationary state one has $dn_2/dt = 0$ and thus

$$\frac{n_1}{n_2} = \frac{A + B\,u_\nu}{C\,u_\nu}, \tag{2.36}$$

which for a system in thermal equilibrium is equal to a Boltzmann distribution

$$\frac{n_1}{n_2} = e^{-(E_1-E_2)/kT} = e^{\hbar\omega/kT}. \tag{2.37}$$

One finds that

$$u_\nu = \frac{A\,n_2}{C\,n_1 - B\,n_2} = \frac{A/C}{e^{\hbar\omega/kT} - B/C}. \tag{2.38}$$

This agrees with Plancks black-body radiation if

$$B = C, \tag{2.39}$$

$$\frac{A}{C} = \frac{8\pi\,\nu^3}{c^3} = \frac{8\pi}{\lambda^3}. \tag{2.40}$$

These results are indeed found in a quantummechanical treatment. Using the energy density for black-body radiation one sees that for emission the ratio of spontaneous/stimulated emission is given by

$$\frac{\text{spontaneous emission}}{\text{stimulated emission}} = \frac{A}{B\,u_\nu} = e^{\hbar\omega/kT} - 1. \tag{2.41}$$

Thus for low frequencies ($\hbar\omega \ll kT$ or $\lambda \gg 2\pi\,\hbar c/kT$) there is no spontaneous emission, e.g. for $T = 1$ K there is no spontaneous emission for $\lambda \gg 1$ cm.

Principle of lasers and masers

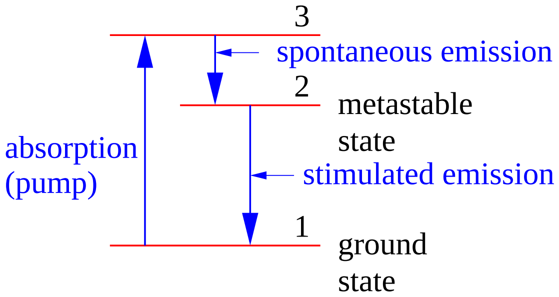
The total emission over absorption ratio is

$$\frac{\text{total emission}}{\text{absorption}} = \frac{n_2}{n_1}\,\frac{A + B\,u_\nu}{C\,u_\nu}, \tag{2.42}$$

which in an equilibrium situation is given by

$$\frac{\text{total emission}}{\text{absorption}} = \frac{n_2}{n_1}\left[1 + \frac{A}{B\,u_\nu}\right] = \frac{n_2}{n_1}\left[1 + \frac{8\pi\,\nu^3/c^3}{u_\nu}\right] \tag{2.43}$$

With u_ν being mostly large the second term (spontaneous emission) can be ignored. Hence to stimulate emission we need to make sure that $n_2 > n_1$. This can be achieved via a two-step mechanism.



Via a pump mechanism electrons are excited to level 3, from which they via spontaneous emission reach a metastable state with a lifetime long enough to achieve $n_2 > n_1$.

Transitions in atoms

The electric dipole operator for a system of Z charges is given by

$$\boldsymbol{D} = \sum_{i=1}^{Z} e_i\,\boldsymbol{r}_i, \tag{2.44}$$

where e_i are the charges and $\boldsymbol{r}_i$ is the position operator. For our purposes, it is important to know that expectation values of the electric dipole operator can be measured via absorption or emission of photons. Since the photon transfers energy to the system in the case of absorption or takes away energy in the case of emission one deals in these cases with transition matrix elements. The details of the interaction with the photon and the use of Fermi's golden rule to find the transition probabilities will be dealt with in courses on Quantum Mechanics and/or Electrodynamics (see Appendices). We will state the for us important results as the Einstein coefficients. For stimulated emission or absorption of a photon with polarization direction $\boldsymbol{\epsilon}$ one obtains via Fermi's golden rule

$$B_{2\to 1} = \frac{\pi}{\epsilon_0 \hbar^2}\,|D_{12}|^2 . \tag{2.45}$$

Here D_{12} is the dipole transition matrix element,

$$D_{12} = \int d^3r\ \psi_1^*(\boldsymbol{r})\,\boldsymbol{D}\cdot\boldsymbol{\epsilon}\,\psi_2(\boldsymbol{r}). \tag{2.46}$$

It depends on the polarization of the photon involved which operator is needed. In fact one needs the operator $\boldsymbol{D}\cdot\boldsymbol{\epsilon}$, where the vector $\boldsymbol{\epsilon}$ gives the photon polarization, which can be chosen as linear polarizations ($\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$ or $\hat{\boldsymbol{z}}$) or given a specific direction of motion (e.g. the z-direction) circular polarizations $\boldsymbol{\epsilon}_\pm \equiv \mp(\hat{\boldsymbol{x}} \pm i\hat{\boldsymbol{y}})/\sqrt{2}$. One has

$$\boldsymbol{D}\cdot\boldsymbol{\epsilon}_+ = -e\,r\sqrt{\frac{4\pi}{3}}\,Y_1^1(\theta,\varphi), \tag{2.47}$$

$$\boldsymbol{D}\cdot\hat{\boldsymbol{z}} = -e\,r\sqrt{\frac{4\pi}{3}}\,Y_1^0(\theta,\varphi), \tag{2.48}$$

$$\boldsymbol{D}\cdot\boldsymbol{\epsilon}_- = -e\,r\sqrt{\frac{4\pi}{3}}\,Y_1^{-1}(\theta,\varphi). \tag{2.49}$$

For spontaneous emission one finds the same dipole matrix element governing the transition. To obtain the result one needs to also quantize the electromagnetic fields. The result for one level to a specific other level is given by

$$A_{2\to 1} = \frac{\omega^3}{\pi\epsilon_0\hbar c^3}\sum_{i=1}^{3}|D_{12}|^2 . \tag{2.50}$$

As we will see a particular transition always involves a photon with a particular polarization. If there is no preferential direction (e.g. caused by an external magnetic field), one can average over the polarizations, giving averaged coefficients

$$\overline{B_{2\to 1}} = \frac{\pi}{3\,\epsilon_0\hbar^2}\,|\boldsymbol{D}_{12}|^2 , \tag{2.51}$$

$$\overline{A_{2\to 1}} = \frac{\omega^3}{3\pi\epsilon_0\hbar c^3}\,|\boldsymbol{D}_{12}|^2 , \tag{2.52}$$

where $|\boldsymbol{D}_{12}|^2 = |\langle 1|D_x|2\rangle|^2 + |\langle 1|D_y|2\rangle|^2 + |\langle 1|D_z|2\rangle|^2$. For transitions involving degenerate levels, the probability is multiplied with the degeneracy of the final states (probability is larger if a level can decay in more ways) and divided by the degeneracy of the initial state (we see an average of the decaying levels). The lifetime of a specific level is given by

$$\tau_1 = \frac{1}{\sum_i A_{i1}}. \tag{2.53}$$

Scaling the dipole operator via a_0 one finds that the typical magnitude of the probabilities for e.g. spontaneous emission is given by

$$A = \frac{\omega^3\, e^2\, a_0^2}{3\pi\epsilon_0\, \hbar c^3}\left(\frac{\langle D\rangle}{e\, a_0}\right)^2 = \frac{\alpha^3}{3}\left(\frac{R_\infty}{\hbar}\right)\left(\frac{\hbar\omega}{R_\infty}\right)^3\left(\frac{\langle D\rangle}{e\, a_0}\right)^2.$$

Taking $\hbar\omega \sim R_\infty$ and $\langle D\rangle \sim e\, a_0$ gives $A \sim (1/137)^3\,(13.6\ \text{eV}/3 \times 6.6 \times 10^{-16}\ \text{eV}\,\text{s}) \approx 1/(8 \times 10^{-10}\ \text{s})$.

Selection rules

Since the relevant operator to calculate dipole transitions is the position operator, the calculation of the matrix elements can be done disregarding the spin wave functions. In fact the spin wave function doesn't change, giving rise to a spin selection rule: $m_{s\,1} = m_{s\,2}$, i.e.

$$\Delta s = \Delta m_s = 0. \tag{2.54}$$

In fact the photon polarization determines which of the components of the position operator is the relevant operator. Using the representation as one of three $Y_1^{m_\gamma}$, one needs (consider one electron) the integral

$$\langle 1|\boldsymbol{r}\cdot\boldsymbol{\epsilon}|2\rangle = \sqrt{\frac{4\pi}{3}}\int d^3r\ \psi^*_{n_1\ell_1m_1}(\boldsymbol{r})\, r\, Y_1^{m_\gamma}(\theta,\varphi)\,\psi_{n_2\ell_2m_2}(\boldsymbol{r}),$$

which factorizes into

$$\langle 1|\boldsymbol{r}\cdot\boldsymbol{\epsilon}|2\rangle = \sqrt{\frac{4\pi}{3}}\int dr\ r\, u_{n_1\ell_1}(r)\, u_{n_2\ell_2}(r)\int d\Omega\ Y_{\ell_1}^{m_1\,*}(\theta,\varphi)\, Y_1^{m_\gamma}(\theta,\varphi)\, Y_{\ell_2}^{m_2}(\theta,\varphi).$$

From the φ-dependence of the spherical harmonics one sees that the matrix element is proportional to

$$\int d\varphi\ e^{-i\,m_1\varphi}\, e^{i\,m_\gamma\varphi}\, e^{i\,m_2\varphi} = 2\pi\,\delta(m_2 + m_\gamma - m_1),$$

giving rise to the selection rule

$$\Delta m_\ell = 0,\ \pm 1, \tag{2.55}$$

each of these corresponding to a specific photon polarization. In fact, the integrals for the φ-dependent part is simple, but more general the same applies for the Y_ℓ^m-functions in case of the full angular integration. One only gets a nonzero result if the addition of angular momenta $|\ell_2, m_2\rangle$ and $|1, m_\gamma\rangle$ can yield the final state $|\ell_1, m_1\rangle$ via the well-known angular momentum addition rules. In fact the result is simply proportional to the Clebsch-Gordan coefficient in this recoupling,

$$\langle 1|\boldsymbol{r}\cdot\boldsymbol{\epsilon}|2\rangle = \sqrt{\frac{4\pi}{3}}\int dr\ r\, u_{n_1\ell_1}(r)\, u_{n_2\ell_2}(r)\, C(1, m_\gamma, \ell_2, m_2; \ell_1, m_1).$$

This leads besides the m-selection rule to $|\Delta\ell| \le 1$ Knowing the parity of the spherical harmonics one immediately gets a *Parity selection rule*, namely $\Pi_1\Pi_2 = -1$ or with $\Pi = (-)^\ell$, one is left with

$$\Delta\ell = \pm 1. \tag{2.56}$$

Rotational invariance also requires that the sum of the total angular momentum in initial and final state is conserved. This becomes relevant if the spin quantum numbers of electrons and/or nuclei are included. In many cases the orbital angular momentum no longer is a good quantum number. Still, even when ℓ and s are coupled to j, or for many particles L and S are coupled to J, the transition operator involves a simple $Y_1^{m_\gamma}$, implying

$$\Delta J = 0, \ \pm 1 \tag{2.57}$$

(with $J = 0 \to J = 0$ forbidden!).

Other transitions

The interactions (absorption or emission) of photons in atoms can also proceed via different operators. The one treated here is known as electric dipole radiation (E1). In order of strength one has also the magnetic dipole radiation (M1), electric quadrupole radiation (E2), etc. For instance electric quadrupole radiation is governed by operators of the type $x_i\, x_j$. Recall from quantum mechanics that the latter operators give rise to transition selection rules in which parity is not changed and since the operators are proportional to $r^2\, Y_2^{m_\gamma}$ one has $\Delta\ell = 2$.

2.4 Refinements in the spectrum of hydrogen

Perturbation theory

Perturbation theory describes a systematic way of obtaining a solution for a hamiltonian $H = H_0 + \lambda V$ in the form of an expansion in the (small) parameter λ, assuming the solutions of H_0 are known, $(H_0 - E_n^{(0)})\,|\phi_n\rangle = 0$. One inserts the expansions

$$E_n = E_n^{(0)} + \lambda\, E_n^{(1)} + \lambda^2\, E_n^{(2)} + \ldots, \tag{2.58}$$

$$|\psi_n\rangle = |\phi_n\rangle + \lambda\, |\psi_n^{(1)}\rangle, \tag{2.59}$$

into the Schrödinger equation $(H - E_n)|\psi_n\rangle = 0$. After ordering the terms according to the power of λ, one finds at first order

$$\lambda\, E_n^{(1)} = \langle\phi_n|\lambda\, V|\phi_n\rangle, \tag{2.60}$$

$$\lambda\, |\psi_n^{(1)}\rangle = |\phi_n\rangle + \sum_{m\neq n} |\phi_m\rangle\, \frac{\langle\phi_m|\lambda\, V|\phi_n\rangle}{E_m^{(0)} - E_n^{(0)}}. \tag{2.61}$$

Perturbation theory is very useful if the first-order shift in the energies is small. The second equation warns us that in the case of degenerate levels for the unperturbed situation one must make sure that the degenerate states must be labeled as eigenstates of the perturbation $\lambda\, V$.

Fine structure in hydrogen

The mass correction

In the hydrogen atom there are a number of additional terms in the hamiltonian that can be attributed to relativistic corrections,

$$H = H_0 + H_{\text{mass}} + H_{\text{Foldy}} + H_{\text{so}} \tag{2.62}$$

The first term is a correction coming from the difference of the relativistic and nonrelativistic kinetic energies,

$$H_{\rm mass} = \sqrt{\boldsymbol{p}^2 c^2 + m^2 c^4} - mc^2 - \frac{\boldsymbol{p}^2}{2m} \approx -\frac{\boldsymbol{p}^4}{8m^3 c^2}. \tag{2.63}$$

Including this correction, the operators $\boldsymbol{\ell}^2$ and ℓ_z still remain compatible with the hamiltonian, but the radial dependence now will be modified. However in *first order perturbation theory* one obtains an accurate estimate of the energy shifts by calculating the expectation value of the correction. We here just state the result (treated in many quantum mechanics books),

$$\Delta E_{\rm mass}(n\ell m) = \langle n\ell m|\frac{\boldsymbol{p}^4}{8m^3 c^2}|n\ell m\rangle = -\alpha^2\,\frac{R_\infty}{n^3}\left(\frac{1}{\ell+\frac{1}{2}} - \frac{3}{4n}\right). \tag{2.64}$$

Another interaction term arises because of the interaction of the spin with the induced magnetic field by the orbital motion. It can be up to a factor 2 be derived with classical arguments, but a proper derivation requires the use of the relativistic Dirac equation for the electron. The result for a particle in a central potential is

$$H_{\rm so} = \frac{1}{2m^2c^2}\,\frac{1}{r}\,\frac{dV_c}{dr}\,\boldsymbol{\ell}\cdot\boldsymbol{s}. \tag{2.65}$$

When applying perturbation theory for this term one must be careful. One cannot simply calculate the expectation value between hydrogen states $|n\ell s m_\ell m_s\rangle$. Since the level is $2(2\ell+1)$-fold degenerate the perturbation mixing these degenerate states. Application of perturbation theory requires a reordering of these states, such that they are compatible with the perturbation. Instead of the brute force way of diagonalizing the matrix $\langle n\ell s m_\ell^\prime m_s^\prime|H_{\rm so}|n\ell s m_\ell m_s\rangle$, there is a smarter way. By rewriting

$$\boldsymbol{\ell}\cdot\boldsymbol{s} = \frac{1}{2}\left[\boldsymbol{j}^2 - \boldsymbol{\ell}^2 - \boldsymbol{s}^2\right],$$

one sees that the operators $\boldsymbol{\ell}^2$, $\boldsymbol{s}^2$, $\boldsymbol{j}^2$ and j_z (which from the theory of addition of angular momenta are known to be compatible with each other) are also compatible with the hamiltonian. This is not true for the set $\boldsymbol{\ell}^2$, $\boldsymbol{s}^2$, ℓ_z and s_z. Hence if we use states $|n\ell s j m\rangle$, the correction term has no off-diagonal elements, hence does not mix the unperturbed states and the splitting for the correct combinations of states is directly found as

$$\begin{aligned}
\Delta E_{\rm so}(n\ell s j m) &= \frac{1}{2m^2c^2}\langle n\ell s j m|\frac{1}{r}\,\frac{dV_c}{dr}\,\boldsymbol{\ell}\cdot\boldsymbol{s}|n\ell s j m\rangle \\
&= \frac{e^2\,\hbar^2}{32\pi\epsilon_0\,m^2c^2}\,\langle n\ell|\frac{1}{r^3}|n\ell\rangle\;[j(j+1) - \ell(\ell+1) - s(s+1)] \\
&= \frac{e^2\,\hbar^2}{32\pi\epsilon_0\,m^2c^2}\,\frac{j(j+1) - \ell(\ell+1) - s(s+1)}{a_0^3\,n^3\,\ell(\ell+1)(\ell+\frac{1}{2})}
\end{aligned} \tag{2.66}$$

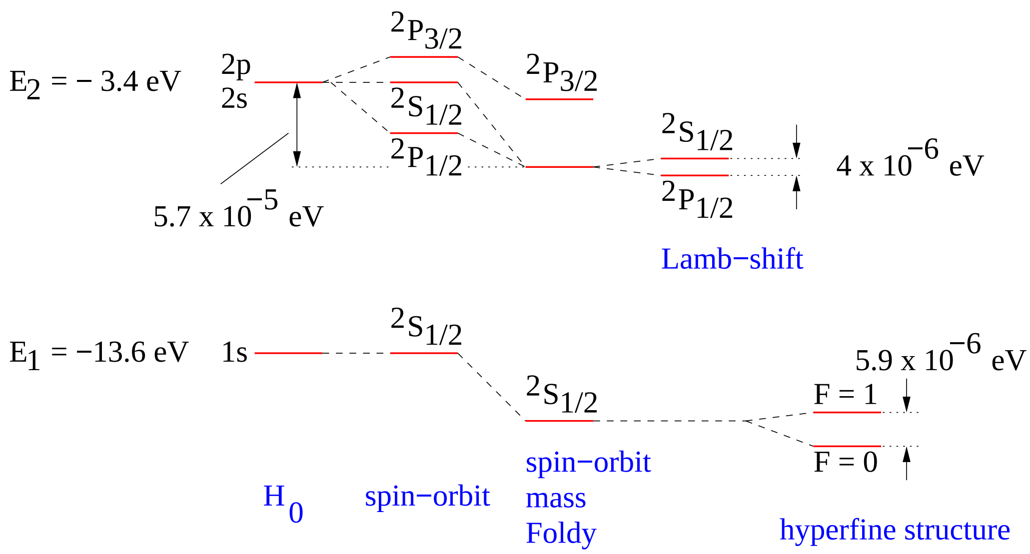
We thus must couple ℓ and s to j-eigenstates. For one electron with a given $\ell \neq 0$ there are two possibilities for j, namely $j = \ell \pm \frac{1}{2}$ giving for $\ell \neq 0$

$$\Delta E_{\rm so}(n\ell j) = \alpha^2\,\frac{R_\infty}{n^3}\left(\frac{1}{\ell+\frac{1}{2}} - \frac{1}{j+\frac{1}{2}}\right) \tag{2.67}$$

and for the combined result

$$\Delta E_{\text{mass + so}} = -\alpha^2 \frac{R_\infty}{n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) \tag{2.68}$$

The Foldy term is a relativistic correction proportional to $\delta^3(\boldsymbol{r})$ and thus only affecting s-waves. It makes the above equation valid also for s-waves. Schematically (not on scale) one has the following fine structure in the hydrogen spectrum



The various terms cause shifts in the order of 10^{-4} eV, giving within a orbit characterized by the principal quantum number n states with well-defined j-values. We denote such a level with a *term symbol*, for hydrogen

$$(n\ell)\,^{(2S+1)}L_J$$

where $(n\ell)$ indicates the spatial part of the electron wave function, $2S+1$ is the total spin multiplicity and L is the total orbital angular momentum of the electrons (using notation $S, P, D, \ldots$ for $L = 0, 1, 2, \ldots$). In this specific case of hydrogen with just one electron $S = 1/2$ and the multiplicity is always 2 while $L = \ell$. The splitting of the $^2S_{1/2}$ and $^2P_{1/2}$, the socalled Lamb shift, is due to several higher order effects. It is about 4×10^{-6} eV and produces a splitting of the Lyman α line. Also transitions between both levels are possible via an E1 transition with frequency of about 1 GHz.

The hyperfine structure in hydrogen

The hyperfine structure in hydrogen is due to the interaction of the magnetic moments of electron and nucleus. Also the proton has a magnetic moment, which induces a magnetic dipole field felt by the electron and vice versa. It produces an interaction term, which for s-waves is of the form

$$V_{ss} = \frac{1}{6\pi\epsilon_0\, c^2}\, \boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p\, \boldsymbol{\nabla}^2\, \frac{1}{r}. \tag{2.69}$$

We know that $\boldsymbol{\mu}_e = g_e\,(e/m_e)\,\boldsymbol{S}$ and $\boldsymbol{\mu}_p = g_p\,(e/M_p)\,\boldsymbol{I}$ (where we use the in atomic physics conventional notation $\boldsymbol{I}$ for the nuclear spin). The splitting thus is proportional to

$$\Delta E_{ss} \propto g_e\, g_p\, \langle|\boldsymbol{S}\cdot\boldsymbol{I}|\rangle = \frac{1}{2}\, g_e\, g_p\, \hbar^2\, \left[F(+F1) - S(S+1) - I(I+1)\right]. \tag{2.70}$$

The proper eigenstates are labeled by eigenstates for the angular momentum operators F^2 and F_z, where $\boldsymbol{F} = \boldsymbol{S} + \boldsymbol{I}$. For normal hydrogen in the ground state ($I = 1/2$), it produces two states with $F = 0$ (para-) and $F = 1$ (ortho-hydrogen). The splitting is much smaller than the fine structure. For the $(1s)\,^2S_{1/2}$ level in hydrogen the splitting is 5.9×10^{-6} eV (see figure in previous section), corresponding to a transition frequency $\nu_{hf} = 1.42$ GHz or a wavelength of 21 cm. Although the radiative transition is heavily suppressed (it is certainly not an electric dipole transition!) it plays a very important role in radio astronomy. It traces the abundant occurence of hydrogen in the universe not in the least since the 21 cm wavelength is not strongly attenuated by interstellar dust.

2.5 Many electron atoms

Permutations for identical particles and the Pauli principle

The hamiltonian for Z electrons in an atom (omitting at this stage fine and hyperfine interactions),

$$H(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z; \boldsymbol{p}_1, \ldots, \boldsymbol{p}_Z) = \sum_{i=1}^{Z} \left(-\frac{\hbar^2}{2m}\, \boldsymbol{\nabla}_i^2 - \frac{Ze^2}{4\pi\epsilon_0\, r_i} \right) + \sum_{i>j}^{Z} \frac{e^2}{4\pi\epsilon_0\, |\boldsymbol{r}_i - \boldsymbol{r}_j|} \tag{2.71}$$

is invariant under *permutations* of the particle labels, $i \leftrightarrow j$, written symbolically as

$$H(1 \ldots i \ldots j \ldots Z) = H(1 \ldots j \ldots 1 \ldots Z). \tag{2.72}$$

Consider first two identical particles and assume an eigenstate $\phi(12)$,

$$H(12)\phi(12) = E\phi(12),$$

Because $H(12) = H(21)$ one has also

$$H(21)\phi(12) = E\phi(12).$$

Since the labeling is arbitrary one can rewrite the latter to

$$H(12)\phi(21) = E\phi(21).$$

Thus there are two degenerate solutions $\psi(1,2)$ and $\psi(2,1)$. In particular one can choose symmetric and antisymmetric combinations

$$\phi^{S/A} = \phi(12) \pm \phi(21), \tag{2.73}$$

which are also eigenstates with the same energy. These are eigenfunctions of the permutation operator P_{ij}, which interchanges two labels, in general $P_{ij}\phi(1 \ldots i \ldots j \ldots) = \phi(1 \ldots j \ldots i \ldots)$ with eigenvalues + and - respectively. This operator commutes with H and the symmetry is not changed in time.

For three particles one has six degenerate solutions, $\phi(123)$, $\phi(213)$, $\phi(231)$, $\phi(321)$, $\phi(312)$ and $\phi(132)$. There is *one* totally symmetric combination,

$$\phi^S = \phi(123) + \phi(213) + \phi(231) + \phi(321) + \phi(312) + \phi(132) \tag{2.74}$$

(any permutation operator gives back the wave function), *one* totally antisymmetric combination

$$\phi^S = \phi(123) - \phi(213) + \phi(231) - \phi(321) + \phi(312) - \phi(132) \tag{2.75}$$

(any permutation operator gives back minus the wave function) and there are four combinations with mixed symmetry. Nature is kind and only uses the *symmetric* wave functions (for *bosons*) or the *antisymmetric* wave function (for *fermions*). Particles with integer spin turn out to be bosons, particles with half-integer spin are fermions. For instance for electrons which have spin 1/2 (two possible spin states) the total wave function must be antisymmetric. This has profound consequences. It underlies the periodic table of elements.

Consider again for simplicity first a two-particle system. When we as a further approximation neglect mutual interactions, one has a separable hamiltonian of the form

$$H = H_0(1) + H_0(2).$$

Suppose the solutions of the single-particle hamiltonian are known,

$$H_0(1)\phi_a(1) = E_a\phi_a(1), H_0(1)\phi_b(1) = E_b\phi_b(1),$$

etc. Considering the lowest two single-particle states available, there are three symmetric states and one anti-symmetric state,

$$\begin{array}{rl} \text{symmetric:} & \left\{ \begin{array}{l} \phi_a(1)\,\phi_a(2) \\ \phi_a(1)\,\phi_b(2) + \phi_b(1)\,\phi_a(2) \\ \phi_b(1)\,\phi_b(2) \end{array} \right. \\ \text{antisymmetric:} & \quad \phi_a(1)\,\phi_b(2) - \phi_b(1)\,\phi_a(2) \end{array}$$

For bosons with a symmetric wave function one sees that they can all reside in the lowest state, while any two fermions cannot be in the same state, known as the *Pauli exclusion principle.*

A general way to obtain the completely antisymmetric wave function for a separable potential is by constructing the antisymmetric wave function as a *Slater determinant*, for instance for three fermions the (properly normalized) antisymmetric wave function constructed from three available states ϕ_a, ϕ_b and ϕ_c is

$$\phi^A(123) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \phi_a(1) & \phi_a(2) & \phi_a(3) \\ \phi_b(1) & \phi_b(2) & \phi_b(3) \\ \phi_c(1) & \phi_c(2) & \phi_c(3) \end{vmatrix}. \tag{2.76}$$

The most well-known application is the consecutive filling of atomic levels $1s$, $2s$, $2p$, $3s$, $3p$, $4s$, $\ldots$, giving the periodic table of elements. The available states for each of the levels is $2(2\ell+1)$ accounting for the spin-degeneracy and the ℓ-degeneracy.

The Helium atom

As a first-order description of the helium atom, one can consider the independent-electron approximation, starting with a hamiltonian in which the electron-electron interaction is neglected, as well as any interactions involving the spin of the electrons. In that case one has a separable hamiltonian and for each of the electrons the solutions are given by hydrogen-like states ($Z = 2$), characterized by $(n\ell)$. Let us investigate the possible ground-state configurations, $(1s)^2$ and the first excited levels $(1s)(2p)$ and $(1s)(2s)$.

- The ground state configurations $(1s)^2$.
  Knowing the two angular momenta involved is sufficient to know the parity of these states, $\Pi = (-)^{\ell_1}(-)^{\ell_2} = +$. The angular momentum recoupling works in the following way.
  - Combining $\ell_1 = 0$ and $\ell_2 = 0$, the only possibility is $L = 0$. The orbital wave function then is symmetric under the interchange of the two electrons 1 and 2.
  - Combining the spins $s_1 = 1/2$ and $s_2 = 1/2$ gives two possibilities, $S = 0$ or $S = 1$. The first possibility is antisymmetric under the interchange of the electrons, the second is symmetric.
  - The total wave function (product of orbital and spin parts) must be antisymmetric for fermions according to the Pauli principle, hence $L = 0$ can only be combined with $S = 0$. This leaves only one possibility for the total angular momentum, $J = 0$. The notation for the only allowed ground state configuration is
$$(n_1\,\ell_1)(n_2\,\ell_2)\ {}^{2S+1}L_{J^\Pi} = (1s)^2\ {}^1S_{0^+}.$$
- The configurations $(1s)(2p)$ with parity $\Pi = -$.
  - We have $L = 1$, but appearing twice. We can construct the symmetric and antisymmetric combinations,
$$\phi^{s/a}_{LM_L} = \frac{1}{\sqrt{2}}\left[\frac{u_{1s}(r_1)}{r_1}\,Y_0^0(\Omega_1)\,\frac{u_{2p}(r_2)}{r_2}\,Y_1^{M_L}(\Omega_2) \pm \frac{u_{2p}(r_1)}{r_1}\,Y_1^{M_L}(\Omega_1)\frac{u_{1s}(r_2)}{r_2}\,Y_0^0(\Omega_2)\right]$$
    for the spatial part.
  - The combination of the spins gives again an antisymmetric $S = 0$ and a symmetric $S = 1$ wave function.
  - The allowed configurations are thus obtained by the appropriate antisymmetric combinations of orbital and spin parts,
$$(1s)(2p)\ {}^1P_{1^-} \qquad \text{and} \qquad (1s)(2p)\ {}^3P_{0^-,1^-,2^-}.$$
- The configurations $(1s)(2s)$ with parity $\Pi = +$.
  - We have $L = 0$, but now also appearing twice in a symmetric and antisymmetric combination.
  - As above, antisymmetric $S = 0$ and symmetric $S = 1$.
  - This gives the allowed configurations
$$(1s)(2s)\ {}^1S_{0^+} \qquad \text{and} \qquad (1s)(2s)\ {}^3S_{1^+}.$$

Summarizing in tabular form

Configurations in Helium							
configuration	$E^{(0)}/R_\infty$	L	S	Parity	Symmetry	J-configurations	# states
$(1s)^2$	-8	0	0	$+$	A	${}^1S_{0^+}$	1
			1	$+$	S	not allowed	3
$(1s)(2p)$ & $(2p)(1s)$	-5	1	0	$-$	S/A	${}^1P_{1^-}$	3
			1	$-$	S/A	${}^3P_{0^-,1^-,2^-}$	9
$(1s)(2s)$ & $(2s)(1s)$	-5	0	0	$+$	S/A	${}^1S_{0^+}$	1
			1	$+$	S/A	${}^3S_{1^+}$	3

Important to note is that although additional terms may be present in the full hamiltonian, the solutions found in this way do form a complete set of states for the atom. Other interaction terms give rise to shifts in the zeroth order energies and they may mix the states.

Refinements for helium

Perturbative approach

Including the ee-interaction the hamiltonian for 2 electrons in an atom is

$$H(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{p}_1, \boldsymbol{p}_2) = \underbrace{\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_1^2 - \frac{Ze^2}{4\pi\epsilon_0\, r_1}\right)}_{H_1} + \underbrace{\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_2^2 - \frac{Ze^2}{4\pi\epsilon_0\, r_2}\right)}_{H_2} + \underbrace{\frac{e^2}{4\pi\epsilon_0\,|\boldsymbol{r}_1 - \boldsymbol{r}_2|}}_{H_{12}},$$

which does not factorize because of the electron-electron interaction term. A way to account for the ee-interaction is by treating it as a perturbation on the result in the previous section. In perturbation theory the shift of the lowest level in the zeroth order approximation for helium, the $(1s)^2\,{}^1S_0$ multiplet, is simply given by the evaluating the ee-interaction term between the unperturbed wave function, which can straightforwardly be calculated

$$\Delta E_{\rm gs} = \int d^3r_1\, d^3r_2\; |\phi_{1s}(\boldsymbol{r}_1)|^2\, |\phi_{1s}(\boldsymbol{r}_1)|^2\, \frac{e^2}{4\pi\epsilon_0|\boldsymbol{r}_1 - \boldsymbol{r}_2|} = \frac{5}{4}\, Z\, R_\infty, \tag{2.77}$$

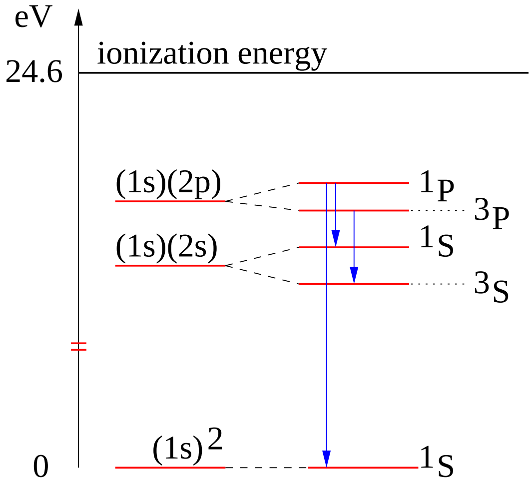
giving as estimate for the binding of the ${}^1S_0$ level $E = \left(-2Z^2 + \frac{5}{4}\,Z\right)\, R_\infty$, which for $Z = 2$ gives $E \approx -5.5\, R_\infty$, considerably higher than the previous result $E^{(0)} = -8$ eV and not bad as compared to the experimental value $E_{\rm gs} = -5.81\, R_\infty$.

For the next multiplets one has a spatially symmetric or antisymmetric wave function of the form $\psi = \psi_1 \pm \psi_2$, the sign depending on the spin wave function and one obtains for the expectation value of the hamiltonian,

$$\begin{aligned} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} &= \frac{\langle\psi_1 \pm \psi_2|H_1 + H_2 + H_{12}|\psi_1 \pm \psi_2\rangle}{\langle\psi_1 \pm \psi_2|\psi_1 \pm \psi_2\rangle} \\ &= E_1 + E_2 + \frac{C \pm K}{1 \pm S}, \end{aligned} \tag{2.78}$$

where

$$\begin{aligned} &\langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = 1 \quad \text{(assumed normalized)}, \\ &\langle\psi_1|H_i|\psi_1\rangle = E_i \qquad \text{(i = 1,2)}, \\ &\langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle = S \qquad \text{(overlap integral)}, \\ &\langle\psi_1|H_i|\psi_2\rangle = \langle\psi_2|H_i|\psi_2\rangle = E_i\, S \qquad \text{(i = 1,2)}, \\ &\langle\psi_1|H_{12}|\psi_1\rangle = \langle\psi_2|H_{12}|\psi_2\rangle = C \qquad \text{(Coulomb integral)}, \\ &\langle\psi_1|H_{12}|\psi_2\rangle = \langle\psi_2|H_{12}|\psi_1\rangle = K \qquad \text{(exchange integral)}. \end{aligned}$$



Looking at the $(1s)(2p)$ and $(1s)(2s)$ configurations and the shifts in perturbation theory, the exchange integral K turns out to be important yielding the lowest energy for the antisymmetric spatial wave function. These are combined with $S = 1$. For the excited levels of helium the $S = 1$ (ortho-helium) multiplets have the lowest energies. The groundstate configuration of helium only has $S = 0$ (para-helium). In the figure some dipole transitions have been indicated.

Variational approach

The variational method is used to obtain an estimate for the ground state energy and the ground state wave function for a given hamiltonian. This is done by taking a trial wave function $|\psi_{[\alpha_1,\alpha_2,\ldots]}\rangle$ depending on a number of parameters α_i and calculating the expectation value for the (given) hamiltonian,

$$E_{[\alpha_1,\alpha_2,\ldots]} = \frac{\langle\psi_{[\alpha_1,\alpha_2,\ldots]}|H|\psi_{[\alpha_1,\alpha_2,\ldots]}\rangle}{\langle\psi_{[\alpha_1,\alpha_2,\ldots]}|\psi_{[\alpha_1,\alpha_2,\ldots]}\rangle}. \tag{2.79}$$

It is a simple exercise to show that if the true solutions and energies of H are given by $(H - E_n)\,|\phi_n\rangle = 0$, that

$$E_{[\alpha_1,\alpha_2,\ldots]} \geq E_0, \tag{2.80}$$

with the equal sign being true if $|\psi_{[\alpha_1,\alpha_2,\ldots]}\rangle = \phi_0$. By minimizing the expectation value of the hamiltonian by varying the parameters,

$$\frac{\partial E_{[\alpha_1,\alpha_2,\ldots]}}{\partial\alpha_i} = 0, \tag{2.81}$$

one hopes to get close to the true ground state. The succes of the method not only depends on the number of parameters used and the calculational power of computers, but also on smart choices for the trial wave function such as choosing the correct symmetry, the correct number of nodes and the correct asymptotic (large and small r) behavior of the wave function.

As a trial function for the He ground a good ansatz is a simple product of wave functions,

$$\psi_T(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{\alpha^3}{\pi\,a_0^3}\,e^{-\alpha\,r_1/a_0}\,e^{-\alpha\,r_2/a_0}. \tag{2.82}$$

By allowing the coefficient α in the exponent to vary, we try to incorporate the screening. We can use the variational approach to see how well we can do. With the results from the sections on the hydrogen atom and those of the previous section we find

$$\langle\psi_T| - \frac{\hbar^2}{2m}\left(\boldsymbol{\nabla}_1^2 + \boldsymbol{\nabla}_2^2\right)|\psi_T\rangle = \frac{\hbar^2}{m\,a_0^2}\,\alpha^2 = 2\,\alpha^2\,R_\infty, \tag{2.83}$$

$$\langle\psi_T|\frac{-Ze^2}{4\pi\epsilon_0}\left(\frac{1}{r_1}+\frac{1}{r_2}\right)|\psi_T\rangle = -\frac{2Ze^2}{4\pi\epsilon_0\,a_0}\,\alpha = 4\,Z\alpha\,R_\infty, \tag{2.84}$$

$$\langle\psi_T|\frac{e^2}{4\pi\epsilon_0\,r_{12}}|\psi_T\rangle = \frac{5}{4}\,\alpha\,R_\infty, \tag{2.85}$$

and thus

$$E_{[\alpha]} = 2\left[\alpha^2 - \left(2Z - \frac{5}{8}\right)\alpha\right]R_\infty, \tag{2.86}$$

which is minimized for

$$\alpha = Z_{\rm eff} = Z - \frac{5}{16} \tag{2.87}$$

with

$$E[\alpha_{\rm min}] = -2\left(Z - \frac{5}{16}\right)^2 R_\infty. \tag{2.88}$$

For He this gives $E_{\rm gs} = -5.7\,R_\infty$, wich is within a few percent of the experimental value of $-5.81\,R_\infty = 79.0$ eV and much better than the perturbative value (which of course is just the result obtained for $\alpha = 2$). As expected the value $Z_{\rm eff} = 27/16$ is less than 2.

Ionization energies and electron affinities

Some results that we have encountered in the previous section are

$$\begin{aligned}
&\mathrm{H}^+ + e^- = \mathrm{H} + \ 13.6\ \mathrm{eV},\\
&\mathrm{He}^{++} + e^- = \mathrm{He}^+ + \ 54.4\ \mathrm{eV},\\
&\mathrm{He}^{++} + 2\,e^- = \mathrm{He} + \ 79.0\ \mathrm{eV}
\end{aligned}$$

Thus one finds

$$\mathrm{He}^+ + e^- = \mathrm{He} + \ 24.6\ \mathrm{eV},$$

An obvious note is that adding electrons one gains less energy if there are already other electrons. The energy one gains in adding the last electron is the *ionization energy*. In many cases one can add additional electrons and gain some energy, which is called the *electron affinity* E.g. for Chlorine

$$\begin{aligned}
&\mathrm{Cl}^+ + e^- = \mathrm{Cl} + \ 13.0\ \mathrm{eV},\\
&\mathrm{Cl} + e^- = \mathrm{Cl}^- + \ 3.6\ \mathrm{eV}.
\end{aligned}$$

The binding energy of Chlorine is 13.0 eV, the electron affinity is 3.6 eV. Electron affinities play a role in molecular binding.

An interesting example is actually the hydrogen atom, which also has a positive electron affinity,

$$\mathrm{H} + e^- = \mathrm{H}^- + \ 0.76\ \mathrm{eV}.$$

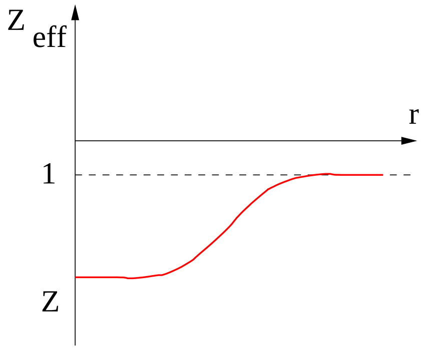
The H atom, however, also illustrates that adding a second electron completely changes the structure of the wave functions. Adding one electron to H^+ or He^{++} one has simple hydrogen-like wave functions. But adding the second electron one has to account for the presence of the other electron as illustrated for He using the variational approach. In that case a product wave function still worked fine. If one tries for a second electron in H^- such a product wave function one does not find a positive electron affinity. In order to find a positive electron affinity for the H-atom (for which an equivalent statement is that the H^--ion has a binding energy of $0.056\, R_\infty = 0.76$ eV) one can use e.g. a trial function of the form

$$\psi_T = C\left[e^{-(\alpha_1 r_1 + \alpha_2 r_2)/a_0} + e^{-(\alpha_1 r_2 + \alpha_2 r_1)/a_0}\right]. \tag{2.89}$$

The form is suggestive for two different orbits with fall-off parameters α_1 and α_2, but as electrons are indistinguishable one must (anti)-symmetrize (depending on spin) the two terms. With a plus sign one has wave functions without nodes giving the lowest energy.

Central field approximation

For many-electron atoms a good starting point is trying to approximate the average effect of the electron-electron repulsion into an effective central potential. The effective charge felt by an electron is expected to behave like

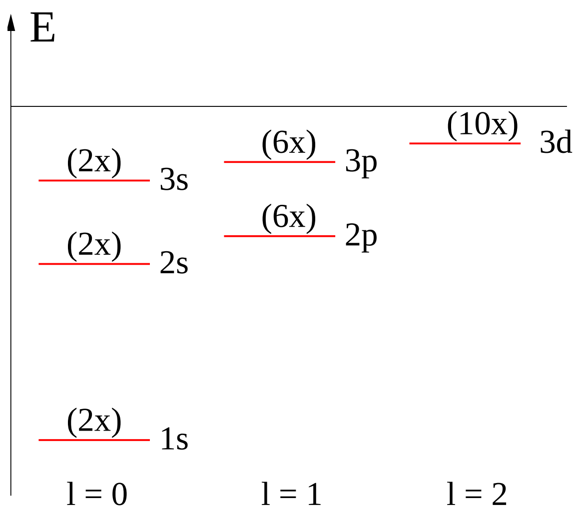


$$Z_{\text{eff}} \quad \begin{cases} \xrightarrow{r\to\infty} 1 \\ \xrightarrow{r\to 0} Z \end{cases}$$

The precise behavior of $Z_{\text{eff}}(r)$ can e.g. be obtained from the electron densities in a self-consistent matter. Thus, one can approximate the many-electron hamiltonian by

$$H(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_Z;\boldsymbol{p}_1,\ldots,\boldsymbol{p}_Z) \approx \sum_{i=1}^{Z}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 - \frac{Z_{\text{eff}}(r)\, e^2}{4\pi\epsilon_0\, r_i}\right) + \ldots \tag{2.90}$$

The advantage of this procedure is that part of the repulsion is taken into account retaining a central interaction and a separable hamiltonian. This will modify the spectrum, lifting the degeneracy between different ℓ-values for given n. In general the higher ℓ values will because of the angular momentum contribution $\hbar^2\, \ell(\ell+1)/2m\, r^2$ in the effective radial potential will feel a smaller charge and hence become less bound.



The (schematic) spectrum for many-electron atoms. A possible parametrization of the levels taking into account the screening effect is

$$E_{n\ell} = -\frac{R_\infty}{(n-\delta_\ell)^2},$$

where δ_ℓ is referred to as quantum defect, and one expects $\delta_\ell \to 0$ for large ℓ-values. This will work particularly well for atoms with one electron outside a closed shell.

Electron configurations for atoms

In the central field approximation, the hamiltonian separates for the different electrons and the solution is an antisymmetrized product of single electron states (Slater determinant), where one needs to keep in mind the spin degeneracy (2 for each level). Operators compatible with the hamiltonian are $\boldsymbol{\ell}_i$, $\boldsymbol{s}_i$ but also $\boldsymbol{L} = \sum_i \ell_i$ and $S = \sum_i s_i$. Also the total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$ is compatible with H as is the parity operator. Hence one has many good quantum numbers. At this level of approximation one can label the states by giving the various $(n\ell)$ levels and their multiplicities, e.g. for the ground state of helium $(1s)^2$, for Carbon $(1s)^2(2s)^2(2p)^2$, etc. Combining the angular momenta and spins to states with definite L, S and J is possible, but not yet relevant, since all multiplets that can be constructed (see next section) are at this level degenerate. This remains true if one refines the picture by using an effective central charge $Z_{\text{eff}}(r)$. The only effect of the latter is the splitting of different ℓ-values corresponding to the same principal quantum number n.

The structure of the periodic table is summarized in the following table of levels given in order of increasing energy

n							summed #	
1	2	3	4	5	6	7	of levels	remarks
$(1s)^2$							2 (He)	
	$(2s)^2$						4	
	$(2p)^6$						10 (Ne)	
		$(3s)^2$					12	
		$(3p)^6$					18 (Ar)	
			$(4s)^2$				20	
		$(3d)^{10}$					30	Fe-group
			$(4p)^2$				36 (Kr)	
				$(5s)^2$			38	
			$(4d)^{10}$				48	Pd-group
				$(5p)^6$			54 (Xe)	
					$(6s)^2$		56	
			$(4f)^{14}$				70	Lanthaniden
				$(5d)^{10}$			80	Pt-group
					$(6p)^6$		86 (Rn)	
						$(7s)^2$	88	
				$(5f)^{14}$			102	Actiniden
					$(6d)^{10}$		112	Pt-group
						$(7p)^6$	118 (?)	

The noble gases correspond with large energy gaps between the filled shell and the next available one. Characteristics of these noble gases are a high ionization energy and a small affinity to other elements, e.g. $E_{\text{ionization}} = 24.6$ eV (He), 21.6 eV (Ne) and 15.8 eV (Ar). The level scheme in the table can also be used to establish the excited states. We already have discussed this for He. The ground state is a $(1s)^2$ configurations, excited states are e.g. $(1s)(n\ell)$ configurations with $(n\ell) \neq (1s)$. Similarly one has for e.g. oxygen a ground state $(1s)^2(2s)^2(2p)^4$ and excited states in the $(1s)^2(2s)^2(2p)^3(n\ell)$ configuration.

Atomic multiplets

In a more realistic atom the ee-interaction term (or what remains after taken into account an effective charge) must also be considered. It breaks rotational invariance in the hamiltonian for the electron coordinate $\boldsymbol{r}_i$, thus $\boldsymbol{\ell}_i$ is no longer compatible with the hamiltonian. We note that $\boldsymbol{L}$ is still compatible with the hamiltonian. Since there is no spin-dependence spin operators $\boldsymbol{s}_i$ and also $\boldsymbol{S}$ are compatible with the hamiltonian and corresponding quantum numbers still can be used.

To illustrate how one easily finds the allowed L and S values given an electron configuration, we consider the ground state configuration of Carbon, $(1s)^2(2s)^2(2p)^2$. The allowed states in a shell can be represented as a number of boxes, e.g. an s-shell as two boxes, a p-shell as six boxes,

$m_s \downarrow\ m_\ell$	0
$+1/2$	
$-1/2$	

$m_s \downarrow\ m_\ell$	-1	0	$+1$
$+1/2$			
$-1/2$			

etc. Putting N electrons in these boxes with at most one electron per box (Pauli principle) one has $6!/N!(6-N)!$ possibilities, e.g. for a filled only one possibility. Obviously then all magnetic quantum numbers combine to zero, $M_L = M_S = 0$ and one also has for the total L and S quantum numbers $L = S = 0$. Hence filled shells can be disregarded for finding total (L, S) values.

As a consequence the specta of atoms with *one* electron outside a closed shell (Li, Na, K, Rb, Cs, Fr) resemble the spectrum of hydrogen, e.g. the configurations for sodium (Na) are $(n\ell)$ with $n \geq 3$. The groundstate for Na is $(3s)^2S_{1/2}$, the first excited states are the $(3p)^2P_{1/2}$ and $(3p)^2P_{3/2}$ levels. The electric dipole transition $^2P \rightarrow^2 S$ is the well-known yellow Na-line in the visible spectrum, which by the fine-structure (see below) is split into two lines corresponding to the transitions $^2P_{3/2} \rightarrow^2 S_{1/2}$ and $^2P_{1/2} \rightarrow^2 S_{1/2}$. For atoms with *two* electrons outside a closed shell (Be, Mg, Ca, Sr, Ba, Ra) the spectra resemble that of helium.

For a particular number of electrons it is easy to look at the number of possibilities to construct particular M_L and M_S values. This is denoted in a Slater diagram

$M_S \downarrow\ M_L$	-2	-1	0	$+1$	$+2$
$+1$	0	1	1	1	0
0	1	2	3	2	1
-1	0	1	1	1	0

It is easy to disentangle this into

$$\begin{array}{|c|c|c|c|c|}\hline 0&0&0&0&0\\\hline 1&1&1&1&1\\\hline 0&0&0&0&0\\\hline\end{array} + \begin{array}{|c|c|c|c|c|}\hline 0&1&1&1&0\\\hline 0&1&1&1&0\\\hline 0&1&1&1&0\\\hline\end{array} + \begin{array}{|c|c|c|c|c|}\hline 0&0&0&0&0\\\hline 0&0&1&0&0\\\hline 0&0&0&0&0\\\hline\end{array}$$

$$(L,S)=(2,0) \qquad\qquad (L,S)=(1,1) \qquad\qquad (L,S)=(0,0)$$

Thus for the Carbon one finds in the groundstate configurations the multiplets

$$^1D \qquad ^3P \qquad ^1S$$

Also for configurations involving more shells that are not completely filled, it is straightforward to find the states in an $M_S - M_L$ diagram. For the ordering in the spectrum a number of phenomenological rules have been formulated, the *Hund rules*. In particular for the groundstate configuration, one has that the terms with highest S-values (highest multiplicity) and then highest L-values have the lowest energy, i.e.

$$E(^3P) < E(^1D) < E(^1S).$$

These phenomenological rules also work well for the lowest excited configurations.

The fine structure of atoms

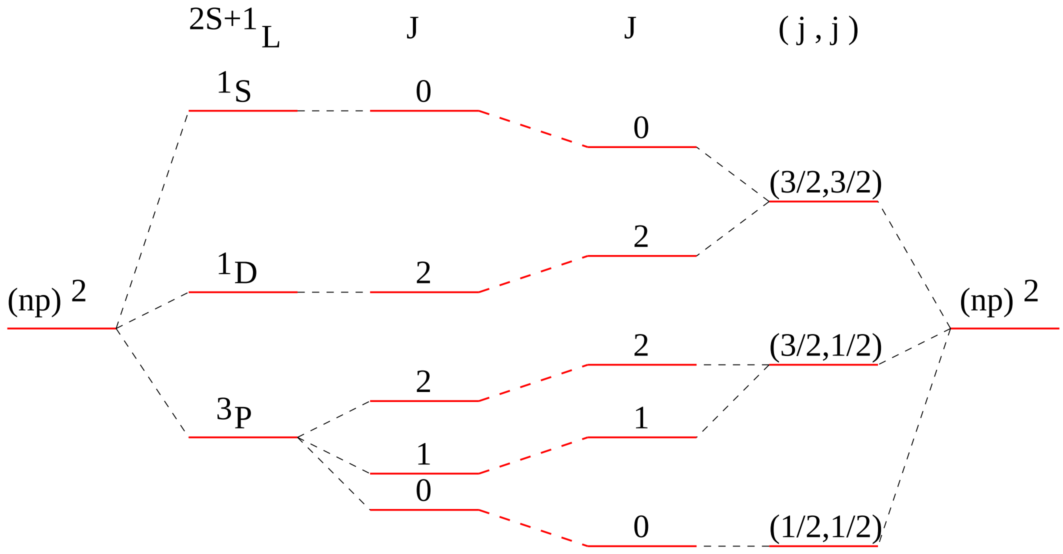
For not too heavy atoms, the fine structure turns out to be described well by a spin-orbit interaction of the form

$$H_{\rm so} = A(L,S)\,\boldsymbol{L}\cdot\boldsymbol{S}, \tag{2.91}$$

with a strenght A depending on the multiplet, coming among others from the radial dependence of the basic interaction. The spin-orbit interaction splits states with different J-values, leading to $^{2S+1}L_J$ multiplets and a magnitude for the splitting being given by

$$\Delta E(LSJM) = \frac{1}{2}A\hbar^2\left[J(J+1) - L(L+1) - S(S+1)\right]. \tag{2.92}$$

An example of the splitting of the three terms for an $(np)^2$ configuration is given below.



Note that the average (beware of degeneracy) of a multiplet gives the energy of the multiplet without the spin-orbit interaction. In cases of shells being less than half filled, the lowest J-value is generally lowest ($A \geq 0$), for shells being more than half filled, the highest J-value is generally lowest ($A \leq 0$).

The pattern of levels can in principle be obtained from atomic spectra. The use of magnetic fields is helpful to determine the degeneracy of the levels, and hence the J-values of levels. But already the spin-orbit splittings contains interesting patterns, such as

$$\frac{E(^{2S+1}L_J) - E(^{2S+1}L_{J-1})}{E(^{2S+1}L_{J-1}) - E(^{2S+1}L_{J-2})} = \frac{J}{J-1}, \tag{2.93}$$

e.g. for

$$r = \frac{E(^3P_2) - E(^3P_1)}{E(^3P_1) - E(^3P_0)},$$

one expects $r = 2$ if LS-coupling describes the fine structure. For carbon the actual ratio is 1.65, for silicium (Si) it is 1.89, but for a heavy atom as lead (Pb) the result is just 0.36, indicating a different type of fine structure. A different scheme is the jj-scheme in which first the orbital angular momenta and spins of the electrons are coupled, which in turn are combined into J-values, illustrated in the figure for the $(np)^2$ configuration. Note that coupling two identical j-values of the electrons, one needs to account for the symmetry of the wave function. The wave function for the maximal $J = 2\,j$ is symmetric, for the next lower J it is antisymmetric, then again symmetric, etc. This explains the J-values in the jj-coupling scheme. In the final result the same J-values must appear, but the spectrum in general is different.

2.6 Magnetic effects in atoms and the electron spin

Interaction of orbital angular momentum with magnetic field

In a magnetic field an additional interaction is added to the hamiltonian,

$$H = \underbrace{-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - \frac{Ze^2}{4\pi\epsilon_0\,r}}_{H_0} + V_{\rm mag}, \tag{2.94}$$

where $V_{\rm mag} = -\boldsymbol{\mu}\cdot B$. Neglecting spin, the magnetic moment of a particle in orbit is given by

$$\boldsymbol{\mu}_\ell = -g_\ell\,\frac{e}{2m}\,\boldsymbol{\ell} \tag{2.95}$$

with $g_\ell = 1$. What are the eigenfunctions and eigenvalues (energies) of this new hamiltonian. For this it is useful to find as many as possible commuting operators. Commuting operators are H, $\boldsymbol{\ell}^2$, ℓ_z (and, although overcomplete, the parity operator). However, the term

$$V_{\rm mag} = \frac{e}{2m}\,\boldsymbol{\ell}\cdot\boldsymbol{B},$$

implies that one only can have ℓ_z as an operator compatible with H if the z-axis is chosen along $\boldsymbol{B}$, i.e. $\boldsymbol{B} = B\,\hat{\boldsymbol{z}}$. In that case it is easy to convince oneself that the eigenfunctions are still the hydrogen wave functions, while the energies are shifted over an amount

$$\Delta E_{n\ell m_\ell} = \langle n\ell m_\ell|\frac{eB}{2m}\,\ell_z|n\ell m_\ell\rangle = m_\ell\,\mu_B B, \tag{2.96}$$

where

$$\mu_B = \frac{e\hbar}{2m} = \frac{1}{2}\,e\,c\,\frac{\hbar}{mc} \approx 5.8\times 10^{-5}\ \text{eV/T} \tag{2.97}$$

is the Bohr magneton.

Interaction of the electron spin with a magnetic field

For a proper description of an electron, one needs to specify in addition to $\psi(\boldsymbol{r},t)$ a spin wave function χ, i.e. an electron is specified by

$$\psi(\boldsymbol{r},t)\,\chi(t).$$

In quantum mechanics we have learned to specify spin states with the quantum numbers s and m_s, corresponding to eigenvalues of $\boldsymbol{s}^2$ (eigenvalue $\hbar^2\, s(s+1)$) and s_z (eigenvalue $\hbar\, m_s$). The possible values for s are $0, 1/2, 1, \ldots$ with for given s the eigenvalue m_s running from s to $-s$ in steps of one, i.e. there are $2s+1$ spin states. For a spin 1/2 particle such as the electron, the spin can take only two values, often referred to as spin-up or spin-down. Thus one sees notations as

$$\chi_{1/2}^{+1/2} = \chi_\uparrow = |1/2, +1/2\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{2.98}$$

$$\chi_{1/2}^{-1/2} = \chi_\downarrow = |1/2, -1/2\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.99}$$

Since the Hilbert space of allowed wave functions contains all linear combinations one immediately sees that after the choice of the spin-up and spin-down basis-states as two-component vectors , the wave function can be written as

$$\begin{pmatrix} \psi_\uparrow(\boldsymbol{r},t) \\ \psi_\downarrow(\boldsymbol{r},t) \end{pmatrix}.$$

With this representation, the spin operators can be given by matrices, $\boldsymbol{s} = \frac{1}{2}\,\hbar\,\boldsymbol{\sigma}$ where $\boldsymbol{\sigma}$ are the three *Pauli matrices*

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.100}$$

Just as the orbital angular momentum, the spin gives in a magnetic field rise to an interaction term in the hamiltonian.

$$V_{\rm mag} = -\boldsymbol{\mu}_s \cdot \boldsymbol{B}, \tag{2.101}$$

with

$$\boldsymbol{\mu}_s = -g_s\,\frac{e}{2m}\,\boldsymbol{s} = -g_s\,\frac{e\hbar}{m}\,\boldsymbol{\sigma}. \tag{2.102}$$

The g-factor for the spin of the electron is $g_s \approx 2$. Actually the deviation from 2 is due to subtle but calculable effects in quantum electrodynamics, $g_e - 2 = \alpha/\pi + \ldots \approx 0.00232$. If the interaction of the spin with the magnetic field is the only interaction (e.g. for s-waves), the result of the interaction term is a simple shift in the energies for the states, that now include also spin quantum numbers.

The Zeeman effect

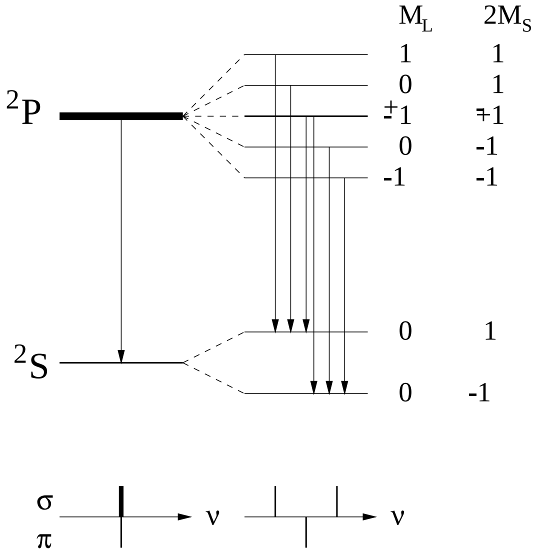
In general a ^{2S+1}L level in a magnetic field is split by an interaction term

$$V_{\rm mag} = -\boldsymbol{\mu} \cdot \boldsymbol{B}, \tag{2.103}$$

where $\boldsymbol{\mu} = -\mu_B(g_L\,\boldsymbol{L} + g_S\,\boldsymbol{S})$, resulting in a number of levels with the splitting given by

$$\Delta E(LSM_LM_S) = -\mu_B B(M_L + 2\,M_S). \tag{2.104}$$

In normal magnetic fields (say smaller or of the order of 1 T), the splittings are only fractions of an eV and there are other effects causing different splitting patterns, such as the $\boldsymbol{L}\cdot\boldsymbol{S}$ spin-orbit interaction. But for very large magnetic fields one does see the above *normal Zeeman splitting* pattern.



Zeeman splitting of levels in a magnetic field (no spin-orbit). Also indicated are the transitions, separated into $\Delta M_L = 0$ (π-transitions) and $\Delta M_L = \pm 1$ (σ-transitions).

Finally we note that the magnetic effects discussed here are those in an external magnetic field. This defines a preferential direction in space and leads to dependence on eigenvalues of the (z-)component of the angular momentum operators. This is also found back in the names *magnetic* quantum numbers for m_ℓ, m_s, etc.

Spin-orbit interaction and magnetic fields

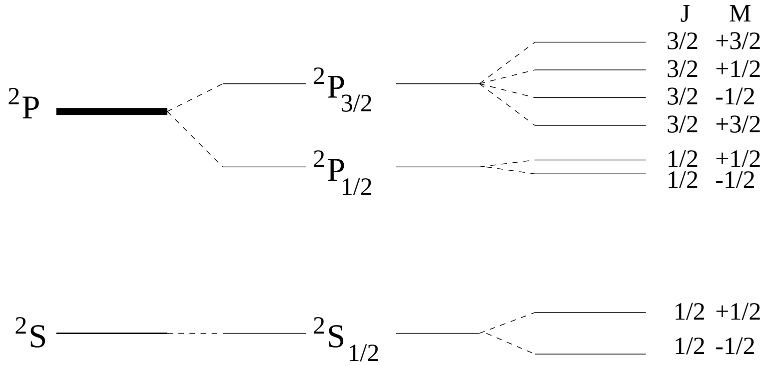
Including the spin-orbit interaction is important to describe the fine structure of atomic spectra and in general turns out to be considerably larger than the magnetically induced splittings. In that case one cannot simply use the results for the normal Zeeman effect when spin plays a role. So consider the situation that one has an interaction term in the atom of the form

$$H_{\text{int}} = A\,\boldsymbol{L}\cdot\boldsymbol{S} - \boldsymbol{\mu}\cdot\boldsymbol{B}, \tag{2.105}$$

with $\boldsymbol{\mu} = \mu_B(g_L\boldsymbol{L} + g_S\boldsymbol{S})/\hbar = \mu_B\,(\boldsymbol{L} + 2\,\boldsymbol{S})/\hbar$. We have already seen what happens in the situations $A = 0$ and $B = |\boldsymbol{B}| = 0$. One has

$$\begin{aligned} A = 0: &\quad \text{eigenstates} \quad |(\ldots)LSM_LM_S\rangle, \\ &\quad \Delta E(LSM_LM_S) = \mu_B B(M_L + 2M_S), \\[1em] B = 0: &\quad \text{eigenstates} \quad |(\ldots)LSJM\rangle, \\ &\quad \Delta E(LSJM) = \frac{1}{2}\,A\hbar^2\,[J(J+1) - L(L+1) - S(S+1)]\,. \end{aligned}$$

The splitting pattern for $A = 0$ has already been given, for $B = 0$ it splits the ${}^{2S+1}L$ multiplet into the different ${}^{2S+1}L_J$ multiplets, for the ${}^2P \rightarrow {}^2S$ transition indicated as the first splitting in the figure below.



The spin-orbit splitting leading to the ${}^{2S+1}L_J$ multiplets for the ${}^2P$ and ${}^2S$ levels and the consecutive splitting in a magnetic field for the case of a small magnetic field.

When one switches on the magnetic field, one deals with an interaction term for which neither $|LSM_LM_S\rangle$, nor $|LSJM\rangle$ are proper states (check compatibility of the relevant operators!). If the magnetic field is small the states will be in first order given by $|LSJM\rangle$ and one can calculate the energy shift via

$$\Delta E_{\text{mag}} = \mu_B B \,\langle(\ldots)LSJM|L_z{+}2S_z|(\ldots)LSJM\rangle = \mu_B B \,\langle(\ldots)LSJM|J_z{+}S_z|(\ldots)LSJM\rangle. \tag{2.106}$$

The part with which we need to be careful is the expectation value of S_z, Evaluating it between states with different M-values belonging to the same J gives zero, because if two M values involve the same M_S, the M_L's must be different (remember that in the coupling $M = M_L + M_S$). Thus we just need

$$\langle LSJM|S_z|LSJM\rangle = M\,\frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \tag{2.107}$$

which follows from a subtle relation involving $\boldsymbol{S}$ and $\boldsymbol{J}$ operators (see e.g. the book of Mandl, Ch. 6), $\boldsymbol{J}^2 J_z + J_z \boldsymbol{J}^2 = 2\,J_z\,(\boldsymbol{J}\cdot\boldsymbol{S})$ leading to

$$\Delta E_{\text{mag}} = \underbrace{\left[1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}\right]}_{g_J} M\,\mu_B B, \tag{2.108}$$

where g_J is called the Landé factor. This splitting is also indicated in the figure. Note that the procedure only works for small B-values. For large B-values (Paschen-Back limit) the assumption of states being approximately given by $|LSJM\rangle$ is not valid and one gets the previously discussed normal Zeeman splitting.

2.7 Exercises

Exercise 2.1

(a) Apply Bohr quantization to a gravitationally bound system. Estimate the quantum number for the orbit of the Earth around the Sun.

(b) Apply Bohr quantization to the harmonic oscillator and the linear potential and determine E_n and r_n.

Exercise 2.2

Evaluate the z-component of the dipole transition amplitude for the Balmer transition $3p \to 2s$. Using Mathematica to evaluate the integral, you can also try the $x \pm iy$-components and vary the m-quantum numbers to check the selection rules.

Exercise 2.3

Consider the Lyman-α transition in atomic hydrogen (transition between $n = 2$ and $n = 1$). What is the isotope shift for this transition going from normal hydrogen to deuterium, having an additional neutron in the nucleus. Calculate also the transition for positronium, a bound state of electron and positron.

Exercise 2.4

Consider a two-level system with energy levels E_2 and E_1 and populations $n_2(t)$ and $n_1(t)$, starting with $n_1(0) = N$ and $n_2(0) = 0$. Solve this equation using an algebraic manipulation program.

(a) Show that for short times, there is a steady growth of population in the excited state.

(b) Look at the behavior for $t \to \infty$.

(c) Show that there is a maximum for n_2 for all times and all intensities u_ν, even for $u_\nu \to \infty$. Give some plots for different values of A/Bu_ν.

Exercise 2.5

Apply the variational principle to find a suitable wave function for H^-. Try the product wave function that has been used for He. What do you find for the electron affinity of H in that case. Then try the two-orbit form proposed in this chapter and show that it at least leads to a positive electron affinity.

Exercise 2.6

(a) Determine the multiplets, their spectroscopic terms and their energy ordering for all $(np)^x$ configurations.

(b) Similar for $(np)(n'p)$ with $n \neq n'$. Compare the levels with those for carbon.

Exercise 2.7

(a) Construct the possible spectroscopic terms of a barium atom in a $(6p)(5d)$ state in the LS-coupling scheme. Include spin-orbit interaction in a second step. Check that there are (as expected) 60 states, which are partly degenerate. Use the Hund rules to order the states.

(b) Give the corresponding construction of allowed J-values in the jj-coupling scheme.

Exercise 2.8

(a) Use for the ^2P states the basis states $|L, S; M_L, M_S\rangle$ and write down the spin-orbit hamiltonian $H_{\rm so} = A\,\boldsymbol{L}\cdot\boldsymbol{S}$ as a matrix. Use for this the explicit expression

$$H_{\rm so} = \frac{A}{2}\,(2\,L_zS_z + L_+S_- + L_-S_+)\,.$$

Determine the eigenvalues and eigenstates. The latter are of course precisely the $|L, S; J, M\rangle$ states.

(b) Do the same for the hamiltonian in an external magnetic field, $H_{\rm int} = A\,\boldsymbol{L}\cdot\boldsymbol{S} - \boldsymbol{\mu}\cdot\boldsymbol{B}$, using the explicit form

$$H_{\rm int} = \frac{A}{2}\,(2\,L_zS_z + L_+S_- + L_-S_+) - \mu_B\,B_0\,(L_z + 2\,S_z)\,,$$

Exercise 2.9

In the section on the Zeeman effect, the splitting of spectral lines $^2P \rightarrow \ ^2S$ (including division into σ- and π-transitions) is given. This is of course also the splitting pattern in the the Paschen-Back limit of the general case (including LS-splitting). Give the splitting of the $^2P \rightarrow \ ^2S$ spectral lines, i.e. the possible transitions, for the small B-field limit in the general case.

Chapter 3

Molecules and chemical binding

Chapter 4

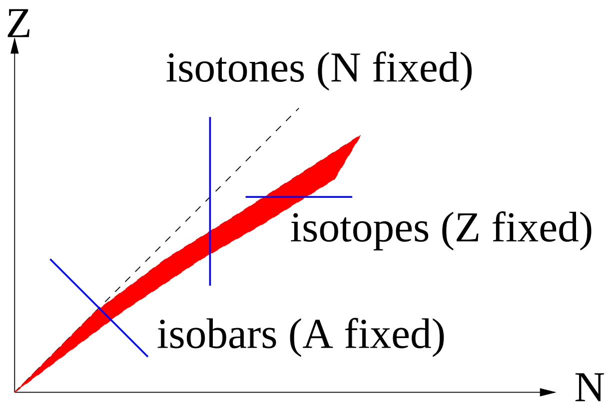
Condensed Matter

Chapter 5

Nuclei

5.1 Properties of nuclei

The atomic nucleus is built from Z protons and N neutrons, containing $A = Z + N$ nucleons. Stable nuclei are found up to $A = 209$ (Bi) and in the laboratory up to about $A = 240$. The diagram of nuclei has been given already in the first chapter. For atomic physics, Z clearly is the most important number, determining the charge of the nucleus.



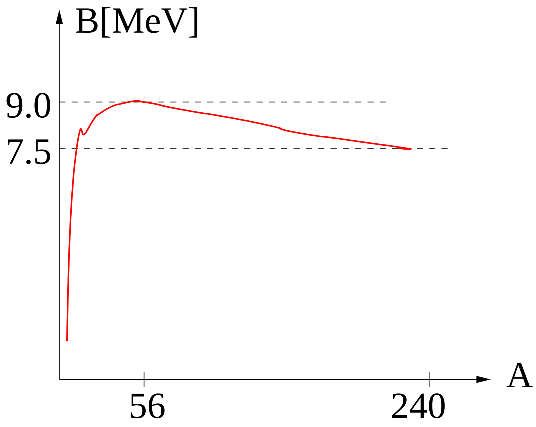
Schematic $N - Z$ diagram of nuclei with definition of *isotopes*, *isotones* and *isobars*. Leaving aside the electromagnetic properties, isobars have very similar properties, showing the *charge independence* of the strong interactions (they are similar for proton and neutron). Examples of isobar states are proton and neutron, ^{3}H and ^{3}He, or ^{14}C and ^{14}N.

Masses of nuclei

The mass of a nucleus is not equal to the sum of proton and neutron masses, but one has

$$M = Z\,m_p + N\,m_n - B/c^2, \tag{5.1}$$

where B is the *nuclear binding energy*. For instance, using MeV's as unit - often these calculations are done in atomic mass units (1 u = 931.478 MeV) - we calculate the binding energies for the deuteron and for ^{12}C. Note that the mass of the Carbon nucleus is 12 u minus 6 electrons, which equals 11.171 80 GeV/c^2.



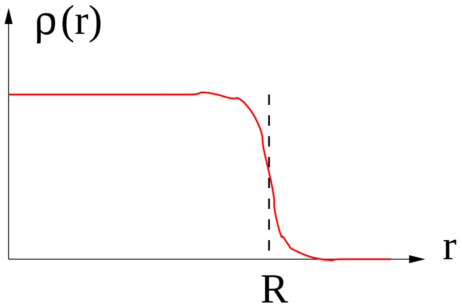
Binding energies per nucleon as a function of A for stable nuclei shows a shape as in the figure. It reaches a maximum around 9 MeV for iron (^{56}Fe) and then gradually decreases to about 7.5 MeV for the largest known A-values. For light nuclei fusion produces energy, for heavy nuclei fission will produce energy.

$$\begin{aligned} m_d &= 1.875\,62 \text{ GeV/c}^2 & m(^{12}\text{C}) &= 11.171\,80 \text{ GeV/c}^2 \\ m_p &= 0.938\,27 \text{ GeV/c}^2 & 6\,m_p &= 5.629\,63 \text{ GeV/c}^2 \\ m_n &= \underline{0.939\,57 \text{ GeV/c}^2} & 6\,m_n &= \underline{5.637\,39 \text{ GeV/c}^2} \\ B &= 0.002\,22 \text{ GeV} = 2 \times 1.11 \text{ MeV} & B &= 0.095\,22 \text{ GeV} = 12 \times 7.93 \text{ MeV} \end{aligned}$$

Binding energies are usually quoted per nucleon. This number is roughly constant. The socalled *separation energy* of a nucleon is found as $E_{\text{separation}}/c^2 = M(A) - M(A-1) - M_N = B(A-1) - B(A)$.

Sizes of nuclei

The charge distribution of a nucleus can be experimentally measured by elastically scattering electrons off the nucleus. Elastic scattering means $e + \text{A} \to e + \text{A}$ (we will return to these scattering processes later). It turns out that the charge, and hence the protons have roughly a constant density. From a variety of other experiments one has also found a more or less constant neutron density.



A roughly constant density implies

$$R = r_0\, A^{1/3}. \tag{5.2}$$

Experimentally the matter distribution (protons and neutrons) requires $r_0 \sim 1.2$ fm, while the charge distribution (protons have a size too!) is about $r_0 \sim 1.4$ fm. This implies a nuclear density of about 10^{15} g/cm^3.

As a general rule, systems that have a size, have some substructure and they can be excited. We have seen this for atoms. As in the case of atoms one could use photons to do this or detect photons if nuclei are excited in other ways, e.g. via collisions with electrons or protons. In this case, however, one needs photons with a quite different wavelength. The typical excitation energy in nuclei go up to the binding energy, i.e. MeV's, corresponding to wavelengths as small as 10^{-12} m.

Spin, parity and magnetic moments of nuclei

The spins of nuclei with A even is always integer, spins of nuclei with A odd are always half-integer, indicating that the nucleons with spin 1/2 are the particles determining the mass number A. In general one has

$$\begin{array}{lll} \text{N even, Z even} & \Rightarrow J = 0 & \text{159 stable nuclei,} \\ \left.\begin{array}{l}\text{N even, Z odd}\\ \text{N odd, Z even}\end{array}\right\} & \Rightarrow J = \text{half} - \text{integer} & \left\{\begin{array}{c}50\\53\end{array}\right\} \text{stable nuclei,} \\ \text{N odd, Z odd} & \Rightarrow J = \text{integer} & \text{just 7 stable nuclei.} \end{array}$$

In general as many neutrons and proton spins as possible are paired to zero. Nuclear states appear to have well-determined parities. This is found by studying selection rules in transitions between excited states in a way similar to that for atoms. Hence, the nuclear force respects mirror symmetry. Some examples are:

nucleus	n	^{1}H	^{2}H	^{3}H	^{3}He	^{4}He	^{6}Li	^{40}Ca	^{41}Ca	^{48}Ca	^{49}Ca
J^π	$\frac{1}{2}^+$	$\frac{1}{2}^+$	1^+	$\frac{1}{2}^+$	$\frac{1}{2}^+$	0^+	1^+	0^+	$\frac{7}{2}^-$	0^+	$\frac{3}{2}^-$
g(A)	-3.83	5.59	1.71	5.96	-4.26	-	1.64	-	-3.19	-	

In this table we also give the magnetic moments for nuclei writing as for nucleons

$$\boldsymbol{\mu}_A = g(A)\,\frac{e\hbar}{2m_p}\,\frac{\boldsymbol{J}}{\hbar}. \tag{5.3}$$

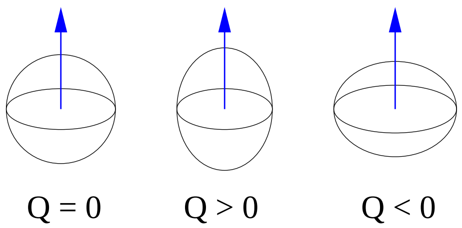
We already discussed that for proton and neutron the results deviate substantially from those of an elementary spin 1/2 particle, $g = 2$. For nuclei, however, one sees that, for example for the deuteron (spin $J = 1$) the result is close to the naively expected $g_p + g_n = 1.76$ (if orbital effects don't play a role), while also the results for ^{3}H and ^{3}He are of the expected order of magnitude if angular momentum doesn't play a role. For higher spins (like the case of ^{41}Ca) the relation with the neutron is less clear.

Electric quadrupole moment

The electric quadrupole moment for a system of charged particles is a tensor given by

$$Q_{ij} = \sum_a Q_a \left(3\, r_{ai} r_{aj} - \boldsymbol{r}_a^2\, \delta_{ij}\right) \tag{5.4}$$

Just as a magnetic moment can be measured in an external $\boldsymbol{B}$-field, the quadrupole moment can be measured in an external $\boldsymbol{E}$-field. It causes a splitting of levels depending only on $|M|$ for spins $J \geq 1$. Note that a state with total angular momentum $J = 0$ has no magnetic moment nor quadrupole moment, while a state with total angular momentum $J = 1/2$ has no quadrupole moment. This is independent of the complexity of the system.



Shapes corresponding to zero, positive or negative values for the quadrupole moment Q_{33}, where the arrow is the z-direction determined by the spin $\boldsymbol{J}$.

5.2 Semi-empirical mass formula

Starting with Weisäcker in 1936 attempts have been made to understand the systematics of nuclear binding energies via an empirical mass formula. The starting point is an average binding energy per particle,

$$B_1 = a_1\,A,$$

a formula that needs several corrections.

(1) The first correction is a correction because a nucleus has a finite size. Nucleons at the surface don't experience the same force. This correction is assumed to be proportional to the surface $\propto R^2 \propto A^{2/3}$. One writes

$$\Delta B_2 = -a_2\,A^{2/3}.$$

(2) A second correction is the electrostatic self-energy. For a uniform charge distribution one has

$$U_Q = \frac{3}{5}\,\frac{Q^2}{R} \propto \frac{Z^2}{A^{1/3}}. \tag{5.5}$$

Therefore one writes

$$\Delta B_3 = -a_3\,\frac{Z^2}{A^{1/3}},$$

(3) A correction is expected to come from the deviation from the fact that N and Z are not equal. A simple model to see what is the expected dependence is assuming a Fermi gas model. Protons and neutrons in nuclei are considered as two (independent) Fermi gases in a volume V, which have similar levels available (the strong interactions are much stronger than electromagnetic effects). Thus for both types one has a level density (see appendix on plane waves) $n(E)dE = V\,d^3p/(2\pi\hbar)^3$. For a spherically symmetric situation one obtains $n(E) \propto V\,\sqrt{E}$. Integrating $n(E)$ and $E\,n(E)$ up to the Fermi energy E_F one gets the number of particles N and the energy U of those particles,

$$\frac{N}{V} \propto \int_0^{E_F} dE\;E^{1/2} = \frac{2}{3}\,E_F^{3/2}, \tag{5.6}$$

$$\frac{U}{V} \propto \int_0^{E_F} dE\;E^{3/2} = \frac{2}{5}\,E_F^{5/2}, \tag{5.7}$$

giving the well-known value of $\frac{3}{5}\,E_F$ for the average energy of particles in a Fermi gas. The equations also tell us that the energy of the N particles is $U \propto V\,E_F^{5/2} \propto N^{5/3}/V^{2/3}$. Thus we have for a system of Z protons and N neutrons in a nuclear volume $V \propto A$,

$$U \propto \frac{Z^{5/3}+N^{5/3}}{A^{2/3}} = A + \frac{5}{9}\,\frac{(N-Z)^2}{A} + \ldots = A + \frac{20}{9}\,\frac{(A/2-Z)^2}{A} + \ldots. \tag{5.8}$$

The expansion around $Z = N$ shows as expected a term in the energy proportional to A, which can be included into a_1 and a correction

$$\Delta B_4 = -a_4\,\frac{(A/2-Z)^2}{A}.$$

(4) The last correction we discuss is the socalled *pairing term* distinguishing even-even, even-odd and odd-odd cases. Empirically it has been found that pairing off spins between identical fermions (protons or neutrons) lowers the energy. The correction is less important for heavy nuclei. One uses

Z	N	# unpaired spins	energy	correction Δ
even	even	0	lower	$+a_5\, A^{-3/4}$
even	odd	1	0	0
odd	even	1	0	0
odd	odd	2	higher	$-a_5\, A^{-3/4}$

The resulting Weisacker formula for the binding energy is

$$B = a_1\, A - a_2\, A^{2/3} - a_3\, \frac{Z^2}{A^{1/3}} - a_4\, \frac{(A/2 - Z)^2}{A} + \Delta. \tag{5.9}$$

The parameters from a best fit are

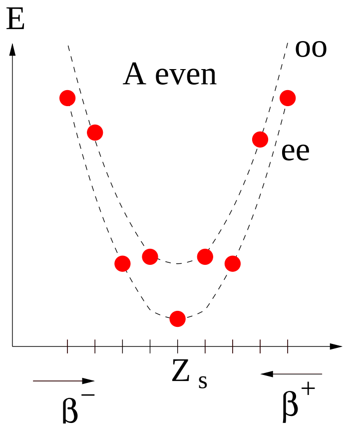
a_1	a_2	a_3	a_4	a_5	
15.76	17.81	0.7105	94.80	39	MeV
0.016 9	0.0191	0.000 763	0.098 55	0.042	u

Stable nuclei

For constant A we can simply find the value for Z for which the binding energy is minimal via $(\partial M/\partial Z)_A = 0$, where $M = A\, m_n + Z\,(m_p - m_n) - B/c^2$. This yields $(m_p - m_n)c^2 - 2\, a_4 (A/2 - Z)\, A^{-1} + 2\, a_3\, Z\, A^{-1/3} = 0$ or

$$Z = \frac{A}{2}\, \frac{\left(1 + \frac{(m_n - m_p)c^2}{a_4}\right)}{\left(1 + \frac{a_3}{a_4}\, A^{2/3}\right)}. \tag{5.10}$$

If A is even, the possibility exist that there is more than one stable nucleus because of the pairing interaction (see figure).



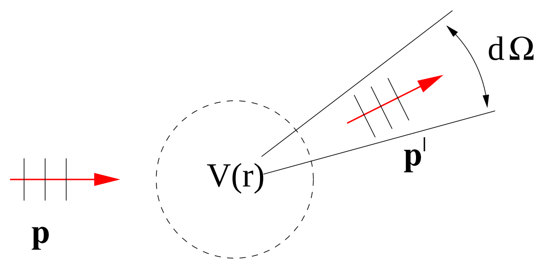
For even A values the (Z, N) combinations will be in turn even-even and odd-odd. In this way we can have several stable nuclei. Between two stable isotopes, there is an unstable nucleus, which can decay via β-decay to be discussed below in more detail. If Δ is too small (depending on the parabolic shape of the $B(Z, A$ fixed) curve, there will be not more than one stable nucleus. This is the case for light nuclei ($A < 35$).

5.3 Scattering theory

Before we discuss models for the nucleon-nucleon force and for nuclear structure, we discuss some aspects of scattering theory needed to understand how experimental information is interpreted.

Cross sections

The quantummechanical treatment of a scattering problem is that of a particle (with mass m and incoming momentum $\boldsymbol{p}$) scattering in a given potential $V(\boldsymbol{r})$. We assume that the particle is scattered into a final state with momentum $\boldsymbol{p}'$. The latter is the result of a measurement with a detector with opening angle $d\Omega$, located under an angle $(\theta,\,\phi)$ with respect to the incoming momentum.



The number of scattered particles per unit time per solid angle, $n(\theta,\phi)$, is proportional to the incoming flux j_{in}, the number of particles per area per unit time,

$$n(\theta,\phi)\,d\Omega = |\boldsymbol{j}_{in}|\,d\sigma(\theta,\phi). \tag{5.11}$$

This is the definition of the *differential cross section* $d\sigma$, from which it should be immediately clear that the unit of cross section indeed is that of an area.

> Typically cross sections have something to do with the area of the target as seen by the incoming particle, e.g. for proton-proton scattering a characteristic cross section is 40 mb, where 1 barn = 1 b $\equiv 10^{-28}$ m^2. The number 40 mb, indeed, is roughly equal to the area of a proton (with a radius of about 1 fm = 10^{-15} m). Besides the area of the target the cross sections also depends on the strength of the interaction. For instance electromagnetic interactions are typically a factor 100 or $(100)^2$ smaller, e.g. $\sigma_{\gamma p} \approx 100$ μb and $\sigma_{ep} \approx 1\mu$b, corresponding to the presence of the fine structure constant α or α^2 respectively, where $\alpha = e^2/4\pi\epsilon_0\hbar c = 1/137$. Weak interactions, e.g. neutrino-proton scattering, again have much smaller cross section in the order of 10^{-2} pb, indicative for the weakness of the "weak" interactions.

Cross section in Born approximation

We use the result of time-dependent perturbation theory to obtain an expression for the cross section, namely the unperturbed situation is the free case, with as possible solutions, the incoming particle in a plane wave, $\phi_i(\boldsymbol{r}) = \sqrt{\rho}\,\exp\left(i\,\boldsymbol{p}\cdot\boldsymbol{r}/\hbar\right)$, with energy $E = \boldsymbol{p}^2/2m$ and the detected final state, $\phi_f(\boldsymbol{r}) = \sqrt{\rho}\,\exp\left(i\,\boldsymbol{p}'\cdot\boldsymbol{r}/\hbar\right)$, with energy $E' = \boldsymbol{p}'^2/2m$. Note that we allow processes in which the energy of the scattered particle changes. writing $Q \equiv E' - E$ one has $Q = 0$ for an elastic scattering process, an energy release, $Q > 0$, for an exothermic process and energy absroption, $Q < 0$, for an endothermic process. The potential V is a perturbation that can cause transitions between plane waves. Using Fermi's golden rule, one obtains the number of particles with momentum $\boldsymbol{p}'$ (of which the direction with respect to $\boldsymbol{p}$ is given by the angles θ,ϕ),

$$n(\theta,\phi)\,d\Omega = \frac{2\pi}{\hbar}\left[|\langle\phi_f|V|\phi_i\rangle|^2\;\rho(E')\right]_{E'=E+Q}. \tag{5.12}$$

In order to get $d\sigma$ we need to know the flux $\mathcal{I}$ in the initial state and the density of states $\rho(E')$ in the final state at the energy E' fixed by energy conservation. For the initial plane wave state the flux is given by $\mathcal{I} = \rho\, v = \rho\, p/m$. The density of final state plane waves is (see appendix D),

$$\rho(\boldsymbol{p}')d^3p' = \frac{1}{\rho}\,\frac{p'^2}{(2\pi\hbar)^3}\,dp'\,d\Omega' = \frac{1}{\rho}\,\frac{m\,p'}{(2\pi\hbar)^3}\,dE'\,d\Omega' = \rho(E')\,dE'\,d\Omega'. \tag{5.13}$$

With the flux and density of final states, we get immediately

$$d\sigma(\theta,\phi) = d\Omega'\left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{p'}{p}\left|\int d^3r\ \exp\left(\frac{i}{\hbar}\,(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{r}\right)\,V(\boldsymbol{r})\right|^2_{E'=E+Q}, \tag{5.14}$$

or introducing the Fourier transform

$$\tilde{V}(\boldsymbol{k}) = \int d^3r\ V(\boldsymbol{r})\ \exp(i\,\boldsymbol{k}\cdot r), \tag{5.15}$$

one obtains the following expression for the differential cross section in the socalled *Born approximation*,

$$\frac{d\sigma}{d\Omega'} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{p'}{p}\,\left|\tilde{V}(\boldsymbol{q})\right|^2, \tag{5.16}$$

where $\hbar\boldsymbol{q} = \boldsymbol{p}-\boldsymbol{p}'$ is the momentum transfer in the process. For an azimuthally symmetric differential cross section one uses $d\Omega = d\cos\theta\,d\phi = 2\pi\,d\cos\theta$ to obtain $d\sigma/d\theta$. Integrating the differential cross section over all angles one obtains the *total cross section*,

$$\sigma(E) = \int d\Omega\,\frac{d\sigma}{d\Omega}(E,\Omega). \tag{5.17}$$

Note that in the case of elastic scattering one has $p' = p$ and the momentum transfer squared is given by

$$\begin{aligned}\hbar^2\boldsymbol{q}^2 &= |\boldsymbol{p}-\boldsymbol{p}'|^2 = p^2 + p'^2 + 2\,pp'\,\cos(\theta)\\ &= 2\,p^2(1-\cos\theta) = 4\,p^2\,\sin^2(\theta/2).\end{aligned} \tag{5.18}$$

A dependence of the differential cross section $(d\sigma/d\Omega)(E,\theta)$ on this combination is a test for the validity of the Born approximation. This dependence is in particular applicable for central potentials, $V(\boldsymbol{r}) = V(r)$, in which case the Fourier transform

$$\begin{aligned}\tilde{V}(\boldsymbol{q}) &= \int d^3r\ V(r)\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}) = 2\pi\int_0^\infty dr\int_{-1}^1 d\cos\alpha\ r^2V(r)\,e^{i\,qr\,\cos\alpha}\\ &= \frac{4\pi}{q}\int_0^\infty dr\ rV(r)\,\sin(qr),\end{aligned} \tag{5.19}$$

only depends on $q = |\boldsymbol{q}|$.

The square well potential

As a first application consider the square well potential, $V(r) = V_0$ for $r \le a$ and zero elsewhere for sufficiently weak potentials at low energies and small angles ($qa \ll 1$). We will come back to the applicability of the Born approximation in a later section. The Fourier transform is given by

$$\begin{aligned}\tilde{V}(\boldsymbol{q}) &= \frac{4\pi\,V_0}{q}\int_0^a dr\;r\,\sin(qr) = \frac{4\pi\,V_0}{q^3}\int_0^{qa} dx\;x\,\sin(x) = \frac{4\pi\,V_0}{q^3}\left[\sin qa - qa\,\cos qa\right] \\ &\overset{qa\ll 1}{\longrightarrow} \frac{4\pi\,V_0}{q^3}\left[qa - \frac{1}{3!}(qa)^3 - qa + \frac{1}{2!}(qa)^3 + \ldots\right] = \frac{4\pi}{3}\,V_0 a^3, \end{aligned} \tag{5.20}$$

leading for $E \to 0$ to

$$\frac{d\sigma}{d\Omega} \approx \frac{1}{9}\left(\frac{2m\,V_0\,a^2}{\hbar^2}\right)^2 a^2 \tag{5.21}$$

The Coulomb potential

The integral

$$\tilde{V}(\boldsymbol{q}) = -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{4\pi}{q}\int_0^\infty dr\;\sin(qr) \tag{5.22}$$

diverges and we need to consider for instance the screened Coulomb potential, multiplied with $\exp(-\mu r)$. In that case one obtains

$$\begin{aligned}\tilde{V}(\boldsymbol{q}) &= -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{4\pi}{q}\int_0^\infty dr\;\sin(qr)\,e^{-\mu r} \\ &= -\frac{Ze^2}{4\pi\epsilon_0}\,\frac{4\pi}{q}\int_0^\infty dr\;\frac{1}{2i}\left(e^{i(q+i\mu)r} - e^{i(q-i\mu)r}\right) \\ &= -\frac{Ze^2}{\epsilon_0}\,\frac{1}{q^2+\mu^2}, \end{aligned} \tag{5.23}$$

allowing even the limit $\mu \to 0$ to be taken. Thus

$$\frac{d\sigma}{d\Omega}(E,\theta) = \left(\frac{m}{2\pi\,\hbar^2}\right)^2\left(\frac{Ze^2}{\epsilon_0}\right)^2\frac{1}{q^4} = \left(\frac{Ze^2}{8\pi\,\epsilon_0\,pv}\right)^2\frac{1}{\sin^4(\theta/2)}. \tag{5.24}$$

This result is known as the Rutherford cross section.

Processes near threshold

If the volume integral over the potential exists, one knows that $\tilde{V}(0)$ is finite and one sees that for small values of the momentum transfer one can write

$$\sigma(E) \;\propto\; \frac{p'}{p} \;=\; \sqrt{\frac{E'}{E}}. \tag{5.25}$$

Thus for an endothermic process (energy absorption or $Q < 0$) one has a threshold value for the incoming energy, $E_{\text{thr}} = |Q|$ and one has for $E \approx E_{\text{thr}}$

$$\sigma(E) \;\propto\; \sqrt{E - E_{\text{thr}}}. \tag{5.26}$$

For an exothermic process (with energy release $Q > 0$) one can scatter for any (positive) energy E and one has near $E \approx 0$

$$\sigma(E) \;\propto\; \frac{1}{\sqrt{E}}. \tag{5.27}$$

Application to two-particle collisions

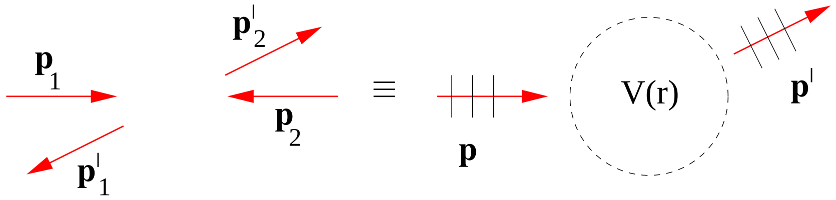
In many applications, the target is not an "external" potential, but rather two particles that collide (*collider experiments*) or one particle that is shot onto another one (*fixed target experiments*). This can in general lead to several possibilities corresponding to several *scattering channels*,

$$\begin{array}{lcll} a+b & \longrightarrow & a+b & \text{(elastic scattering)} \\ & \longrightarrow & \left.\begin{array}{l} c_1+c_2 \\ d_1+d_2+d_3 \end{array}\right\} & \text{(inelastic scattering)} \end{array} \tag{5.28}$$

Nevertheless, one can deal with these processes, at least the two → two ones, by considering the problem in the center of mass (CM) system. Considering two particles with momenta $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ and masses m_1 and m_2, for which the only translationally invariant interaction that is allowed must be of the form $V(\boldsymbol{r}_1 - \boldsymbol{r}_2) = V(\boldsymbol{r})$ with $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ the relative coordinate. Since the flux factor is just given by

$$\mathcal{I} = \rho\,|\boldsymbol{v}_1 - \boldsymbol{v}_2| = \rho\left|\frac{\boldsymbol{p}_1}{m_1} - \frac{\boldsymbol{p}_2}{m_2}\right| = \rho\,\frac{\boldsymbol{p}}{\mu}, \tag{5.29}$$

where $\boldsymbol{p}$ is the relative momentum and μ the reduced mass one sees that the collision of *two* particles indeed can be described by considering the scattering of *one* particle with reduced mass μ having the relative momentum $\boldsymbol{p}$, scattering of the potential $V(\boldsymbol{r})$.



Notes:

- Note that in the scattering of *one* particle in an "external" potential, there is no translation invariance, hence no momentum conservation, while for *two* particles with a potential depending on the relative coordinate there is translation invariance. The latter requires conservation of the total momentum $\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2$, but not of the relative momentum.

- In the limit that one of the masses becomes very large, the light particle's momentum and mass, indeed, coincide with relative momentum and reduced mass, so one finds (consistently) that the heavy particle can be considered as scattering center.

Scattering off a composite system

Consider the scattering of an electron off an extended nucleus consisting of Z protons (and N neutral neutrons). The interaction between the scattering electron and the nucleus is given by,

$$V = -\sum_{j=1}^{Z} \frac{e^2}{4\pi\,\epsilon_0\,|\boldsymbol{r} - \boldsymbol{r}_j|}. \tag{5.30}$$

We consider the nucleus to be initially in a state $|\Phi_A\rangle$ with energy ϵ_A and after the collision in a state $|\Phi_B\rangle$ with energy ϵ_B. Depending on the energy of the incoming electron this will be an elastic or endothermic process with $Q = \epsilon_A - \epsilon_B \le 0$, i.e. part of the energy of the scattering electron is absorbed and brings the nucleus into an excited state. The wave functions of the scattering electron in initial and final states are plane waves characterized by the momenta $\boldsymbol{p} = \hbar\boldsymbol{k}$ and $\boldsymbol{p}' = \hbar\boldsymbol{k}'$, respectively. The full initial state and final state wave functions are taken to be $\Psi_i(\boldsymbol{r}, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) = \sqrt{\rho}\,\exp(i\,\boldsymbol{k}\cdot\boldsymbol{r})\,\Phi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z)$ and $\Psi_f(\boldsymbol{r}, \boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) = \sqrt{\rho}\,\exp(i\,\boldsymbol{k}'\cdot\boldsymbol{r})\,\Phi_B(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z)$, respectively. The Fourier transform of the potential needed to calculate the transition rate and the cross section is

$$
\begin{aligned}
V(\boldsymbol{q}) &= \int d^3r \int \left(\prod_{k=1}^{Z} d^3r_k\right)\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r})\,\Phi_B^*(\boldsymbol{r}_1\ldots\boldsymbol{r}_Z)\left(\sum_{j=1}^{Z}\frac{-e^2}{4\pi\,\epsilon_0\,|\boldsymbol{r}-\boldsymbol{r}_j|}\right)\Phi_A(\boldsymbol{r}_1\ldots\boldsymbol{r}_Z) \\
&= -\frac{e^2}{4\pi\,\epsilon_0}\sum_{j=1}^{Z}\int\left(\prod_{k=1}^{Z} d^3r_k\right)\,\Phi_B^*(\boldsymbol{r}_1\ldots\boldsymbol{r}_Z)\,\Phi_A(\boldsymbol{r}_1\ldots\boldsymbol{r}_Z)\int d^3r\ \ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r})\,\frac{1}{|\boldsymbol{r}-\boldsymbol{r}_j|} \\
&= -\frac{e^2}{4\pi\,\epsilon_0}\sum_{j=1}^{Z}\int\left(\prod_{k=1}^{Z} d^3r_k\right)\,\Phi_B^*\,\Phi_A\,\exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}_j)\int d^3r'\ \ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}')\,\frac{1}{r'} \\
&= -\frac{e^2}{4\pi\,\epsilon_0}\,\frac{4\pi}{q^2}\,F_{BA}(\boldsymbol{q}), \qquad (5.31)
\end{aligned}
$$

where we have introduced the nuclear form factor

$$
\begin{aligned}
F_{BA}(\boldsymbol{q}) &= \sum_{j=1}^{Z}\int\left(\prod_{k=1}^{Z} d^3r_k\right)\ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}_j)\,\Phi_B^*(\boldsymbol{r}_1\ldots\boldsymbol{r}_Z)\,\Phi_A(\boldsymbol{r}_1\ldots\boldsymbol{r}_Z) \qquad (5.32) \\
&= \int d^3s\ \ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{s})\ \underbrace{Z\int\left(\prod_{k=2}^{Z} d^3r_k\right)\ \Phi_B^*(\boldsymbol{s},\boldsymbol{r}_2\ldots\boldsymbol{r}_Z)\,\Phi_A(\boldsymbol{s},\boldsymbol{r}_2\ldots\boldsymbol{r}_Z)}_{\rho_{BA}(\boldsymbol{s})},
\end{aligned}
$$

which is the Fourier transform of the one-nucleon (transition) density $\rho_{BA}(\boldsymbol{s})$. We note that the wave functions Φ_A and Φ_B are fully antisymmetric. The result for the cross section is

$$
\frac{d\sigma_{BA}}{d\Omega} = \left(\frac{m\,e^2}{2\pi\,\epsilon_0\,\hbar^2\,q^2}\right)^2\frac{p'}{p}\,|F_{BA}(\boldsymbol{q})|^2 . \qquad (5.33)
$$

and shows the possibility to determine the distribution of nucleons in a nucleus.

Form factors

From the measurements of form factors one obtains via the Fourier transform the charge density,

$$
F(\boldsymbol{q}) = \int d^3r\ \ \exp(i\,\boldsymbol{q}\cdot\boldsymbol{r})\,\rho(\boldsymbol{r}). \qquad (5.34)
$$

As before, in discussing the potential in momentum space, one has for a spherically symmetric density,

$$
F(q) = \frac{4\pi}{q}\int dr\ r\,\rho(r)\,\sin(qr). \qquad (5.35)
$$

For a spherical distributions it is trivial to find by expanding the exponential $\exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}) = 1 + i\,\boldsymbol{q}\cdot\boldsymbol{r}$ - $\frac{1}{2}\,(\boldsymbol{q}\cdot\boldsymbol{r})^2 + \ldots$, that

$$F(q) = Q - \frac{1}{6}\,q^2\,\langle r^2\rangle + \ldots, \tag{5.36}$$

where $Q = \int d^3r\;\rho(r)$ is the total charge and $\langle r^2\rangle = \int d^3r\;r^2\,\rho(r)$ is the charge radius squared. The small-$\boldsymbol{q}$ behavior of a form factor can thus be used to determine the charge radius of an atom, a nucleus or a nucleon.

Some examples of form factors corresponding to specific densities are:

- A uniform density

  $$\rho(r) = \rho_0 \qquad \text{for } x \le R \tag{5.37}$$

  (and zero elsewhere). If $\rho_0 = 3/4\pi\,a^3$, i.e. the integrated density is one, the Fourier transform is given in terms of the Bessel function j_1,

  $$F(q) = \frac{3\,j_1(qR)}{qR}, \quad \text{where} \quad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}. \tag{5.38}$$

  Note that

  $$\frac{3\,j_1(x)}{x} \approx 1 - \frac{1}{10}\,x^2 + \ldots, \tag{5.39}$$

  and, indeed, the charge radius of a uniform distribution is $\langle r^2\rangle = \frac{3}{5}\,R^2$. Examples of uniform densities are the nuclear densities, although agreement with data can be improved by introducing a smooth fall-off at the edge.

- A (normalized) Yukawa distribution

  $$\rho(r) = \frac{\mu^2}{4\pi}\,\frac{e^{-\mu r}}{r}, \tag{5.40}$$

  has as form factor

  $$F(q) = \frac{\mu^2}{q^2+\mu^2} = \frac{1}{1+q^2/\mu^2}, \tag{5.41}$$

  which is called a *monopole* form factor. We have encountered this same Fourier transform already earlier where we derived the momentum space screened Coulomb potential.

- The form factor of the (normalized) exponential distribution

  $$\rho(r) = \frac{\mu^3}{8\pi}\,e^{-\mu r}, \tag{5.42}$$

  is simply found by differentiation of the Yukawa form factor with respect to μ, yielding

  $$F(q) = \frac{1}{(1+q^2/\mu^2)^2}, \tag{5.43}$$

  which is called a *dipole* form factor. The charge density of the proton behaves in this way, with the experimental formfactor having $\mu^2 \approx 0.71$ GeV^2.

- Finally a normalized Gaussian distribution

  $$\rho(r) = \rho_0\,e^{-\frac{1}{2}r^2/R^2} \tag{5.44}$$

  has also a Gaussian form factor

  $$F(q) = e^{-\frac{1}{2}q^2\,R^2}. \tag{5.45}$$

5.4 The nucleon-nucleon force

The most important properties of the force between two nucleons, deduced from scattering experiments between nucleons, are:

1. The force is short-ranged, i.e. of the order of fm's ($1\text{ fm} = 10^{-15}$ m, also referred to as 1 Fermi). This is deduced from scattering experiments between nucleons.

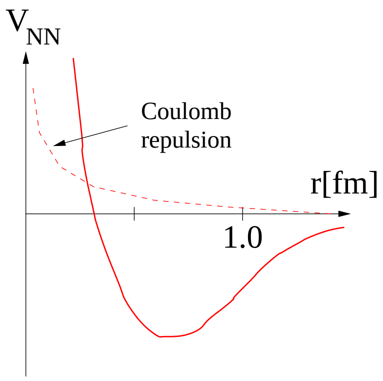
2. The force is *charge independent*, which means that the charge between two protons is the same as between proton-neutron and between two neutrons. Indications for this come from

   - Light nuclei have equal number of protons and neutrons.
   - The binding energy per nucleon is roughly constant.
   - The mass difference between *mirror nuclei* (same A on opposite side of $Z = N$) is tiny, e.g. for ^{3}H and ^{3}He.

3. The force between nucleons depends on the spin of the nucleons, again something which can be deduced from scattering experiments.

4. The force is not central. It depends on the spin orientations with respect to the relative coordinate of the two nucleons. This means that the orbital angular momentum $\boldsymbol{\ell}$ is not compatible with the hamiltonian (ℓ is not a good or conserved quantum number).

5. At short range the force is repulsive.



The nucleon-nucleon potential, which for pp includes a Coulomb repulsion. A reasonable approximation for the deuteron is a square well potential with depth $-V_0$ and range a (possibly with a hard core, $V(r) \to \infty$ at a distance $r \leq b$).

In order to study the two-nucleon system, it is necessary to look at the possible spin and spatial wave functions. The two nucleons have spin 1/2, from which one can construct one antisymmetric spin 0 wavefunction and three symmetric spin 1 wave functions. Next consider the relative orbital angular momentum ℓ, which can be $\ell = 0, 1, \ldots$. It is ℓ, which also determines the parity of the two-nucleon system, $\Pi = (-)^\ell$. In the case of two protons or two neutrons, one cannot simply combine any orbital wave function with any of the two spins. The total wave function must be antisymmetric. As far as the orbital part is concerned exchanging the particles is the same as changing the relative coordinate, thus also the exchange symmetry is $(-)^\ell$. Including spin one obtains the configurations indicated as $^{2S+1}\ell_J$ in the first row. In the table is indicated if the Pauli principle allows such configuration for pp, nn or pn.

${}^{2S+1}\ell_J$	pp	nn	pn	$(NN)_{I=0}$	$(NN)_{I=1}$
${}^1S_0$	yes	yes	yes	-	yes
${}^3S_1$	-	-	yes	yes	-
${}^1P_1$	-	-	yes	yes	-
${}^3P_{0,1,2}$	yes	yes	yes	-	yes
${}^1D_2$	yes	yes	yes	-	yes
${}^3D_{1,2,3}$	-	-	yes	yes	-
${}^1F_3$	-	-	yes	yes	-
${}^3F_{2,3,4}$	yes	yes	yes	-	yes

The similarity of the strong interactions for protons and neutrons have led to the introduction of *isospin* symmetry. Proton and neutron are considered as two possible nucleon states, which are labeled by isospin I and third component of isospin I_3, in complete analogy with spin. The two-state nucleon system is assigned $I = 1/2$ and $I_3 = \pm 1/2$,

$$|p\rangle = |1/2, +1/2\rangle, \qquad |n\rangle = |1/2, -1/2\rangle.$$

As seen in the table above, the use of isospin is not necessary, but it is often convenient. When one uses isospin, the *generalized Pauli principle* requires antisymmetry of the full wave function, which now incorporates orbital part, spin part and isospin parts. Just as for spin, the isospin singlet $I = 0$ is the antisymmetric wave function and it can be combined with an antisymmetric spin wave function $S = 0$ only for an antisymmetric orbital wave function (ℓ odd).

The deuteron

The deuteron is a proton-neutron bound state with $J^\Pi = 1^+$. There is no proton-neutron state with $J^\Pi = 0^+$, nor are there proton-proton or neutron-neutron bound states. The binding-energy of the deuteron is small, $B = 2.22$ MeV. The conclusion is that the NN potential is spin-dependent. It appears that the groundstate in the two-nucleon system is a weakly bound ${}^3S_1$ state (isosinglet with $I = 0$), while the ${}^1S_0$ states (isotriplet with $I = 1$) are not bound. For a bound state, we know that the wave function for large r-values approaches $u(r) \to e^{-\alpha\, r}$, where $B = \hbar^2\,\alpha^2/2m$. Thus $\alpha \approx 46$ MeV $\approx 1/4$ fm^{-1} (note that the reduced mass $m = 0.5\, m_N$). This weak fall-off indicates indeed a weakly bound state. To estimate the parameters of the nucleon-nucleon potential assume a square well with depth $-V_0$ and size a. Taking as an approximation $\alpha = 0$ (a bound state at the edge of the square well called *zero-binding approximation*) the wave function in the well must satisfy $u'(a) = 0$. The wave function in the well is given by

$$u(r) \quad \propto \quad \sin(K\, r) \quad \text{with} \quad K = \sqrt{\frac{2m(E + V_0)}{\hbar^2}},$$

which with $E \approx 0$ gives

$$\sqrt{\frac{2m\, V_0}{\hbar^2}}\, a = \frac{\pi}{2} \quad \Rightarrow \quad V_0\, a^2 = \frac{\pi^2\, \hbar^2 c^2}{8mc^2} \approx 2.5 \text{ GeV}^{-1} \approx 0.1 \text{ GeV fm}^2.$$

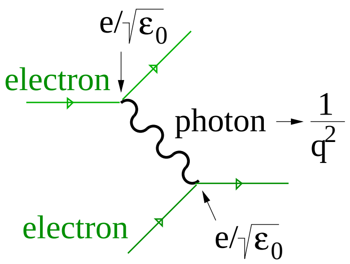
Using results from NN scattering (with $d\sigma/d\Omega \sim 15$ mb/sr at threshold) one obtains $a \approx 1.5$ fm and hence $V_0 \approx 45$ MeV.

Actually, if the deuteron would be a pure ${}^3S_1$ bound state, it would have a quadrupole moment $Q = 0$. Experimentally, one has found $Q \neq 0$. Furthermore, the magnetic moment deviates (slightly) from the sum of the proton and neutron magnetic moments. These effects indicate that the actual groundstate is not a pure S-wave, but is a mixture of ${}^3S_1$ and ${}^3D_1$, both of which can contribute in a $J^\Pi = 1^+$ state. The ${}^3P_1$ state cannot contribute to a positive parity state. Calculations indicate about a 6 % admixture of D-wave, i.e. $\Psi \approx 0.97\,\psi({}^3S_1) + 0.25\,\psi({}^3D_1)$.

Summarizing, the nucleon-nucleon force has various contributions, among them a central, a spin-spin and a tensor contribution,

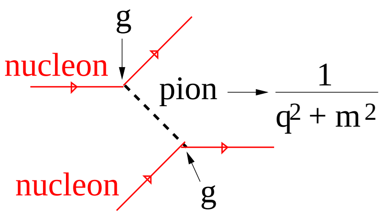
$$V_{NN}(\boldsymbol{r}) = V_c(r) + V_{\rm s}(r)\,\boldsymbol{s}_1\cdot\boldsymbol{s}_2 + V_{\rm t}(r)\left[\frac{3(\boldsymbol{s}_1\cdot\boldsymbol{r})(\boldsymbol{s}_2\cdot\boldsymbol{r})}{\boldsymbol{r}^2} - \boldsymbol{s}_1\cdot\boldsymbol{s}_2\right], \qquad (5.46)$$

The tensor contribution is responsible for the mixture between different ℓ-waves. For such a potential ℓ is not a good quantum number, although the total spin turns out to be still a good quantum number. The spin-spin interaction turns out to be repulsive for $S = 1$, rendering the $I = 1$ nucleon-nucleon ${}^1S_0$ wave (with pp and nn) unbound. Also parity is a good quantum number for the above potential and for the strong interactions in general. A potential as above can be derived from the exchange of pions between the nucleons. It is the same mechanism as the exchange of photons that is used to derive the Coulomb potential. In such derivations (for which one needs to use methods from quantum field theory) one needs a coupling of the particles, e.g. $e/\sqrt{\epsilon_0}$ for photons to charged particles or g for pions coupling to nucleons and the propagators for exchanged particles, $G \propto 1/(\boldsymbol{q}^2 + m^2c^2/\hbar^2) = 1/(\boldsymbol{q}^2 + \lambda\!\!\!^{-}_\pi{}^{-2})$.



$$V(\boldsymbol{q}) = \frac{e^2}{\epsilon_0}\frac{1}{\boldsymbol{q}^2}$$

$$\Rightarrow\quad V(r) = \frac{e^2}{4\pi\,\epsilon_0}\frac{1}{r}.$$

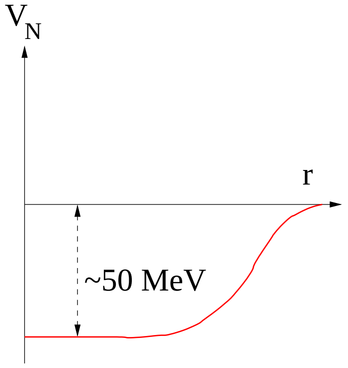


$$V(\boldsymbol{q}) = g^2\,\frac{1}{\boldsymbol{q}^2 + m_\pi^2c^2/\hbar^2}$$

$$\Rightarrow\quad V(r) = \frac{g^2}{4\pi}\,\frac{\exp(-r/\lambda\!\!\!^{-}_\pi)}{r}.$$

5.5 The nuclear shell-model

For larger nuclei an approach similar as in the atom is taken. A nucleon is considered in the potential produced by all other nucleons.

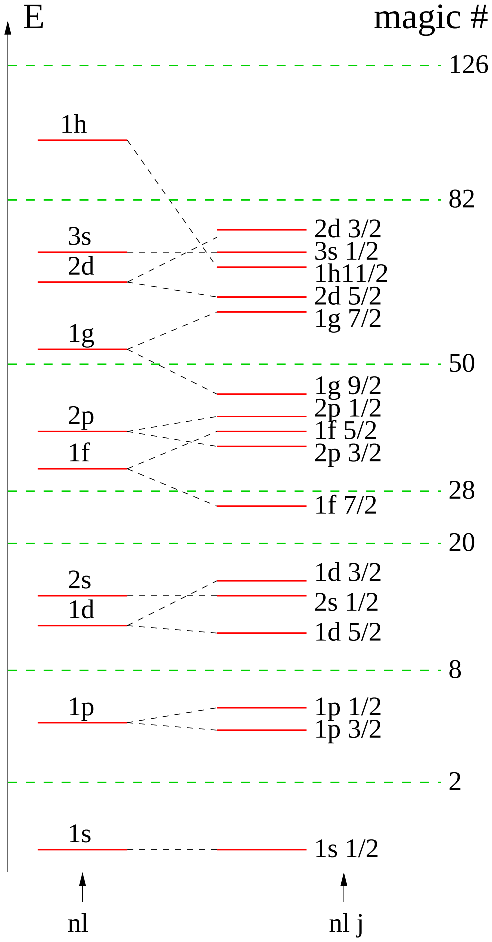


A typical ansatz for this is a well-like potential, or a bit more sophisticated, a Woods-Saxon potential of the form

$$V(r) = \frac{V_0}{1 + \exp[(r-a)/t]}, \tag{5.47}$$

which falls to half its central value at $r = a$ with the thickness t determining how much it deviates from a square well ($t \to 0$). The shape of the effective potential, not surprisingly, resembles the nuclear density.

In spite of the fact that nucleons are pretty big themselves with $R_N \approx 0.8$ fm, the nuclear wave function is well described in a shell model, in which nucleons occupy consecutive orbits in the nuclear potential, with only as a refinement some additional correlations reflecting the short-range repulsion between pairs. As in atoms, the wave function can be written down as a Slater determinant, a properly antisymmetrized product of single-particle wave functions.



The effective level structure available for nucleons (protons and neutrons) in a nucleus. The order of magnitude is MeV's. In a nucleus there is a strong spin-orbit splitting,

$$V_{\rm ls}(r) = -\frac{a_{\rm ls}^2}{r}\frac{dV}{dr}\,\boldsymbol{\ell}\cdot\boldsymbol{s}, \tag{5.48}$$

so the orbital angular momentum and spin of a nucleon must be coupled to the total angular momentum j. Important is the sign of the spin-orbit interaction, which causes the highest j-values to come down in energy.

A spin-orbit interaction with this sign is actually found by solving the relativistic Dirac equation for light particles in a square well, instead of the Schrödinger equation. A whole Dirac phenomenology is built upon this treatment, in which the typical 50 MeV potential added to the mass $M + V$ is replaced by a sum of $M - V_{\rm scalar} + V_{\rm vector}$, with $V_{\rm scalar}$ being of the order of several hundreds of MeV.

The dashed lines in the spectrum of nuclear levels indicate filled groups of levels separated from the higher ones with a sufficiently large gap. This leads to the socalled magic numbers for Z and N with relatively stable nuclei. For nuclei with one additional proton or neutron (or one missing) one immediately finds the J^Π values of the nucleus. The nuclear shell model has been very successful in providing reasonable wave functions, excitation spectra, and several nuclear properties, such as magnetic moments, transition rates and transition form factors.

Measuring the 'single particle orbits'

In a process like

$$e + A \longrightarrow e + \underbrace{(A-1) + p}_{B} \tag{5.49}$$

one can obtain the wave function squared via the emitted proton p in the process. The principle is the same as in measuring densities via the form factor as explained above. One again calculates the transition amplitude, but the final state wave function is the remainder nucleus (A-1) and the emitted proton with momentum $\boldsymbol{p}$ (we will neglect the recoil of the $(A-1)$ nucleus). Thus $\Phi_B(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) = \exp(i\,\boldsymbol{p}' \cdot \boldsymbol{r}_1)\,\Phi_{A-1}(\boldsymbol{r}_2, \ldots, \boldsymbol{r}_Z)$. One obtains in analogy to Eq. 5.31

$$\begin{aligned} V(\boldsymbol{p}', \boldsymbol{q}) &= \langle A-1; p(\boldsymbol{p}'), e(\boldsymbol{k}')|V|A; e(\boldsymbol{k})\rangle \\ &= -\frac{e^2}{4\pi\,\epsilon_0}\,\frac{4\pi}{q^2}\sum_{j=1}^{Z}\int\left(\prod_{k=1}^{Z} d^3r_k\right)\,\exp(i\,\boldsymbol{q}\cdot\boldsymbol{r}_j)\,\exp(-i\,\boldsymbol{p}'\cdot\boldsymbol{r}_1) \\ &\qquad\qquad \times\,\Phi^*_{A-1}(\boldsymbol{r}_2, \ldots, \boldsymbol{r}_Z)\,\Phi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z). \end{aligned}$$

When the nuclear wave function is written as a product of single particle wave functions, $\Phi_A(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_Z) = \phi_a(\boldsymbol{r}_1)\,\phi_b(\boldsymbol{r}_2)\ldots\phi_z(\boldsymbol{r}_Z)$ and $\Phi_{A-1}(\boldsymbol{r}_2, \ldots, \boldsymbol{r}_Z) = \phi_b(\boldsymbol{r}_2)\ldots\phi_z(\boldsymbol{r}_Z)$ one sees that

$$V(\boldsymbol{p}', \boldsymbol{q}) = -\frac{e^2}{4\pi\,\epsilon_0}\,\frac{4\pi}{q^2}\,\tilde{\phi}_a(\boldsymbol{p}' - \boldsymbol{q}) \tag{5.50}$$

where $\tilde{\phi}_a$ is the momentum-space single-particle wave function. The cross section thus is simply proportional to $|\tilde{\phi}_a(\boldsymbol{p}' - \boldsymbol{q})|^2$, where (in the limit of heavy nuclei) the momentum $\boldsymbol{p}' - \boldsymbol{q}$ is just the momentum of the *struck* nucleon. Note that we have skipped here some (if $\boldsymbol{p}'$ and $\boldsymbol{q}$ are sufficiently high minor) complications. Furthermore one should include proper antisymmetrization, but this is straightforward.

5.6 Nuclear reactions and decay

Beta-decay

We already mentioned the neutron decay,

$$\beta^- - \text{decay}: \qquad n \longrightarrow p + e^- + \bar{\nu}_e. \tag{5.51}$$

For the neutron the lifetime is about 15 minutes. In nuclei, this decay is possible provided the energy difference between initial and final nucleus is larger than one electron mass. This causes decay of nuclei with $Z < Z_{\text{stable}}$ along an isobar line in steps $\Delta Z = +1$ towards the stable nucleus. An example is the decay of tritium (^{3}H) into ^{3}He. The maximum energy available to the electron depends on the mass of the neutrino. This was the first (obvious) attempt to obtain limits on the mass of the neutrino. These experiments (see next chapter) led only to upper limits in the order of eV's. The transition of a proton into a neutron,

$$\beta^+ - \text{decay}: \qquad p \longrightarrow n + e^+ + \nu_e, \tag{5.52}$$

is not possible for a free proton ($m_p < m_n + m_e + m_\nu$) but is possible in nuclei, causing decay of nuclei with $Z > Z_{\text{stable}}$ along an isobar line in steps $\Delta Z = -1$ towards the stable nucleus.

In an atom, the presence of electrons can lead to the socalled *electron capture* for which the underlying process is

$$\text{e} - \text{capture}: \qquad e^- + p \longrightarrow n + \nu_e. \tag{5.53}$$

Gamma-decay

Emission (and in principle also absorption) of photons with typical energies of the order of 1 MeV occur in 1-particle transition, where one proton or neutron switches from one to another level belonging to the excitation spectrum of the same nucleus ($\Delta Z = \Delta N = 0$).

As selection rules one has parity and spin, which are good quantum numbers. Photon emission and absorption proceeds via operators that are connected to the position operator, such as the dipole operator, quadrupole operator, which enter via an expansion of the photonic plane wave. One distinguishes electric ($E\ell$) and magnetic ($M\ell$) multipole transitions with $\ell = 1$ (dipole), 2 (quadrupole), 3 (octupole), etc. The selection rules are

$$\begin{aligned} E\ell: &\quad P = (-)^\ell \quad \text{and} \quad |\Delta J| \le \ell, \\ M\ell: &\quad P = (-)^{\ell+1} \quad \text{and} \quad |\Delta J| \le \ell. \end{aligned}$$

The typical strength of multipole transitions is proportional to

$$\text{strenght} \quad \propto \quad \left(\frac{\text{size of system}}{\text{wavelength of photons}}\right)^\ell,$$

while furthermore magnetic transitions are weaker than electric ones. This explains why for atoms ($d/\lambda \sim 10^{-3}$) only electric dipole transitions are relevant, while for nuclei ($d/\lambda \sim 10^{-1}$) higher multipoles are also important.

Photons with smaller energies, $E_\gamma \sim 100$ keV can be used to study vibrational and rotational excitations of the nucleus. These are collective phenomena to be compared with the vibrations and rotations of molecules.

Alpha-decay

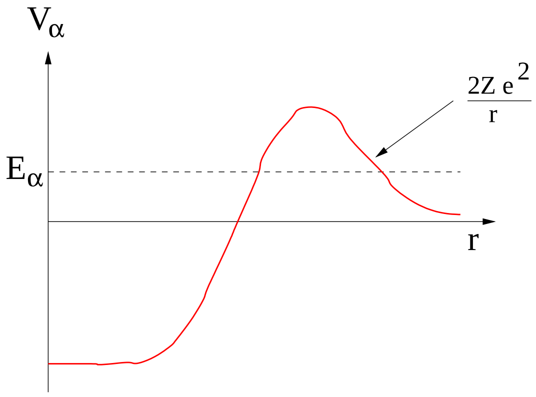
Alpha decay is the emission of α-particles, a process possible for heavy nuclei,

$$\alpha - \text{decay}: \qquad {}^A_Z X \longrightarrow {}^{A-4}_{Z-2} X' + \alpha. \tag{5.54}$$

Some radioactive chains are:

$$\begin{aligned} &{}^{238}\text{Th} \longrightarrow (1.5 \times 10^{10}\ \text{yr}) \longrightarrow\ {}^{208}\text{Pb} \qquad (\text{running via nuclei with } A = 4n) \\ &{}^{237}\text{Np} \longrightarrow (2.2 \times 10^{6}\ \text{yr}) \longrightarrow\ {}^{205}\text{Tl} \qquad (\text{running via nuclei with } A = 4n+1) \\ &{}^{238}\text{U} \longrightarrow (4.5 \times 10^{9}\ \text{yr}) \longrightarrow\ {}^{206}\text{Pb} \qquad (\text{running via nuclei with } A = 4n+2) \\ &{}^{235}\text{U} \longrightarrow (7 \times 10^{9}\ \text{yr}) \longrightarrow\ {}^{207}\text{Pb} \qquad (\text{running via nuclei with } A = 4n+3) \end{aligned}$$

The ^{4}He nucleus is the most optimal nucleus to be emitted, because its binding energy is much larger than that of the lighter nuclei, while the probability to find a ^{4}He-like configuration (with both protons and neutrons paired to spin 0) is large compared to configurations of more protons and neutrons. The reaction will only occur if some energy Q is released. The enormous diversity in lifetimes can be easily understood in terms of



To understand α-decay, one uses an effective potential for the α-particle with respect to the ${}^{A-2}_{Z-2}$X. Somehow the α is bound at the energy $M({}^A_Z\mathrm{X})c^2$ in a metastable state caused by a barrier, which behaves for $r \geq r_0\, A^{1/3}$ roughly as $V(r) \approx 2Ze^2/4\pi\epsilon_0\, r$. The α particle can tunnel the barrier.

the tunneling (see figure) through the barrier showed above. From quantum mechanics we know that the transition probability for tunneling a barrier is given by

$$T \approx \exp\left(-2\int_R^{R_1} dr\,\sqrt{\frac{2m\,(V(r)-E)}{\hbar^2}}\right). \tag{5.55}$$

The tunneling explains the tremendous energy sensitivity of the lifetimes for α-decay. With a typical resonance time of the α in the nucleus of $\tau_0 \sim 2R/v$, where R is the size of the nucleus and v is the velocity of the α-particle one obtains (with $E = Q = 2Ze^2/4\pi\epsilon_0\, R_1$),

$$\tau = \tau_0\,\exp\left(2\int_R^{R_1} dr\,\sqrt{\frac{2m\,(V(r)-Q)}{\hbar^2}}\right) = \tau_0\,\exp\left(2\sqrt{\frac{2m\,Q}{\hbar^2}}\int_R^{R_1} dr\,\sqrt{\frac{R_1}{r}-1}\right). \tag{5.56}$$

It results in $\ln\tau \sim a/\sqrt{Q} - b$, ranging from fractions of a second to more than 10^9 years when changing Q from a few MeV towards 10 MeV.

Fusion and Fisson

We already mentioned collective excitations in nuclei that are excited by photons. Similarly the capture of thermal neutrons can produce an instable nucleus, e.g.

$$^{235}U + n \longrightarrow \left(^{236}U\right)^*.$$

The latter nucleus is instable and (like a droplet) fissions into two fragments. The net energy result is about 240 nucleons gaining some 0.7 MeV binding energy.

For light nuclei fusion will produce energy. This process is the engine of stars burning Hydrogen into heavier elements, in particular into Helium.

Exercises

Exercise 5.1

Construct the spin wave functions for ppn and argue which of these is the one relevant for ^3He in the ground state.

Exercise 5.2

Estimate the size of the a_3 term in the semi-empirical mass formula using Eq. 5.5

Exercise 5.3

Check the stability line $Z(A)$ as calculated from the semi-empirical mass formula for a few examples, using the island of stability figure in Chapter 1 or some table of stable nuclei. Find some A's for which you expect more than one stable nucleus.

Exercise 5.4

Determine the depth of the deuteron potential, using a square well potential with a hard core for $r \leq b = 0.4$ fm and a range $a = 1.5$ fm. Do this in the zero-binding approximation and numerically [e.g. using Mathematica].

Exercise 5.5

Given that the proton charge form factor is a dipole form factor with $\mu^2 = 0.71$ GeV^2, calculate the charge radius of the proton.

Exercise 5.6

Look for the spectrum of a square-well or (with an algebraic manipulation program) a Woods-Saxon potential (with a small thickness parameter, say $t = 2$ fm with depth V_0 and a 'nuclear' size $r_0\,A^{1/3}$ depending on A. Play a bit with the depth, so as to get consistency, that means you need at least sufficient orbits to place all neutrons. If you really get going, add a repulsive Coulomb interaction and solve for the proton levels.

Exercise 5.7

Determine the spin and parity of the following nuclei: ^{36}Ar, ^{37}Ar, ^{38}Ar, ^{39}Ar and ^{40}Ar.

Exercise 5.8

Show the $\ln\tau \sim a/\sqrt{Q} - b$ behavior for α-decay using the tunneling through a Coulomb potential of the form $V(r) = 2Ze^2/4\pi\epsilon_0\,r$ from R to R_1, where $Q = 2Ze^2/4\pi\epsilon_0\,R_1$. Take characteristic values $Z = 90$ and $A = 220$. To estimate the velocity of the α-particle in the nucleus use a typical value for the kinetic and potential energy of 50 MeV.

Exercise 5.9

Estimate the energy release of a ^{235}U nucleus splitting into two (roughly equal) fragments. How much energy can be released from 10 kg ^{235}U. Convert this into Joules.

Exercise 5.10

The half-life of ^{235}U is 7.04×10^8 yr, while that for ^{238}U is 4.468×10^9 yr. Assuming as much of both isotopes when the Earth was formed en the present abundance of the 235-isotope of 0.72 %, deduce the lifetime of the Earth.

Chapter 6

Particles

6.1 Introduction

In chapter 1 we have discussed some basic features of elementary particles. Observed elementary particles fall into three classes, *hadrons*, *leptons* and *force-carriers* (also referred to as *gauge bosons*). Hadrons are composite and built from *quarks*. Quarks, leptons and gauge bosons are (as far as we know presently) elementary.

ELEMENTARY PARTICLES						COMPOSITE PARTICLES	
		spin	interactions				spin
			strong	EM	weak		
leptons $(\ell, \overline{\ell})$		1/2	no	yes	yes		
						baryons (qqq)	half-integer
quarks $(q, \overline{q})$		1/2	yes	yes	yes	mesons $(q\overline{q})$	integer
gauge bosons	electroweak $(\gamma, W^{\pm}, Z^0)$	1	no	yes	yes		
	strong (gluons)		yes	no	no		

The concept of a particle and unstable states

Particles that travel macroscopic distances are most easily to conceive. Tracks of electrons or protons can be made visible in bubble chambers (used from the 1950's to around 1980) relying for their operation on a superheated liquid, e.g. hydrogen or deuterium, in which bubbles form along the particle tracks. The momentum can be determined by embedding the whole setup in a magnetic field, in which charged particles describe circular (or spiraling) orbits. Instead of the bubble chambers one nowadays uses many other detecting techniques, e.g. wire chambers, in which induced currents indicate the presence of charged particles. Often one has all kinds of detector elements specifically aimed at certain particles, such as muons or photons. The key property of such a particle is its mass, determined from a measurement of energy E and momentum $\boldsymbol{p}$ via

$$M^2 = E^2 - \boldsymbol{p}^2. \tag{6.1}$$

We will mostly set $\hbar = c = 1$, as discussed in Chapter 1. Keeping c one would have $M^2c^4 = E^2 - \boldsymbol{p}^2c^2$. The relation is valid in any reference frame. In the restframe one has $E = Mc^2$.

In particle physics one often deals with extremely unstable particles, decaying in fractions of a second. For particles living of the order of $\tau = 10^{-12}$ s the lifetime can still be determined in a classical way, such as from the length of of a track within the detector ($c\tau \approx 3$ cm). For particles that live much shorter (and we will see many typical lifetimes of the order of $\tau = 10^{-24}$ s) this is impossible. In that case one employs the corresponding energy uncertainty.

Consider for this an unstable particle decaying into two other particles $R \to 1 + 2$. The probability P to find the particle R decreases in time,

$$P(t + dt) = P(t)\;(1 - \Gamma\, dt) \quad\Longrightarrow\quad \frac{dP}{dt} = -\Gamma\, P(t), \tag{6.2}$$

where Γ is the *decay rate* or decay probability per unit time. The solution is

$$P(t) = P(0)\, e^{-\Gamma\, t} = P(0)\, e^{-t/\tau}, \tag{6.3}$$

with $\tau = \hbar/\Gamma = 1/\Gamma$ the *lifetime*. The quantity Γ is referred to as the *width* of a state. Rather than a plane wave, the wave function of particle R is

$$|\psi_R(t)\rangle \propto e^{-i\,E_R t - \Gamma_R t/2}, \tag{6.4}$$

at least for $t \geq 0$. We can expand a decaying state in eigenmodes according to

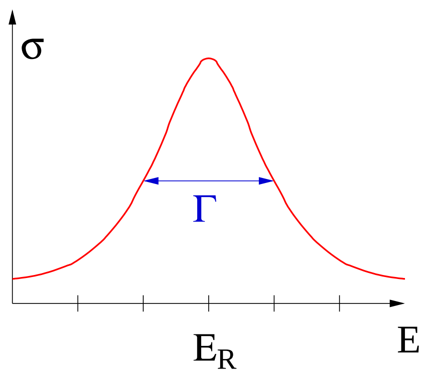
$$e^{-i\,E_R t - \Gamma_R t/2}\,\theta(t) = \int_{-\infty}^{\infty} \frac{dE}{2\pi}\, c(E)\, e^{-i\,Et}, \tag{6.5}$$

and calculate $c(E)$ in the following way

$$\begin{aligned} c(E) &= \int_0^\infty dt\; e^{+i\,(E - E_R + i\Gamma_R/2)t} \\ &= \frac{-i}{E - E_R + i\Gamma_R/2}\, e^{+i\,(E - E_R + i\Gamma_R/2)t}\Big|_0^\infty \\ &= \frac{i}{E - E_R + i\Gamma_R/2}. \end{aligned} \tag{6.6}$$

In the decay of unstable states $R \to 1{+}2$ one thus has a transition amplitude proportional to $c(E_1 + E_2)$ and a distribution of final state energy distribution in $E_{12} = E_1 + E_2$ proportional to

$$I(E_{12}) \propto |c(E_{12})|^2 \propto \frac{1}{(E_R - E_{12})^2 + \Gamma_R^2/4}, \tag{6.7}$$



Normalizing to the peak intensity, one finds

$$I(E) = I_0\, \frac{\Gamma_R^2/4}{(E - E_R)^2 + \Gamma_R^2/4}. \tag{6.8}$$

It shows the reason for the name width. The quantity Γ_R is precisely the width of the peak at half-maximum intensity, when plotting I as a function of the final state energy E_{12}. The function is known as a Lorentzian or Breit-Wigner distribution.

The mass is an example of an invariant (the same in any reference frame) quantity for one particle. The corresponding invariant quantity for two particles is

$$s \equiv (p_1 + p_2)^2 = (E_1 + E_2)^2 - (\boldsymbol{p}_1 + \boldsymbol{p}_2)^2, \tag{6.9}$$

referred to as the center of mass energy squared for the obvious reason that in the center of mass (where $\boldsymbol{p}_1 + \boldsymbol{p}_2 = 0$) one has $s = (E_{12}^{\rm cm})^2$. The relativistic Breit-Wigner is found by rewriting the above expression for $I(E)$ in the rest-frame of the decaying particle in terms of the invariants, i.e. $E_R = M_R$ and $E_{12} = \sqrt{s}$. One has

$$I(s) = I(M_R^2)\,\frac{\Gamma_R^2/4}{(\sqrt{s} - M_R)^2 + \Gamma_R^2/4},$$

which near resonance ($s \approx M_R^2$) coincides with the (relativistic) Breit-Wigner

$$I(s) = I(M_R^2)\,\frac{M_R^2\Gamma_R^2}{(s - M_R^2)^2 + M_R^2\Gamma_R^2}. \tag{6.10}$$

If an unstable state has more than one decay mode, the initial equation 6.2 has more terms each involving partial widths Γ_R^i that must be summed to find the total decay rate $\Gamma_R = \sum_i \Gamma_R^i$, which determines the lifetime

If a resonance R is an intermediate state in a process $a + b \to R \to c + d$, the cross section near $s \approx M_R^2$ behaves like

$$\sigma(s) \propto \frac{M_R^2\Gamma_R^{ab}\Gamma_R^{cd}}{(s - M_R^2)^2 + M_R^2\Gamma_R^2} \tag{6.11}$$

Production of particles

Scattering processes in accelerators, or in particular in the early days in cosmic ray physics, have produced many particles beyond the well-known nucleons (proton and neutron) and electrons, e.g. muons or pions, shortlived resonances like the Δ-particle in pion-proton scattering. With higher energies one produces particle-antiparticle pairs or the heavy gauge bosons in e^+e^- annihilation processes.

In accelerator physics one distinguishes *fixed target experiments* in which a *beam* is aimed at a *target* and *collider experiments*. The (fixed) target in essence consists of stable particles (protons, atomic nuclei or atoms). Note for instance that a neutron target necessarily requires the use of nuclei, e.g. deuterium. As beams one has somewhat more possibilities, e.g. electrons, protons, nuclei but also relatively short-lived particles such as muons, pions or kaons, if they are produced with sufficiently large energies enhancing their lifetime in the accelerator with the well-known factor $\gamma = E/M$.

This same factor is responsible that muons (mass m_μ = 106 MeV and lifetime $\tau = 2.2 \times 10^{-6}$ s, i.e. $c\tau = 660$ m) produced in the upper atmosphere with energies of several GeV's can travel the tens of kilometers to the detector on Earth.

In collider experiments one collides two beams of particles. In high-energy experiments, the produced *final state* particles in colliders have a more or less isotropic distribution around the scattering point, while in fixed target experiments they are focussed in the forward direction.

In general one specifies for an accelerator or collider the maximal energy via the invariant s. For very high energies one easily can see that in a collider $s \approx 4\,E_1\,E_2$, while for a fixed target experiment one has $s = 4\,M_{\rm target}E_{\rm beam}$ (explain this!). Another important property of an accelerator is the achievable flux factor, referred to as *luminosity*, the proportionality constant that relates the event rate (events/s) to the cross section, $R = \mathcal{L}\sigma$. Typical luminosities in present day accelerators are of the order of 10^{32} cm^{-2}s^{-1}. For the performance of an experiment or accelerator one talks of *integrated luminosities*, e.g. in a certain period (say 10^6 s) one might achieve $\int dt\,\mathcal{L}$ of about 10^{38} cm^{-2} = 100 pb^{-1}, implying 100 event over the integrated time interval for a cross section as small as 1 pb or 10^5 events for a cross section of 1 nb, but only 1 event for typical neutrino cross sections of 10^{-2} pb. Depending on the detection of the final state one distinguishes *exclusive* measurements in which the full final state is measured and *inclusive* measurements, in which all final states are taken together.

Examples of specific scattering processes are socalled *elastic* scattering processes in which initial and final state are the same,

$$a + b \longrightarrow a + b,$$

(in particle reactions the + is usually omitted) yielding information on the forces working between the particles, e.g. as we have seen in proton-proton scattering in Chapter 5. Knowing the forces for particle a, these processes can be used to study system b, for instance knowing the electromagnetic interactions of the (elementary) electron, can be used to study electromagnetic properties of composite particles via $ep \rightarrow ep$, such as the charge distribution in the proton. If the energy available is high enough, one has in general many more *inelastic* processes,

$$\begin{array}{lcll}
a+b & \longrightarrow & a+b' & \text{(excitation of b)} \\
a+b & \longrightarrow & a+b+\ldots & \text{(production of \ldots)} \\
a+b & \longrightarrow & c+d+\ldots & \text{(scattering into other channels)} \\
a+b & \longrightarrow & R \longrightarrow 1+2 & \text{(resonance formation)} \\
a+\bar{a} & \longrightarrow & \ldots & \text{(annihilation),}
\end{array}$$

or combinations. Examples are resonance formation such as in $\pi^+n \rightarrow \Delta^+ \rightarrow \pi^0 p$ and $\pi^+n \rightarrow \Delta^+ \rightarrow \pi^+ n$, production processes like $pp \rightarrow pp\pi^0$, associated production of two *strange* particles $\pi^-p \rightarrow K^-\Sigma^+$ (subsequently decays $K^- \rightarrow \mu^-\overline{\nu}_\mu$ and $\Sigma^+ \rightarrow p\pi^0$) or $K^-p \rightarrow \Lambda^0\pi^0$ (subsequent decay $\Lambda \rightarrow \pi^-p$ or $\Lambda \rightarrow \pi^0 n$). The annihilation process $e^+e^- \rightarrow \ldots$ is a particularly clean process to scan energy ranges and study new resonances, or production thresholds e.g. $e^+e^- \rightarrow \rho^0 \rightarrow \pi^+\pi^-$ and $e^+e^- \rightarrow \phi \rightarrow K^+K^-$ in the GeV-range or $e^+e^- \rightarrow Z^0 \rightarrow \ldots$ and $e^+e^- \rightarrow W^+W^-$ in the 100 GeV range.

For the understanding of these processes the *conservation* (or violation of conservation) for certain quantum numbers in going from initial to final state is an important guide. Absolutely conserved turn out to be the *total energy* and *total momentum*. It is important to stress that this is true for the initial and final state and not necessarily in the intermediate state, where the energy uncertainty is related to the interaction time, such as made quantitative in the above treatment of resonances. Conservation of energy requires in a decay process $a \rightarrow 1 + 2$ that $M_a \geq M_1 + M_2$, while for $a + b \rightarrow c + d$ one must have $\sqrt{s} \geq M_c + M_d$. Note that because of energy and momentum conservation s can be calculated from initial or (full) final state, e.g. for $ab \rightarrow cd$ one has $s = (p_a + p_b)^2 = (p_c + p_d)^2$.

The minimal value for s in a particular reaction channel, $s_{min}(cd) = M_c + M_d$ for the reaction channel cd, is referred to as the *threshold* for this channel. Another quantity that is strictly conserved in going from initial to final state is the total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$, i.e. the quantum numbers J and M (eigenvalues $J(J+1)\hbar^2$ and $M\hbar$ of $\boldsymbol{J}^2$ and J_z respectively) are the same in initial and final state, where J and M are obtained by combining all orbital angular momenta and all spins of the particles involved. Also the total *electric charge* and the total *number of baryons* are conserved. In contrast, a quantity like parity is not always conserved. This turns out to depend on the type of interactions that are responsible for a particular process.

For plots of the cross sections and complete overview of particle properties we refer to the *Particle Data Review*, which can be found at **http://pdg.lbl.gov**. A number of particles, some properties and decay modes are listed below.

LEPTONS				
name	mass (MeV/c^2)	lifetime	J^P	main decay mode(s)
e^-	0.511	stable ($> 4 \times 10^{24}$ yr)	$1/2^+$	
ν_e	$< 3 \times 10^{-6}$ s	stable (see 6.6)	1/2	
μ^-	105.7	$\tau = 2.2 \times 10^{-6}$ s	$1/2^+$	$\mu^- \to e^- \overline{\nu}_e \nu_\mu$
ν_μ	< 0.19	stable (see 6.6)	1/2	
τ^-	1777.0	$\tau = 0.29 \times 10^{-12}$ s	$1/2^+$	$\tau^- \to e^- \overline{\nu}_e \nu_\tau$ (17.8 %) $\tau^- \to \mu^- \overline{\nu}_\mu \nu_\tau$ (17.4 %) $\tau^- \to \nu\tau q_{[-1/3]} \overline{q}_{[+2/3]}$ (e.g. $\tau^- \to \pi^- \nu_\tau, \ldots$)
ν_τ	< 18	stable (see 6.6)	1/2	

MESONS ($B = 0$)				
name	mass (MeV/c^2)	lifetime/width	J^P	main decay mode(s)
$\pi^\pm$	139.6	$\tau = 2.6 \times 10^{-8}$ s	0^-	$\pi^+ \to \mu^+ \nu_\mu$
π^0	135.0	$\tau = 8.4 \times 10^{-17}$ s	0^-	$\pi^0 \to \gamma\gamma$

MESONS ($B = 0$) continued				
name	mass (MeV/c^2)	lifetime/width	J^P	main decay mode(s)
η	139.6	$\Gamma = 1.2$ keV	0^-	$\eta \to \gamma\gamma$ $\eta \to \pi^0\pi^0\pi^0$
$K^\pm$	493.6	$\tau = 1.24 \times 10^{-8}$ s	0^-	$K^+ \to \mu^+\nu_\mu$ $K^+ \to \pi^+\pi^0$ and $\pi^+\pi^+\pi^-$
K_S^0	497.7	$\tau = 0.9 \times 10^{-10}$ s	0^-	$K_S^0 \to \pi\pi$ ($\pi^+\pi^-$ and $\pi^0\pi^0$)
K_L^0	497.7	$\tau = 5.2 \times 10^{-8}$ s	0^-	$K_L^0 \to \pi\pi\pi$
$\rho^\pm$, ρ^0	770	$\Gamma = 150$ MeV	1^-	$\rho \to \pi\pi$
ω	783	$\Gamma = 8.4$ MeV	1^-	$\omega \to \pi^+\pi^-\pi^0$
ϕ	1019	$\Gamma = 4.5$ MeV	1^-	$\phi \to KK$ (K^+K^- and $K_L^0K_S^0$)
$D^\pm$	1869	$\tau = 1.1 \times 10^{-12}$ s	0^-	$D^+ \to \overline{K}^0\ell^+\nu_\ell$ ($\ell = e, \mu$) $D^+ \to \overline{K}\pi\ell^+\nu_\ell$ $D^+ \to \overline{K}^0\pi^+$
D^0, $\overline{D}^0$	1865	$\tau = 0.4 \times 10^{-12}$ s	0^-	$D^0 \to K^-\ell^+\nu_\ell$, $\overline{K}\pi\ell^+\nu_\ell$ and $\overline{K}\pi$
J/ψ	3110	$\Gamma = 87$ keV	1^-	$J/\psi \to \ell^+\ell^-$ ($\ell = e, \mu$)
Υ	9460	$\Gamma = 53$ keV	1^-	$\Upsilon \to \ell^+\ell^-$ ($\ell = e, \mu, \tau$)

BARYONS ($B = 1$)				
name	mass (MeV/c^2)	lifetime/width	J^P	main decay mode(s)
p	938.3	stable ($\tau > 10^{32}$ yr)	$1/2^+$	
n	939.6	$\tau = 887$ s	$1/2^+$	$n \to pe^-\overline{\nu}_e$
Λ	1116	$\tau = 2.6 \times 10^{-10}$ s	$1/2^+$	$\Lambda \to N\pi$ ($p\pi^-$ and $n\pi^0$)
Σ^+	1189	$\tau = 0.8 \times 10^{-10}$ s	$1/2^+$	$\Sigma^+ \to N\pi$ ($p\pi^0$ and $n\pi^+$)
Σ^0	1193	$\tau = 7.4 \times 10^{-20}$ s	$1/2^+$	$\Sigma^0 \to \Lambda\gamma$
Σ^-	1197	$\tau = 1.5 \times 10^{-10}$ s	$1/2^+$	$\Sigma^- \to n\pi-$
Ξ^0	1315	$\tau = 2.9 \times 10^{-10}$ s	$1/2^+$	$\Xi^0 \to \Lambda\pi^0$
Ξ^-	1321	$\tau = 1.6 \times 10^{-10}$ s	$1/2^+$	$\Xi^- \to \Lambda\pi^-$
$\Delta^-, \ldots, \Delta^{++}$	1232	$\Gamma = 120$ MeV	$3/2^+$	$\Delta \to N\pi$
Ω^-	1672	$\tau = 0.8 \times 10^{-10}$ s	$3/2^+$	$\Omega^- \to \Lambda K^-$, $\Xi^0\pi^-$ and $Xi^-\pi^0$

Notes:

- Neutrino oscillations will be discussed in section 6.6.
- With $q_{[-1/3]}$ and $\overline{q}_{[+2/3]}$ we indicate the underlying decay into quarks (q) and antiquarks ($\overline{q}$) with particular charges.
- K^+ and π^+ also decay to $e^+\nu_e$, but with only a small fraction ($\sim 10^{-4}$).
- The kaon system will be discussed in section 6.5. The mass difference between the physical states is $M_{K_L} - M_{K_S} = 3.5 \times 10^{-12}$ MeV $= 0.53 \times 10^{10}$ s^{-1} $= 1/(15.5$ m$)$.

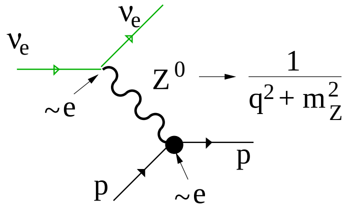
6.2 Forces between elementary particles

Traditionally four types of forces are distinguished. Some general facts are summarized in the following table.

FORCES				
	gravitation	weak interaction	electromagnetism	strong force
strength	10^{-39}	10^{-10}	10^{-2}	1
range	$\propto 1/r^2$	10^{-18} m	$\propto 1/r^2$	10^{-15} m
source	mass	weak charges	electric charge	color charge
carrier particle	graviton	$W^{\pm}$, Z^0	γ	gluons
spin-parity	2^+	1^-	1^-	1^-
indirect forces	-	-	van der Waals force	nuclear force
stable systems	solar system, ...	-	atom, molecule	proton, nucleus

The interactions in the domain of subatomic physics are described via the exchange of spin-1 particles. The example of electromagnetic interactions has been discussed in the chapter on nuclear physics. There, it was compared with the exchange of pions producing the nuclear force. We will see below how this latter force actually arises as a derivative of the true strong force, which is mediated by gluons.

Also the weak interactions are mediated by spin-1 particles, but these bosons are very heavy (on the scale of the nucleon). For instance, the Z^0-boson is exchanged in the case of a neutrino interacting with a proton. The basic interaction strength, the coupling, for the weak interactions is actually comparable to the electromagnetic interactions, but the fact that the exchanged particle is heavy, $M_Z \approx 91$ GeV/c^2, makes the interaction extremely short-ranged ($\lambda\!\!\!^{-}_Z = 0.011$ GeV$^{-1} \approx 2.2 \times 10^{-18}$ fm).



$$V(\boldsymbol{q}) \approx \frac{e^2}{(\boldsymbol{q}^2 + M_Z^2 c^2)}$$

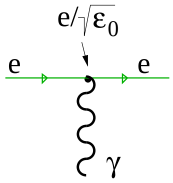
$$\Rightarrow \quad V(r) \approx \alpha \hbar c\, \frac{\exp\left(-r/\lambda\!\!\!^{-}_Z\right)}{r}$$

One immediately sees in the cross section, which is proportional to $|V(\boldsymbol{q})|^2$ the appearance of a factor $1/M_Z^4$. Comparing this with the typical mass of the hadron used in the scattering process, gives a factor $(M_N/M_Z)^4 \sim 10^{-8}$. Together with phase space factors, this leads to characteristic neutrino-nucleon cross sections, which are of the order of 10^{-2} pb, indeed roughly 8 orders of magnitude weaker than characteristic electromagnetic cross sections.

Gauge theories for electromagnetic and strong forces

Electromagnetic interactions

Without going into technical details (for which one needs methods from quantum field theory), we state the important ingredients in the diagrammatic approach (Feynman diagrams) used to describe the interactions, the *propagators* and the *interaction vertices.* We will focus on the interaction terms. In QED we have seen the the interaction term

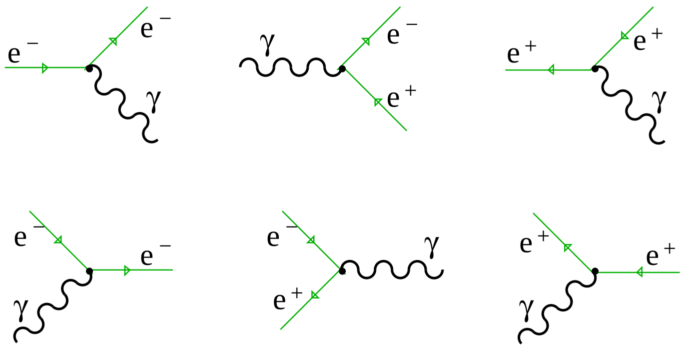


$$\Longleftrightarrow \qquad H_{\text{int}} = \frac{e}{\sqrt{\epsilon_0}}\, \mathrm{e}^{\dagger} Q \mathrm{e} \gamma. \tag{6.12}$$

The interaction term contains the coupling constant, the charge operator Q (e.g. giving -1 for an electron) and fields for the various particles, here just represented by the particle's name. The fields are in essence a sum of annihilation operator for the particle and the creation operator of an antiparticle, i.e.

$$\begin{array}{rcl} \mathrm{e} & \longleftrightarrow & \text{annihilate a particle} \\ & & \qquad\quad \text{or} \\ & & \text{create an antiparticle} \\ \mathrm{e}^\dagger & \longleftrightarrow & \text{create a particle} \\ & & \qquad\quad \text{or} \\ & & \text{annihilate an antiparticle} \end{array}$$

The interaction term thus incorporates not only the absorption and emission of a photon by an electron, but also the annihilation of an electron and its anti-particle, the positron, into a photon, the creation of an electron-positron pair out of a photon and the absorption and emission of a photon by the positron, in total six possibilities:



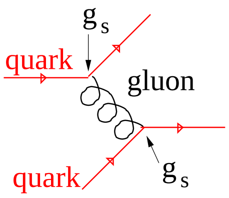
(Note that to keep track of particle or antiparticle nature one uses an arrow on the particle's line).

The strong interactions

The strong force, at the elementary level acting on quarks and gluons, is of the same nature, except that the *charges* are of a different type. We have already seen (chapter 1) that quarks come in 3 colors, which we group together

$$q = \begin{pmatrix} q_r \\ q_g \\ q_b \end{pmatrix}.$$

Instead of having many type of couplings, one for each $q_i^\dagger q_j\, G_a$ vertex, involving a quark with color i a quark with color j and a gluon of type a, each with its own particular strength, these couplings obey an underlying symmetry, [in group theory language described by $SU(3)$, the unitary transformations among the three colors]. There is in fact only *one* coupling constant g_s. All relative couplings are determined by the requirement that transformations in color space do not alter the theory, the *gauge principle*. This leads to strong constraints on the interaction term.



The exchange of gluons between colored quarks underlies the strong interactions. All possible quark-quark-gluon vertices are summarized in

$$H_{\rm int} = g_s\, q_i^\dagger (F_a)_{ij} q_j\, G_a, \qquad (6.13)$$

The charge operators $(F_a)_{ij}$ form just the set of (eight) hermitean matrices in color space [corresponding to the generators of the SU(3) symmetry].

The eight hermitean matrices in the 3-dimensional color space are just the extension of the three hermitean matrices in the 2-dimensional spin space, where one has $\boldsymbol{S} = \boldsymbol{\sigma}/2$ with

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

satisfying $\mathrm{Tr}(\sigma_i\sigma_j) = 2\,\delta_{ij}$. For the 3-dimensional space one has 8 hermitean matrices F_a $(a = 1,\ldots,8)$ which are written as $F_a = \lambda_a/2$, known as the Gell-Mann matrices,

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \qquad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \lambda_8 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

which satisfy $\mathrm{Tr}(\lambda_a\lambda_b) = 2\,\delta_{ab}$. For the quarks, coming in 3 colors and coupling to 8 gluons, these eight matrices are precisely the ones fixing all the relative $8 \times 3 \times 3$ couplings (55 of them being zero!).

An important difference between QED and QCD is the *nonabelian* character of the latter. In a nonabelian theory the charges(matrices!) do not commute. Without going into the details, we also mention that this has the important consequence that the gluons themselves carry a color, which means that they can interact with themselves, i.e. there exist vertices connecting three gluons $G_aG_bG_c$.

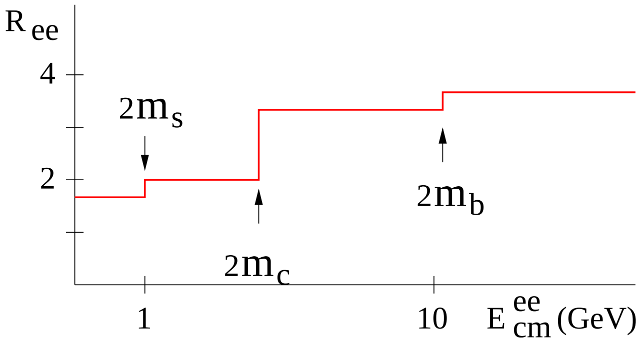
In chapter 1 we already discussed that there exist six kinds of quarks, referred to as *flavors*. All flavors couple to gluons with the same strength, in other words gluons are flavor-blind. The production of the various flavors in an electromagnetic interaction can actually nicely be seen in electron-positron annihilation and the subsequent quark-antiquark creation. One can have

$$e^+e^- \rightarrow e^+e^-,\ \mu^+\mu^-,\ \tau^+\tau^-,\ u\overline{u},\ d\overline{d},\ s\overline{s},\ c\overline{c},\ b\overline{b},\ t\overline{t}.$$

The ratio

$$R = \frac{\sigma(e^+e^- \rightarrow \text{hadrons})}{\sigma(e^+e^- \rightarrow \mu^+\mu^-)}, \qquad (6.14)$$

where the cross section into hadrons is initiated by the creation of a quark-antiquark pair, nicely shows jumps corresponding to thresholds where the next quark flavor comes in.



A schematic representation of the expected behavior of the ratio R in e^+e^- annihilation is given in the figure. The physical thresholds are of course determined by the lowest two-meson or baryon-antibaryon threshold containing the indicated quarks.

The ratio R turns out to be well reproduced by the incoherent sum of contributions,

$$R = 3\sum_q e_q^2, \tag{6.15}$$

where the sum depending on the energy runs over quark flavors that can be produced. The factor 3 is a consequence of the fact that there are 3 colors. The quark-antiquark pair can be produced in any of the color combinations $r\overline{r}$, $b\overline{b}$ and $g\overline{g}$.

6.3 Electroweak interactions

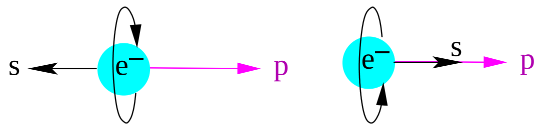
The weak interactions, mediated by heavy gauge bosons, can be considered in a unified framework together with the electromagnetic interactions in a way similar to the color interactions. In essence all coupling constants are related via symmetries.

6.3.1 Leptons and electroweak interactions

Leptons only experience electroweak interactions (and gravity via their masses). They do not feel strong interactions. Leptons are fermions with half-integer spin. We will consider two particular choices for fermions, *helicity states* and *chirality states*. Choosing the momentum direction as quantization axis fermions can have helicities

$$\lambda = \frac{\boldsymbol{s}\cdot\boldsymbol{p}}{|\boldsymbol{p}|} = \pm\frac{1}{2}. \tag{6.16}$$

A particle with spin along the momentum has positive helicity, with spin opposite to the momentum negative helicity. Helicity is a property that can be measured, but depends on the observer. It is not an intrinsic property of particles except for a particle without mass. In that case, positive and negative helicity coincides with socalled *right-handed* and *left-handed* chirality states for fermions.



$\lambda = -1/2$ $\quad\updownarrow\quad$ lefthanded

$\lambda = +1/2$ $\quad\updownarrow\quad$ righthanded

(for massless particles)

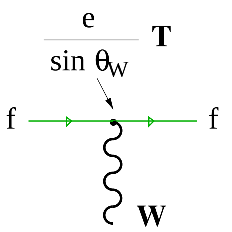
Chirality is an intrinsic property of fermions, also for massive fermions, such as electrons or muons and plays a crucial role in the weak interactions, which behave different for righthanded and lefthanded states, e.g. e^-_R and e^-_L. Neutrinos even only appear left-handed, while antineutrinos only appear right-handed. All the interactions of fermions with spin-1 particles do not change chirality, but they can change helicity. In order to expand chirality states into (physical) helicity states one needs the overlap factors,

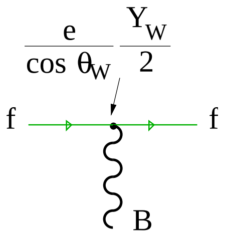
$$\langle L|\lambda = -1/2\rangle = \langle R|\lambda = +1/2\rangle = \frac{1+\gamma(1+\beta)}{2\sqrt{\gamma(\gamma+1)}} \quad \xrightarrow{\gamma\gg 1} \quad \frac{1+\beta}{2} \quad \xrightarrow{\beta\to 1} \quad 1,$$
$$\langle L|\lambda = +1/2\rangle = \langle R|\lambda = -1/2\rangle = \frac{1+\gamma(1-\beta)}{2\sqrt{\gamma(\gamma+1)}} \quad \xrightarrow{\gamma\gg 1} \quad \frac{1-\beta}{2} \quad \xrightarrow{\beta\to 1} \quad 0.$$

The latter factor can also be expressed as $\langle L|\lambda = +1/2\rangle = M/(\sqrt{E}(\sqrt{E+M}+\sqrt{E-M}))$, showing that for $M = 0$ chirality = helicity. The factors explains why the decay of a π^- into $e^-\overline{\nu}_e$ is heavily suppressed with respect to the decay into $\mu^-\overline{\nu}_\mu$ (see exercise 6.2).

The electroweak interactions are also of the gauge type discussed before, but one needs a 2-dimensional space (referred to as weak isospin) and an additional quantum number. In group theoretical language the symmetry is referred to as $SU(2)_W \otimes U(1)_Y$ (W stands for weak isospin, Y for weak hypercharge).

The basic expression for the interaction term can be written in a fairly simple way as interactions of fermions with three W-bosons via three weak-isospin operators $\boldsymbol{T}$ and with one B-boson via a socalled weak hypercharge operator Y_W.





The corresponding interaction terms are written

$$H_{int} = \frac{e}{\sin\theta_W}\, f^\dagger \boldsymbol{T} f \cdot \boldsymbol{W} + \frac{e}{\cos\theta_W}\, f^\dagger \frac{Y_W}{2} f\, B, \tag{6.17}$$

The key issue is that different particles such as neutrino's and electrons are considered as *one* fermion with different electroweak charges. To be precise the lefthanded electron and the neutrino (only lefthanded!) form a doublet, while the righthanded electron forms a singlet. This same structure repeats itself three times for the different lepton families,

$$L = \begin{pmatrix} \nu_{eL} \\ e^-_L \end{pmatrix}, \begin{pmatrix} \nu_{\mu L} \\ \mu^-_L \end{pmatrix}, \begin{pmatrix} \nu_{\tau L} \\ \tau^-_L \end{pmatrix}; \quad R = e^-_R,\ \mu^-_R,\ \tau^-_R. \tag{6.18}$$

The weak-isospin operators for the doublets are the hermitean 2×2 matrices, $\boldsymbol{T} = \boldsymbol{\tau}/2$ (with τ_i being the Pauli matrices),

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The treatment of doublets is completely analogous to spin. The doublets are assigned a weak-isospin quantum number $T = 1/2$, the members of the doublets are eigenstates of T_3 (diagonal matrix) with quantum numbers $T_3 = +1/2$ and $T_3 = -1/2$, respectively. For the singlets, one can (like spin) also write down the weak-isospin operators but they are trivial,

$$T_1 = (0)\,, \quad T_2 = (0)\,, \quad T_3 = (0)\,,$$

implying for the singlets $T = T_3 = 0$. For doublets and singlets, the weak hypercharge is a diagonal operator, of which the value can be calculated via

$$Q = T_3 + \frac{Y_W}{2}. \tag{6.19}$$

The fact that lefhanded particles form doublets and righthanded singlets, implies e.g. that the W-bosons only interact with lefthanded particles, which means *maximal parity violation*.

For antiparticles one has opposite quantum numbers. The righthanded antileptons belong to doublets while the lefthanded antifermions are singlets, i.e. we have

$$\begin{pmatrix} e_R^+ \\ \overline{\nu}_{eR} \end{pmatrix}, \begin{pmatrix} \mu_R^+ \\ \overline{\nu}_{\mu R} \end{pmatrix}, \begin{pmatrix} \tau_R^+ \\ \overline{\nu}_{\tau R} \end{pmatrix}; \qquad e_L^+,\ \mu_L^+,\ \tau_L^+. \tag{6.20}$$

In the same way as the full rotational symmetry for a collection of spins in a cristal can be *spontaneously* broken when all spins (for whatever reason) align, nature has choosen a symmetry breaking mechanism for the weak interactions with only one surving symmetry [referred to as $SU(2)_W \otimes U(1)_Y \longrightarrow U(1)_Q$]. The operator corresponding with the surviving symmetry is precisely the charge operator Q related to T_3 and Y_W via Eq. 6.19. The gauge boson coupling to the charge operator in the hamiltonian is (of course) our photon. This requires a redefinition of the B and W gauge bosons. Using, instead of these bosons in Eq. 6.17 the linear combinations,

$$W^{\pm} \equiv \frac{1}{\sqrt{2}}\left(W_1 \pm i\, W_2\right), \tag{6.21}$$

$$Z \equiv \cos\theta_W\ W_3 - \sin\theta_W\ B, \tag{6.22}$$

$$\gamma \equiv \sin\theta_W\ W_3 + \cos\theta_W\ B, \tag{6.23}$$

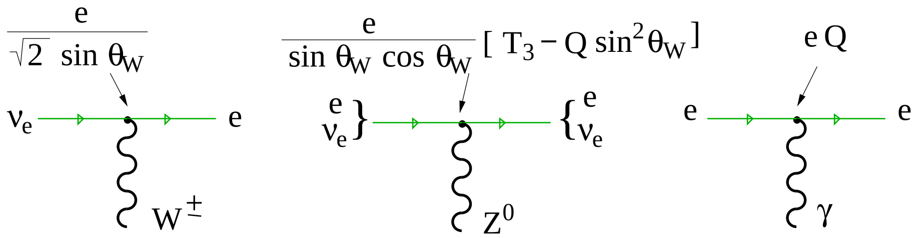
Eq. 6.17 becomes

$$\begin{aligned} H_{\text{int}} &= \frac{e}{\sin\theta_W\ \sqrt{2}}\left(f^\dagger T_+ f\, W^- + f^\dagger T_- f\, W^+\right) \\ &\quad + \frac{e}{\sin\theta_W\ \cos\theta_W}\, f^\dagger \left[T_3 - Q\,\sin^2\theta_W\right] f\, Z + e\, f^\dagger Q f\ \gamma, \end{aligned} \tag{6.24}$$

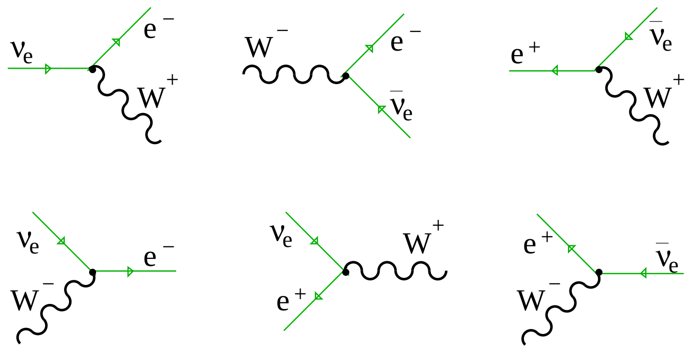
where $T_{\pm} = T_1 \pm i\, T_2$ are weak-isospin raising and lowering operators. The first line in this interaction hamiltonian is known as *charged current* interaction, the second part as the *neutral current* interaction. The interaction vertices for the electroweak part of the standard model can now be read off after just inserting the lepton doublets and singlets. E.g. for the doublet the first term explicitly contains

$$f^\dagger T_+ f\, W^- = \begin{pmatrix} \nu_e^\dagger & (e_L^-)^\dagger \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \nu_e \\ e_L^- \end{pmatrix} W^- = \nu_e^\dagger e_L^-\ W^-.$$

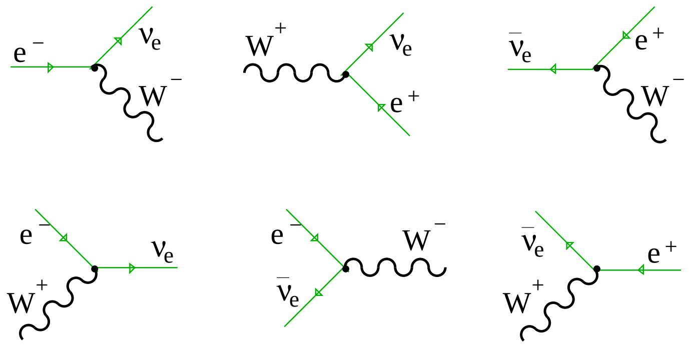
Pictorially, we have



Note that, just as in the case of the $ee\gamma$ vertex, each diagram actually represents a large number of possibilities, e.g. for the first vertex

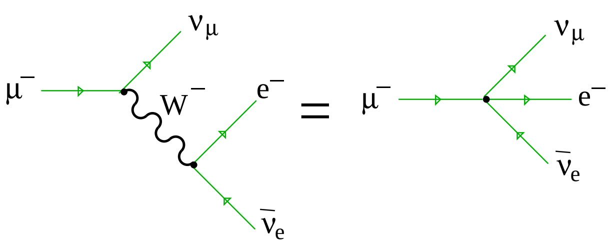


For the antiparticles one has



As discussed the interactions felt by the leptons can change the nature of the lepton, in particular one can have $\nu_e \to e^- W^+$, which has been incorporated as a change of weak-isospin T_3. There are, however, no transitions that change particles of one family into those belongng to a different family, e.g. in the decay of the τ^--lepton always a ν_τ appears. To incorporate this one has introduced quantum numbers L_e, L_μ and L_τ, called *lepton numbers*, that must be conserved (note that anti-leptons get opposite lepton number). The exchanged W^-, however, couples with the same strength to particles of any family, known as *universality* of the electroweak interactions. E.g. the decay probabilities of the τ into an e^- and a μ^- are about the same. The remaining differences can be explained by the phase space.

Dating back to Fermi, one used to introduce for the weak interactions a four-fermion interaction. We now can easily understand the origin of this. Look at the muon decay. It is described by the left diagram below, but at low energies, where $1/(\boldsymbol{q}^2 + M_W^2) \to 1/M_W^2$, it is not distinguishable from a four-fermion interaction,



$$\frac{e^2}{2\sin^2\theta_W}(\nu_\mu^\dagger\, \mu_L)\,\frac{1}{\boldsymbol{q}^2 + M_W^2}\,(e_L^\dagger \nu_e) \quad\Longrightarrow\quad H_{\rm int} = 2\sqrt{2}\, G_F\, (\nu_\mu^\dagger\, \mu_L)\,(e_L^\dagger \nu_e), \tag{6.25}$$

with

$$\frac{G_F}{\sqrt{2}} = \frac{e^2}{8\,\sin^2\theta_W\;M_W^2}. \tag{6.26}$$

The numerical values of G_F and θ_W are

$$G_F = 1.166\,39(1) \times 10^{-5}\ \mathrm{GeV}^{-2}, \tag{6.27}$$

$$\sin^2\theta_W = 0.231. \tag{6.28}$$

Actually, the weak mixing angle plays also a role in the masses of the gauge bosons. The combination forming the photon is massless, while a relation between the heavy boson masses is found,

$$M_Z^2 = \frac{M_W^2}{\cos^2\theta_W}. \tag{6.29}$$

We end this paragraph with a summary of the gauge bosons that are exchanged and which themselves also carry electroweak interactions, an important property of nonabelian gauge theories such as those based on the symmetry groups $SU(2)$ and $SU(3)$. For instance the

ELECTROWEAK GAUGE BOSONS					
gauge boson	mass (GeV/c^2)	width (GeV)	decay modes	T_3	Y_w
γ	0	∞		0	0
Z^0	91.188	2.495	$Z \rightarrow \ell^+\ell^-$ $Z \rightarrow \overline{q} + q$	0	0
$W^\pm$	80.4	2.12	$W^+ \rightarrow \ell^+\nu_\ell$ $W^+ \rightarrow q_{[+2/3]}\overline{q}_{[-1/3]}$	± 1	0

$W^+W^-Z^0$ vertex has strength $e\,\cot\theta_W$, while the $W^+W^-\gamma$ has the (expected) strength e. The vertices of W- and Z-bosons to leptons provide also their dominant decay channels, e.g. the leptonic decays $Z^0 \rightarrow \ell^+\ell^-$ for $\ell = e$, μ and τ. Since their masses are (compared to the Z^0-mass) irrelevant, these decay modes have exactly equal widths (universality).

6.3.2 Quarks and electroweak interactions

The main interactions for quarks are the strong interactions, which we will discuss in the next section. They, however, also interact electromagnetically and weakly. The latter actually determines their lifetime and that of the hadrons built from them.

For quarks, one has, just as for the leptons, that the righthanded quarks (u_R, d_R, etc.) are weak isosinglets, $T = 0$, while the lefthanded quarks can also be grouped into doublets with $T = 1/2$,

$$\left(\begin{array}{c} u_L \\ d'_L \end{array}\right), \left(\begin{array}{c} c_L \\ s'_L \end{array}\right), \left(\begin{array}{c} t_L \\ b'_L \end{array}\right). \tag{6.30}$$

The states that are relevant for weak interactions, however, are not the (dominant) strong interaction eigenstates but combinations. The mixing is described by the (unitary) Cabibbo-Kobayashi-Maskawa matrix,

$$\begin{pmatrix} d' \\ s' \\ b' \end{pmatrix} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix}. \tag{6.31}$$

In a two-family world, for which the mixing was first suggested by Cabbibbo, the matrix would be determined by one angle, referred to as the Cabibbo angle,

$$\begin{pmatrix} d' \\ s' \end{pmatrix} = \begin{pmatrix} \cos\theta_c & \sin\theta_c \\ -\sin\theta_c & \cos\theta_c \end{pmatrix} \begin{pmatrix} d \\ s \end{pmatrix}. \tag{6.32}$$

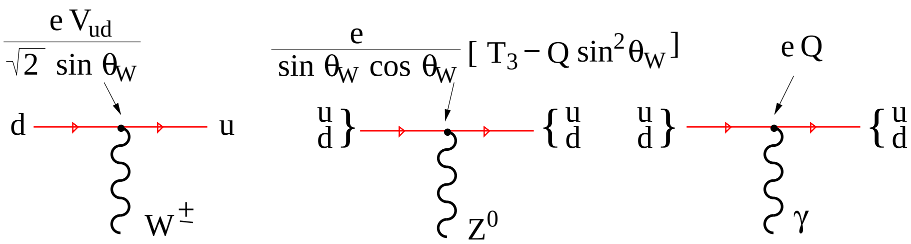
This matrix e.g. implies that, using $g = e/\sin\theta_W$, the vertex $s \rightarrow u + W^-$ has strength $(g/\sqrt{2})\,\sin\theta_c$, while the vertex $d \rightarrow u + W^-$ has strength $(g/\sqrt{2})\,\cos\theta_c$. The latter vertex is needed in neutron β-decay. Note that in a unitary 2×2 matrix the entries can always be made real by absorbing complex fases in the two states. For a 3×3 matrix, the third state can be used to absorb one additional complex phase. However, one complex phase remains, showing up in some of the matrix elements. This phase allows CP-violation in the quark sector, which we will discuss in a later section.

The magnitudes of the entries in the CKM-matrix are nicely represented in the a socalled Wolfenstein parametrization

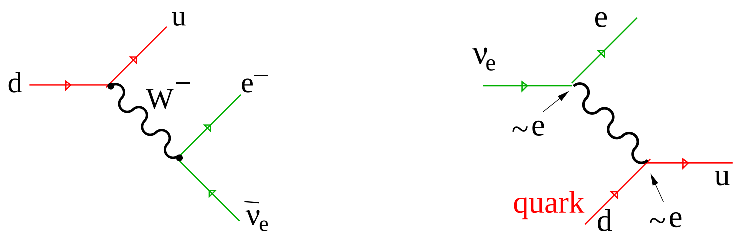
$$V = \begin{pmatrix} 1-\frac{1}{2}\lambda^2 & \lambda & \lambda^3 A(\rho - i\,\eta) \\ -\lambda & 1-\frac{1}{2}\lambda^2 & \lambda^2 A \\ \lambda^3 A(1-\rho-i\,\eta) & -\lambda^2 A & 1 \end{pmatrix}.$$

with $\lambda \approx 0.24$, $A \approx 0.84$ and $\rho \approx 0.2$ and $\eta \approx 0.3$. The imaginary part $i\,\eta$ gives rise to CP violation in decays of K and B-mesons (containing s and b quarks, respectively).

Just as for leptons, we thus have for quarks interaction vertices of the following type:



These underly interactions like neutron decay, $n \rightarrow pe^-\overline{\nu}_e$ or $\nu_e n \rightarrow e^- p$, a process with extremely small cross section which nevertheless is very important in measuring the solar neutrino flux.



$d \rightarrow ue^-\overline{\nu}_e$ $\qquad$ $\nu_e\, d \rightarrow e^- u$

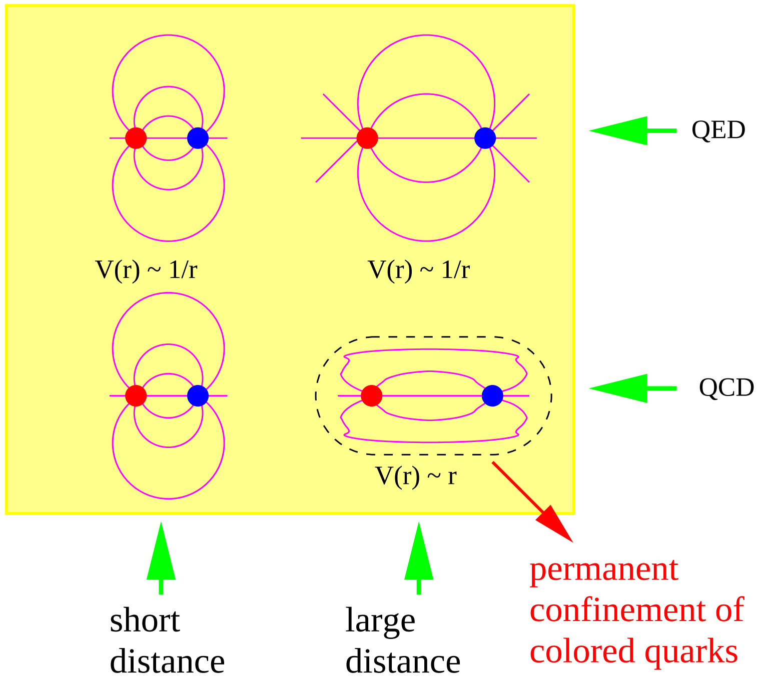
QUARKS									
	mass	lifetime		isospin					
quarks	(GeV/c^2)	(s)	decay modes	I	I_3	S	C	B	T
u	0.35		$u \to d\, e^+\, \nu_e$	1/2	+1/2	0	0	0	0
d	0.35		$d \to u\, e^-\, \overline{\nu}_e$	1/2	−1/2	0	0	0	0
s	0.5	$\sim 10^{-10}$	$s \to u\, d\, \overline{u}$	0	0	−1	0	0	0
			$s \to u\, e^-\, \overline{\nu}_e$						
			$s \to u\, \mu^-\, \overline{\nu}_\mu$						
c	1.5	$\sim 10^{-12}$	$c \to s\, u\, \overline{d}$	0	0	0	+1	0	0
			$c \to s\, e^+\, \nu_e$						
			$c \to s\, \mu^+\, \nu_\mu$						
b	5.0	$\sim 10^{-12}$	$b \to c\, d\, \overline{u}$	0	0	0	0	−1	0
			$b \to c\, e^-\, \overline{\nu}_e$						
			$b \to c\, \mu^-\, \overline{\nu}_\mu$						
			$b \to c\, \mu^-\, \overline{\nu}_\mu$						
t	174	$\sim 5 \times 10^{-25}$	$t \to b\, W^+$	0	0	0	0	0	+1

Summary of quark properties

We have now sufficient information to give an overview of the quantum numbers of all the quarks. As mentioned already, the different types of quarks are referred to as *flavors* and flavor quantum numbers strangeness (S), charm (C), bottomness (B) and topness (T) are assigned. Since the interactions of the gluons are blind for flavor, flavor quantum numbers are conserved in strong interaction processes. But as discussed above the weak interactions allow the decay of quarks and can change flavor quantum numbers. The masses in the table are socalled *constituent* masses that used linearly give a rough indication of the masses of the hadrons formed from the quarks. Also the lifetimes are only indicative for the lifetimes of hadrons containing the respective quarks. Note that the top quark decays (although through weak interactions) in such a short time that formation of hadrons is irrelevant. By the time the quark decays, a region with a radius less than 1 fm knows of its existence.

6.4 Hadrons

Strong interactions at the microscopic level are mediated by gluons. Although the strong interaction resembles the electromagnetic interaction, mediated by the exchange of photons, an important difference is the possibility that gluons exchange gluons among themselves. One consequence that has been found is that there is an important difference in the strength of the elementary coupling in different energy/momentum ranges (or equivalently different length scales). While $\alpha = e^2/4\pi$ becomes actually stronger at short distances, the strong coupling constant $\alpha_s = g_s^2/4\pi$ becomes weaker, known as *asymptotic freedom*. Catastrophe at large distances is avoided by *confinement* of color charge over distances larger than about 1 fm. The corresponding energy scale is 200 MeV. From the excitation spectrum of mesons built from light (u and d) quarks, one obtains for the long-range tail



The potentials in QED and QCD at short and large distances, respectively.

of the quark-antiquark potential,

$$V(r) \quad \overset{r\to\infty}{\Longrightarrow} \quad T_0\, r \tag{6.33}$$

with $T_0 \approx 0.9$ GeV/fm $= 0.18$ GeV^2. The short-distance behavior looks much more like a Coulomb potential. We will see this when we consider bound states of heavy quarks.

Color singlets

The long-range behavior of the potential between color charges forces the formation of color neutral bound states. How to neutralize color. First consider the case of two colors which may be compared with spin quantum numbers. Neutralizing 'spin' can be done by pairing two spin 1/2 particles to a spin 0 object, taking the antisymmetric wave function $(\uparrow\downarrow - \downarrow\uparrow)$. The charges of the quarks come in 3 colors and they can actually be neutralized in the same way by taking the antisymmetric combination

$$|\text{color singlet}\rangle = \frac{1}{\sqrt{6}}\,(rgb - grb + brg - rbg + gbr - bgr)\,. \tag{6.34}$$

Such a color singlet wave functions requires three quarks to join. These qqq bound states are referred to as *baryons*. A second possibility to make color singlets is to join the color of a quark and the anticolor of an antiquark[1],

$$|\text{color singlet}\rangle = \frac{1}{\sqrt{3}}\left(r\overline{r} + g\overline{g} + b\overline{b}\right). \tag{6.35}$$

[1]Note that in a world with two colors the anti-color would be just the other color. This is not true in the case of three colors. In that case the anti-color is like the antisymmetric combination of the two other colors.

The $q\overline{q}$ bound states are referred to as *mesons*. Taking away a quark from a baryon would result into colored states, but at the same time creating a quark-antiquark pair leads to the emission of a meson

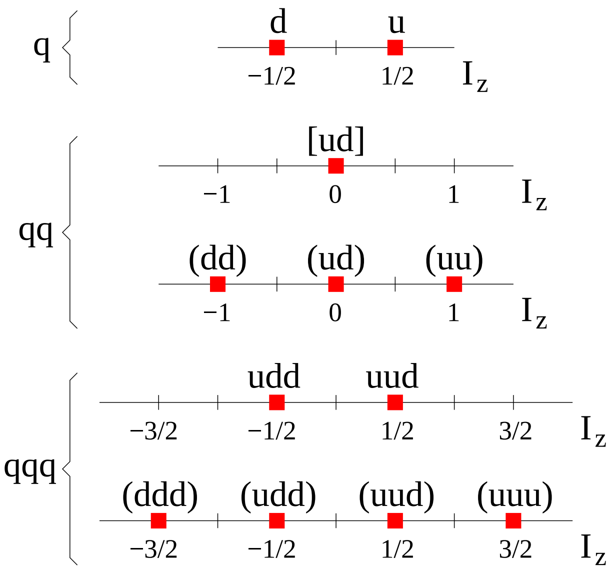
$$B = (qqq) \longrightarrow (qq - -q) \longrightarrow (qq - q\overline{q} - q) \longrightarrow (qqq)(\overline{q}q) = BM,$$

e.g. the (effective) $NN\pi$ vertex used to describe the nucleon-nucleon force (chapter 5).

In building hadrons one can combine quarks of any flavor. The color forces are identical for all flavors. In particular for the two lightest quarks, which have masses very much lower than the typical QCD scale of 200 MeV, this naturally leads to treating them together, i.e. considering u and d as two isospin charges of a quark. Sometimes this is even useful including the third flavor s.

Light hadrons

For building baryons one must combine three quarks of any flavor. Doing this for the two lightest flavors, up and down, it is extremely useful to do this via the assignment of isospin. Since the role of the two lightest quarks is identical as far as the strong interactions is concerned, the isospin symmetry will be important in the spectrum and the interactions.



The two nonstrange quarks are assigned isospin $I = 1/2$ (as for spin $I(I+1)$ is the eigenvalue of $\boldsymbol{I}^2$), for which we have two states with different I_z values. Just as for spin, the isospin doublets can be coupled for a qq-system to $I = 0$ (antisymmetric wave function, denoted by brackets $[ud]$) or $I = 1$ (symmetric wave function, denoted by (ud)). For a three-quark qqq-system, the isospin can be $I = 1/2$ or $I = 3/2$. The isospin $1/2$ combination can be obtained in two ways (via $0 \otimes 1/2$ or $1 \otimes 1/2$), the isospin $3/2$ can only be obtained in one way. It is a fully symmetric wave function.

To get the full baryon wave functions, one must combine the isospin wave functions with spin, color and spatial wave functions. The color part is simply the antisymmetric wave function discussed before; this is the only possibility! For the ground state baryons, the most obvious spatial wave function is a full S-wave, no orbital angular momentum. So let's try that. Since the color wave function is antisymmetric, the spatial wave function is symmetric, the isospin-spin part must be symmetric. For the symmetric isospin $I = 3/2$ state, this implies a fully symmetric spin wave function, i.e. $S = 3/2$. To be explicit one has a uuu-state with all spins parallel, which is the $M_I = +3/2$ and $M_S = +3/2$ member of a particle multiplet, known as the Δ-resonance,

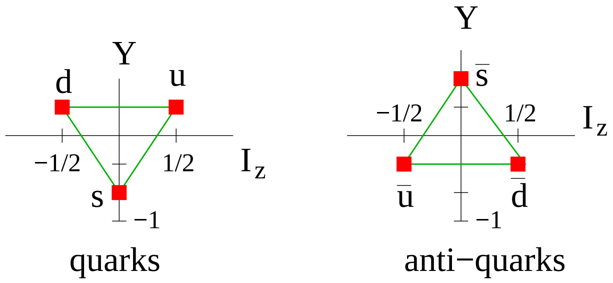
$$\Delta^{++}_{(S_z=+3/2)} = u_\uparrow u_\uparrow u_\uparrow \otimes \psi_{\text{color}} \otimes \psi_{\text{space}}. \tag{6.36}$$

From this Δ state with $I_z = S_z = +3/2$ the other members of the multiplet are obtained with isospin and spin lowering operators. The experimental existence of this state indicated the necessity of an antisymmetric (three)-color wave function.

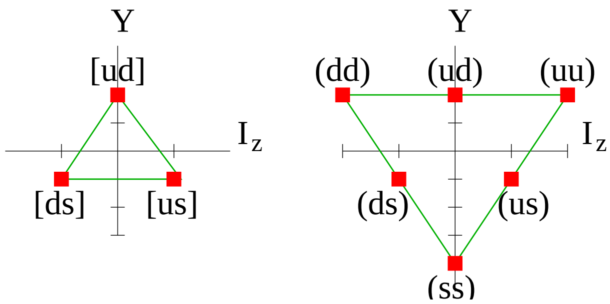
To get the wave function of the nucleons one can start in various ways, e.g. take an $I = 0$ isospin $[ud]$ wave function, combine it (necessarily, why?) with an $S = 0$ spin $[\uparrow\downarrow]$ wave function. Combining with e.g. an $u_\uparrow$-quark, we get after symmetrization the proton wave function (for $M_S = +1/2$),

$$\begin{aligned} p_{(S_z=+1/2)} \quad &= \quad \frac{1}{\sqrt{18}}(2\,u_\uparrow u_\uparrow d_\downarrow + 2\,u_\uparrow d_\downarrow u_\uparrow + 2\,d_\downarrow u_\uparrow u_\uparrow - u_\uparrow u_\downarrow d_\uparrow - u_\downarrow u_\uparrow d_\uparrow - u_\uparrow d_\uparrow u_\downarrow \\ &\qquad - u_\downarrow d_\uparrow u_\uparrow - d_\uparrow u_\uparrow u_\downarrow - d_\uparrow u_\downarrow u_\uparrow) \otimes \psi_{\text{color}} \otimes \psi_{\text{space}}. \end{aligned} \tag{6.37}$$

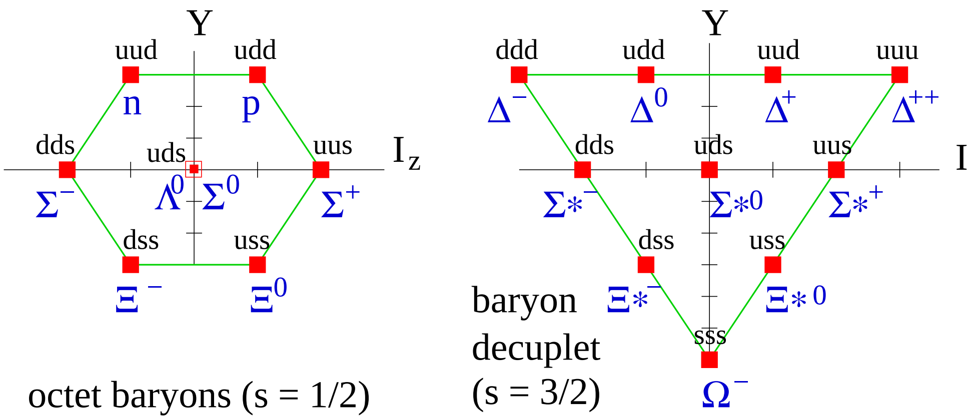
Including the strange s-quark, one constructs $SU(3)_F$ (F for flavor) multiplets. Starting with the quarks and antiquarks one has the basic multiplets $\underline{3}$ and $\underline{3}^*$, given in a plot of $Y = S + B$ versus I_z, where B is the baryon number, being 1/3 for a quark.

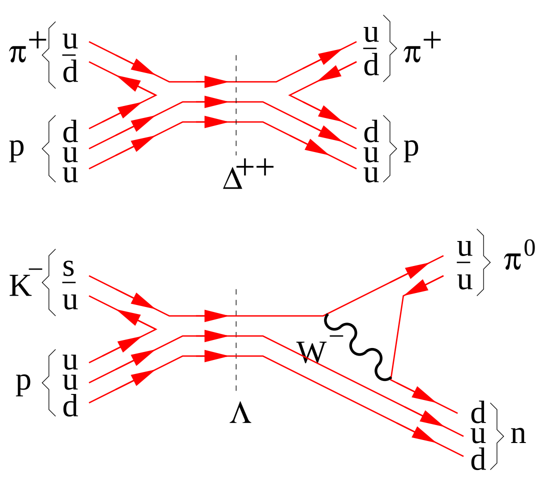


One can construct 9 qq-states, 3 antisymmetric ones (forming again a $\underline{3}^*$ triplet) and 6 symmetric ones (forming a sixtet $\underline{6}$).



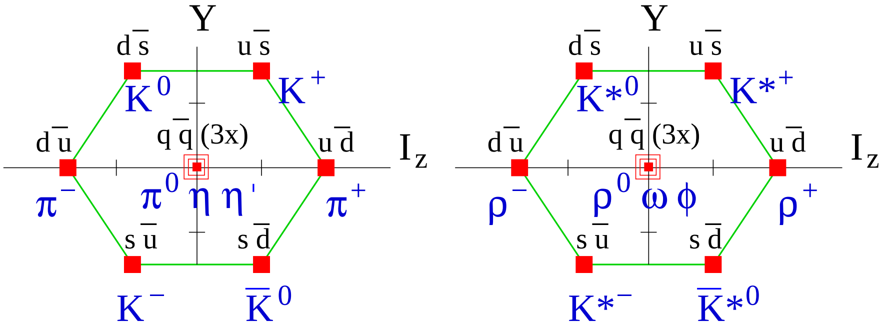
Combining these states with another triplet leads to 27 states, but after symmetrization including spin wave function one is left with a symmetric decuplet ($\underline{10}$) with $s = 3/2$ and a mixed-symmetric octet ($\underline{8}$) with $s = 1/2$.





Examples of quarkline diagrams. In these diagrams showing the gluons which are exchanged between quarks would not make sense. These do not only play a role in the scattering process, but also in the existence of the hadrons themselves. Processes like the upper one, are strong interaction processes, the second example shows a weak process. Here a W is exchanged and produces a quark-antiquark pair. The quarkline diagram immediately shows the nonconservation of flavor quantum numbers in weak processes.

For the mesons one has $q\overline{q}$ states without restrictions from the Pauli principle, yielding two nonets, one with $s = 0$ and one with $s = 1$.



pseudoscalar nonet (s = 0) vector meson nonet (s = 1)

Although a nonet mathematically can be split into an octet and a singlet (the latter with wave function $(u\overline{u} + d\overline{d} + s\overline{s})/\sqrt{3}$), this splitting may not be the one that is physically most relevant. While in the $s = 0$ nonet the $\eta'(938)$ has a wave function that is close to the singlet, one has in the spin $s = 1$ nonet the situation that the physical states are much closer to what is referred to as ideal mixing in which quarks with the same masses combine. The flavor parts of the wave function become

$$\rho^0 = \frac{1}{\sqrt{2}}\left(u\overline{u} - d\overline{d}\right), \tag{6.38}$$

$$\omega = \frac{1}{\sqrt{2}}\left(u\overline{u} + d\overline{d}\right), \tag{6.39}$$

$$\phi = s\overline{s}, \tag{6.40}$$

where for the light u and d quark-antiquark pairs the ω-meson is the isospin $I = 0$ state. Ideal mixing is a natural consequence of the mass difference between s-quark and light u- and d-quarks. Already in the 1950s several of the above hadrons had been found. Often, they were produced in pairs, socalled *associated production*, e.g.

$$\pi^- p \rightarrow \Lambda K^0 \tag{6.41}$$

followed by a decay in one of the in general many modes, e.g.

$$\Lambda \rightarrow \begin{cases} p\pi^- \\ n\pi^0 \\ pe^-\overline{\nu} \\ \ldots \end{cases} \tag{6.42}$$

Associated production was 'explained' with a new quantum number *strangeness*, with the Λ-particle having $S = -1$ and the kaon having $S = +1$. In the quark model this quantum number arose naturally as the identity of a third quark that was needed in addition to the *nonstrange* up and down quarks. The lambda is a baryon containing the s quark, the kaon a meson containing the $\overline{s}$ antiquark. The creation of a quark-antiquark pair is a strong interaction process (conserving strangeness), while the decay is a weak process involving e.g. the weak decay of the s-quark,

$$s \rightarrow ue^-\overline{\nu}. \tag{6.43}$$

This explained why these abundantly produced particles live for such a long time ($\tau_\Lambda = 2.6 \times 10^{-10}$ s) compared to the short lifetime of e.g. a (nonstrange) Δ-particle, which immediately decays again,

$$\pi^+ n \rightarrow \Delta^+ \rightarrow \pi^0 p, \tag{6.44}$$

and only shows up as a resonance with a half-width $\Gamma_\Delta = 120$ MeV, corresponding to a lifetime of $\tau_\Delta = \hbar/\Gamma_\Delta = 5 \times 10^{-24}$ s.

Masses of light hadrons

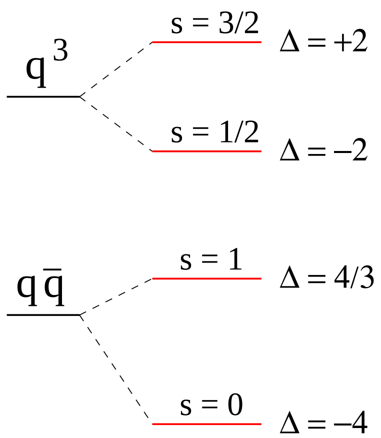
A rough estimate of the masses of the light baryons and mesons can be obtained by adding contributions of the various quarks. This works because for the light hadrons the sizes (determined via elastic scattering, in which one obtains the (squared) form factors) turn out to be roughly the same, about 1 fm, which is the characteristic distance connected with QCD. Light hadrons form sort of bubbles within which the quarks are more or less free. The momentum of a quark confined in such a cavity is proportional to $p_{\rm quark} \propto 1/R$ with the proportionality constant ranging from 2.04 for a massless quark (for this one needs the Dirac equation) to π for a heavy quark (this is the well-known quantummechanical result following from $\sin pR = 0$). Even with almost massless quarks a contribution per quark of about 360 MeV is obtained, referred to as the *constituent quark mass*. The actual masses of the up and down quark turn out to be around 10 MeV, but because of the large momentum ($\propto 1/R$) their precise mass is for the masses and properties of hadrons not very relevant. This and the fact that the basic strong interactions (gluon exchange) are identical for u and d quarks leads to isospin symmetry. A consequence is the appearance of particles in isospin multiplets, of which the members have roughly the same mass. The small mass differences between members of the same multiplet, e.g. the proton and neutron or the pions, $M_{\pi^\pm} = 139.6$ MeV and $M_{\pi^0} = 135.0$ MeV are attributed to small effects like the differences between up and down quark masses and electrostatic contributions of order $e^2/4\pi\epsilon_0\, R$.

The strange quark mass contributes about 500 MeV towards hadron masses. The difference of about 150 MeV per strange quark is clearly seen in the masses of the decuplet baryons, which show a remarkably equidistance between the isospin multiplets

$\Delta(1232)$, $\Sigma^*(1385)$, $\Xi^*(1530)$ and $\Omega(1672)$. Masses are given in MeV between brackets. This mass equidistance was actually what led to the prediction and discovery of the Ω^- baryon. Looking at the differences between the nucleon doublet $N(939)$ and the $\Delta(1232)$ quadruplet one sees the spin-spin force at work. A pairwise interaction of the form

$$H_{\text{int}} \propto \frac{\alpha_s}{R} \sum_{i>j} (F_i \cdot F_j)(\sigma_i \cdot \sigma_j), \tag{6.45}$$

turns out to work very well, splitting not only the $s = 1/2$ and $s = 3/2$ baryons ($M_\Delta - M_N \approx 300$ MeV), but also the $s = 0$ and $s = 1$ mesons (e.g. $M_{K^*(892)} - M_{K(496)} \approx 400$ MeV).

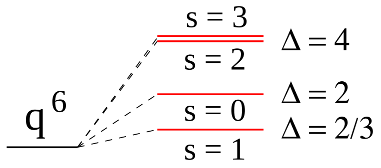


Splitting caused by the interaction proportional to

$$\Delta = -\sum_{i>j} (F_i \cdot F_j)(\sigma_i \cdot \sigma_j)$$

for mesons ($q\bar{q}$) and baryons (q^3). To derive the values of Δ one just calculates from the Gell-Mann matrices that for one quark $F_i \cdot F_i = 4/3$. Using $(F_q + F_{\bar{q}})^2 = 0$ one finds for a meson $F_q \cdot F_{\bar{q}} = -4/3$ and using $(F_1 + F_2 + F_3)^2 = 0$ one finds for a baryon $F_i \cdot F_j$ = -2/3. Furthermore one has $\sigma_i \cdot \sigma_j = +1$ for $s = 1$ and -3 for $s = 0$.

If one would replace in the color-hyperfine interaction in Eq. 6.45 the color charges $(F_i \cdot F_j)$ by ordinary electric charges $e_i\, e_j$ one would get wrong results for the baryon and meson splittings, giving another argument for color. While the $\rho(770)$ and $\omega(783)$ are nearly degenerate, the $\Lambda(1116)$ and $\Sigma(1192)$ baryons have an appreciable mass difference of 76 MeV. This indicates actually that Eq. 6.45 needs refinements depending on quark masses. Note that in a Λ baryon, the isospin $I = 0$ implies an antisymmetric $[ud]$ wave function for the nonstrange quarks and hence also an antisymmetric $[\uparrow\downarrow]$. The spin of the nonstrange quarks combines to zero and thus the spin of the Λ is carried by the s-quark. For the Σ baryons, however, with $I = 1$ one has a different situation with symmetric isospin and spin wave functions for the two nonstrange quarks.



The color-hyperfine splitting discussed above, actually also gives a qualitative explanation of the hard core in the NN interaction. Unlike for the case of $q\bar{q}$ and q^3, one has for six quarks always a repulsion, irrespective of the spin and isospin.

Properties of light hadrons

In the chapter on nuclei we already discussed the charge distribution for the proton, obtained from the form factor, for instance measured in elastic electron-proton scattering. The electric form factor of the nucleon is very well approximated by a dipole form factor,

$$G_E(q^2) = \frac{1}{(1 + q^2/\Lambda^2)^2}, \tag{6.46}$$

indicating an exponential charge density with charge radius $\sqrt{\langle r^2\rangle_E} \approx 0.8$ fm. In such experiments one has also determined the magnetic moments of the proton and neutron and found the g-factors deviating strongly from the value of an elementary fermion ($g = 2$), namely $g_p \approx 5.586$ and $g_n \approx -3.826$. Assuming for up and down quarks a magnetic moments of the form

$$\boldsymbol{\mu}_i = 2\, e_i\, \mu_q\, \boldsymbol{s}_i = e_i\, \mu_q\, \boldsymbol{\sigma}_i, \tag{6.47}$$

and using the proton and neutron spin wave functions to obtain the expectation values

$$\langle p, s_z = +1/2|\sum_i e_i\, \sigma_{i\,z}|p, s_z = +1/2\rangle = 1,$$
$$\langle n, s_z = +1/2|\sum_i e_i\, \sigma_{i\,z}|n, s_z = +1/2\rangle = -2/3.$$

one obtains $g_p = 2\,\mu_N/\mu_q$ and $g_n = (-2/3)\, g_p$, indicating that $\mu_q \approx 2.8\,\mu_N$. Writing $\mu_q = e_q/2m_q$ this implies a mass $m_q \approx 340$ MeV, in good agreement with the beforementioned constituent mass (see Exercise 6.5).

Hadrons in high-energy scattering processes

The quark structure of hadrons has been confirmed and studied in scattering processes and becomes in particular evident at high energies, where high means sufficiently large as compared to the QCD scale. In fact, high-energy scattering experiments in which the total center of mass energy $\sqrt{s} \sim 50 - 100$ GeV or higher, the initial stages of the production of hadrons,

$$\begin{array}{lcll} e^+e^- & \rightarrow & q\overline{q} & \text{(quark-antiquark)}, \\ & \rightarrow & q\overline{q}\,G & \text{(quark-antiquark-gluon)}, \\ & & \vdots & \end{array}$$

remains visible in the distribution of final state hadrons, which appear as showers of hadrons peaked along the high momenta of the initiating processes, socalled *jets*. Also for the decay of an in the intermediate state produced resonance such as the Z^0 one can clearly distinguish the isolated tracks of e^+e^- or $\mu^+\mu^-$ pairs from hadronic channels initiated by $q\overline{q}$ pairs. Missing momenta in these processes indicate neutral or (almost) non-interacting particles like neutrinos.

Another important class of processes are those involving a hadron, in practice mostly a proton, and a lepton. The lepton does not feel the strong interactions and interacts via electromagnetic or weak interactions directly with the quarks in the proton. This can be used to probe the quarks and from the scattering angle of the lepton also the momentum of the struck quark (in fact the fraction x of the proton's momentum carried by the quark). For example, electron-proton scattering,

$$e + p \rightarrow e' + \text{anything},$$

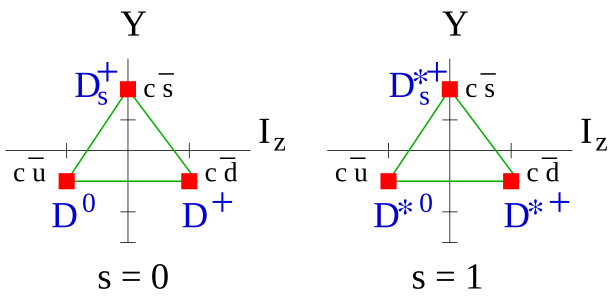
is an electromagnetic process in which a photon with momentum $q = k_e' - k_e$ is exchanged. When this exchanged momentum (more precisely the squared momentum $|q^2|$) is large, the cross section is found to be dependent on only one variable, the Bjorken scaling variable $x = -q^2/2P\cdot q$ (where P is the proton momentum). This can be understood as a consequence of independent scattering off the proton's constituents. One derives that the cross section can be expressed in terms of quark and antiquark distribution functions $q(x)$ and $\overline{q}(x)$,

$$\sigma^{ep}(P,q) \propto \sum_q e_q^2 \, \left(q(x) + \overline{q}(x)\right). \tag{6.48}$$

For this one needs that the underlying process is γ + quark $\rightarrow$ quark, for which the cross section would simply be proportional to the quark charge squared, $\sigma^{eq} \propto e_q^2$. One introduces quark momentum distributions $f_q(x)$ or short $q(x)$ and similarly $\overline{q}(x)$ for each of the (anti-)quark flavors (u, d, s, etc.), where the x is the quark momentum's fraction in the proton, $k = x\,P$. The ep cross section is then obtained by folding the eq cross section with the distribution functions. Using the fact that the scattering off a quark is elastic, i.e. $k^2 = (k+q)^2$, thus $2k\cdot q + q^2 = 0$ and inserting $k = x\,P$ one finds that the momentum fraction is, indeed, identified with the Bjorken variable x. By using different probes, such as neutrinos, which via W-exchange only scatter off negatively charged (anti-)quarks or antineutrinos, which only scatter off positively charged (anti-)quarks one has been able to determine the quark distributions in a nucleon, showing that for small momentum fractions, there are actually many antiquarks, but such that e.g. obvious sumrules like $\int_0^1 dx\ \left(u(x) - \overline{u}(x)\right) = 2$ hold. By looking at the cross sections in more detail, in particular scaling violations, one has also found evidence for gluons. For instance the momentum of quarks and antiquarks together only gives $\sum_q \int dx\ \ (q(x) + \overline{q}(x)) \approx 0.5$, the other 50 % being carried by gluons.

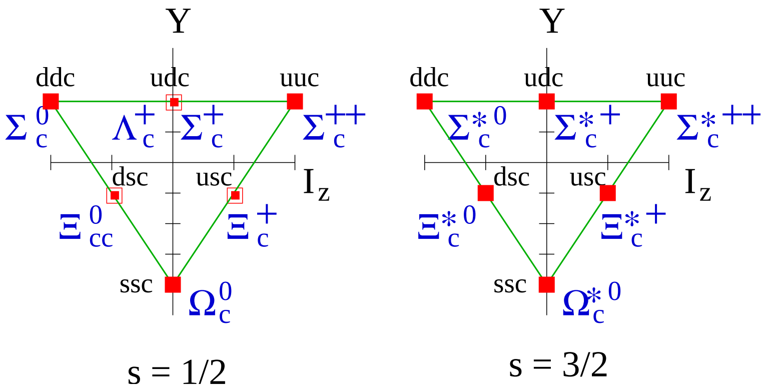
Heavy quarks

For heavy quarks the mass spectrum naturally separates into sectors containing one heavy (anti-)quark, two heavy (anti-)quarks, etc. Taking the charmed c-quark as an example, one finds $C = 1$ mesons with spin 0 and spin 1, by combining the heavy quark with the light antiquark-triplet. One finds the $D(1867)$ and $D_s(1968)$ pseudoscalar ($s = 0$) mesons and the $D^*(2008)$ and $D_s^*(2112)$ vector ($s = 1$) mesons of which the quark structure is found by combining the antiquark $\underline{3}^*$ triplet with the c-quark.

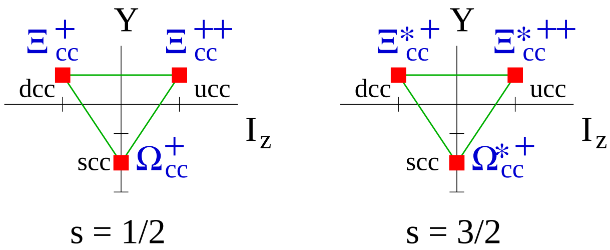


The masses are a way to obtain an indication for the c-quark mass given in the quark summary table. The lifetime of the D and D_s mesons is of the order of 10^{-12} s reflects the c-quark lifetime before its weak decay. As can be argued from the weak interaction vertices given for the quarks, the $c \rightarrow s$ transition is the preferred one, leading to kaons in the final state.

Similarly the two-quark diagrams for up and down quarks discussed before can be used to obtain the structure of $C = +1$ baryons,



or $C = +2$ baryons.



Of course, there is also a $C = +3$ baryon, necessarily only with $s = 3/2$, the Ω_{ccc}^{++} baryon.

Returning to the mesons, one of course has $C = -1$ mesons, which are just the antiparticles $\overline{D}$, $\overline{D}_s$, etc. Furthermore, one has purely charmed mesons consisting of a c-quark and its $\bar{c}$ antiquark, socalled *charmonium* states. One finds a spectrum of states with as groundstate the ${}^1S_0$ bound-state $\eta_c(2980)$ and the ${}^3S_1$ state $J/\psi(3097)$. These states are both below the threshold for decay into two charmed particles, the $D\overline{D}$-threshold (about 3735 MeV). For the η_c the $c\bar{c}$ couple can annihilate into (three) gluons, which in turn produce light quark pairs going into light mesons, e.g. $\eta_c \to \eta'\pi\pi$. This is not possible for the J/ψ-resonance which has a longer lifetime ($\Gamma = 87$ keV). The resonance decays via electromagnetic interactions, e.g. $J/\psi \to e^+e^-$, $J/\psi \to \mu^+\mu^-$ or $J/\psi \to \pi\pi\pi$. For the charmed mesons the P-states lie just above 3400 MeV, while the first radially excited S-wave lies just below the $D\overline{D}$ threshold. The spectrum can be well-understood in a potential with a short-range α_s/r behavior and a long-range linear part as discussed before. In particular the $1/r$ part is important in determining the shape of the wave function of the S-wave ground states. This is even more so if one looks at the corresponding *bottomonium* spectrum for b-quarks. Several $b\bar{b}$-mesons are known, the most stable one being the ${}^3S_1$ state $\Upsilon(9460)$ which is even more stable than the J/ψ with $\Gamma_\Upsilon = 53$ keV. In the same way one also has bottom (sometimes called beauty) mesons (be aware of the charge assignments!) such as $B^\pm(5279)$, which give a good indication of the b-quark mass and its lifetime ($\tau_{B^\pm} \sim 10^{-12}$ s). The preferred weak transition of the b-quark is $b \to c$, i.e. often D-mesons are seen in the decay chain of B-mesons.

6.5 Symmetries and conservation laws

6.5.1 Space-time symmetries

There is an intimate connection between symmetries and conservation laws. The most well-known examples are inversion symmetry, translation invariance and rotational invariance. In all of these cases one determines the basic operators that generate the transformations related to the symmetries in question, e.g. for translations and rotations

$$\begin{aligned}
\psi(x+a,y,z) &\stackrel{a\to 0}{=} \psi(x) + a\,\frac{\partial}{\partial x}\,\psi + \ldots \\
&\equiv \left(1 + \frac{i}{\hbar}\,a\,P_x + \ldots\right)\psi, && (6.49) \\
\psi(r,\theta,\phi+\alpha) &\stackrel{\alpha\to 0}{=} \psi(r,\theta,\phi) + \alpha\,\frac{\partial}{\partial \phi}\,\psi + \ldots \\
&\equiv \left(1 + \frac{i}{\hbar}\,a\,L_z + \ldots\right)\psi. && (6.50)
\end{aligned}$$

If the symmetry leaves the hamiltonian invariant, the symmetry-generating operators commute with the hamiltonian, e.g. in case of translation invariance for a system of many particles one has

$$[\boldsymbol{P}, H] = 0, \qquad (6.51)$$

for $\boldsymbol{P} = \sum \boldsymbol{p}_i$. One needs to sum over all particles, because translation invariance is found after translating the whole system, i.e. all particles. Similarly rotational invariance leads to

$$[\boldsymbol{J}, H] = 0, \qquad (6.52)$$

for the total angular momentum, $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S} = \sum_i (\boldsymbol{\ell}_i + \boldsymbol{s}_i)$, which is the sum of orbital angular momentum and spin. As a consequence one can use the total momentum and total angular momentum as *good* properties of a system, which are conserved. It leads to conservation of energy, momentum (three continuous quantum numbers $\boldsymbol{P}$) and angular momentum (two discrete quantum numbers J and M_J).

Inversion symmetry is an example of a socalled discrete symmetry (this is a symmetry without a continuous parameter like the angle in the case of rotations). The corresponding operator is the parity operator, $P\psi(\boldsymbol{r}) = \psi(-\boldsymbol{r})$ with two possible eigenvalues $\Pi = \pm 1$. When this operator commutes with the hamiltonian, $[P, H] = 0$, the parity of a system is conserved. Not all interactions respect inversion symmetry. In particular the weak interactions with completely different behavior for left- and righthanded fermions do not respect the symmetry. They even maximally violate inversion symmetry. We will come back to other discrete space-time symmetries in the section on discrete symmetries.

Conservation of energy and momentum

These are *absolute* conservation laws, holding for all interactions. The conservation in a scattering process applies to the *total* energy of all particles involved in the process. Important to realize is that one needs to use the relativistic relation between energy and momentum, which was discussed in section 6.1. This is important in case of excitation processes, already at the level of atoms or nuclei (binding energies in initial and final state are different), and in inelastic scattering processes in which one has particles with different masses in the final state or annihilation/creation of particles and antiparticles in which particles disappear or appear. Conservation of total momentum applies to the vector sum $\boldsymbol{P} = \sum_i \boldsymbol{p}_i$) which must be the same in initial and final state.

Let us consider as an example

$$\gamma \;\rightarrow\; e^+e^-. \qquad (6.53)$$

According to energy conservation, this process could occur if $E_\gamma \geq 2\,m_e c^2$. But, also taking into account momentum conservation, one finds that the process can actually not occur. To see this, one should realize that $E_\gamma \geq 2\,m_e c^2$ must hold in any reference frame. Moreover, since the photon is massless one has (also in every reference frame) $|\boldsymbol{p}_\gamma| = E_\gamma/c$, thus also in the center of mass (CM) frame of the electron and positron. But in that frame $\boldsymbol{p}_{e^+} + \boldsymbol{p}_{e^-} = 0$, which would not be allowed by momentum conservation. We note that the creation process can occur near another particle, e.g. a nucleus. One then has in essence $\gamma + A \rightarrow A + e^+ + e^-$, a process where energy and momentum conservation can easily be realized.

In general, we have already seen in section 6.1 that for the decay of a particle into a final state with a number of particles with masses M_i one needs $M \geq \sum_i M_i$ and for a scattering process into a multiparticle final state $s \geq \sum_i M_i$.

Conservation of angular momentum

The total angular momentum obtained by combining all orbital angular momenta and all spins according to the rules of quantummechanics is conserved. To be precise the quantum numbers J and M_J related to the eigenvalues $J(J+1)\,\hbar^2$ and $M_J\hbar$ of the operators $\boldsymbol{J}^2$ and J_z are the same in initial and final state of a scattering process. As an already discussed example, we refer to the fact that processes with on the one side an even and on the other side an odd number of feremions are forbidden, e.g. $n \not\leftrightarrow p + e^-$.

Conservation of parity

As mentioned already, this is not an absolute conservation law. It holds for electromagnetic and strong interactions. Let us illustrate how conservation in strong interactions can be used to determine the parity of the pion. This was first done by looking at the process

$$\pi^- + d \longrightarrow n + n, \tag{6.54}$$

at very low energies. The pion is at these energies actually first caught in an atomic orbit forming a socalled *mesonic atom*, which is in its (s-wave) groundstate. With $\ell = 0$, $S_d = 1$ and $S_\pi = 0$ one has in initial state $J = 1$. Looking at the nn states (see chapter on nuclei) the only allowed $J = 1$ state is the $^3P_1$ wave with negative parity. The full parity analysis gives

$$\Pi_\pi\,\Pi_d\,(-)^0 = (\Pi_n)^2\,(-)^1.$$

Knowing $\Pi_d = +$ one finds $\Pi_\pi = -$.

6.5.2 Internal quantum numbers

In discussing the basic forces in nature, we have encountered electroweak and color charges. Furthermore we have encountered families and for the quarks flavors. These lead to a number of conservation laws. We start with the electroweak quantum numbers. All the internal quantum numbers are additive with opposite values for antiparticles.

Conservation of charge

Conservation of the total charge is again an *absolute* conservation law. Without going in detail here, we mention that it is related to a symmetry, in this case a gauge symmetry. The charge operator generates phase rotations of the wave functions, $\psi(x) \rightarrow e^{i\alpha\,Q}\psi(x)$. Invariance of a gauge symmetry also requires the presence of massless gauge bosons, in this case the photon, which is described with the vector potential $\boldsymbol{A}$ which enters because the symmetry requires *minimal substitution*, the replacement $\boldsymbol{\nabla} \rightarrow \boldsymbol{\nabla} + i\,eQ\,\boldsymbol{A}$.

Conservation of lepton number

As far as the weak interactions do not mix families, this would lead to what one could call a 'family' quantum number. The existence of such a quantum number would not be spoiled by strong interactions because the gluons do not distinguish between families or quark flavors. Certainly in the quark sector the family number is not useful, because the family structure involves a mixing of flavors (CKM matrix). Remains a family number for the leptons, referred to as *lepton number*. In the laboratory this quantum number is conserved and e.g. explains why

$$
\begin{aligned}
n &\rightarrow p + e^- + \overline{\nu}_e, \\
n &\not\rightarrow p + e^- + \nu_e \\
n &\not\rightarrow p + e^- + \overline{\nu}_\mu.
\end{aligned}
$$

At a completely different timescale, the possibility of neutrinos changing from one kind to another (see section on Neutrinos) allows violation of the lepton number.

Conservation of baryon number

Attributing baryon number $B = +1$ to baryons and $B = -1$ to antibaryons, one has an absolute conservaton law. Baryon number can be traced back to fermion number conservation at the quark level and conservation of this number in creation and annihilation processes. In quark-line diagrams the conservation requires arrows to continue on fermion lines throughout the diagram.

Conservation of flavor quantum numbers

In strong interactions, flavors of quarks will not change, as discussed in the section on hadrons. The flavors stay the same, or they are created or annihilated in (oppositely flavored) quark-antiquark pairs. This leads to conservation of I_3, S, C, B and T in strong interactions. Via a coupling to W-bosons, i.e. weak interactions, the flavor quantum numbers can change. The conservation laws, hence, are not absolute ones.

For the strong interactions, the mass difference between u- and d-quarks and electromagnetic effects are secondary effects. Without these secondary effects one could treat u and d as properties of one quark with isospin $I = 1/2$. This implies that not only I_3 is a good quantum number for the strong interactions, but also the I quantum number ($I(I+1)$ is eigenvalue of $\boldsymbol{I}^2$). All strong interaction particles are members of isospin multiplets (as we have explicitly constructed before), but also the isospin in initial and final state must be the same. To find the total isospin of a system of states one must add the isospins of the particles in the same way as done for spins. As an example, consider

$$K^+ \rightarrow \pi^+\pi^0. \tag{6.55}$$

This process has in initial state $I = 1/2$ and in final state an isospin obtained from two pions, each member of an $I = 1$ multiplet. The final state isospin hence is $I = 0, 1, 2$. The process will not be a strong interaction process. Actually also I_3, strangeness S and parity P are not conserved, which would lead one to the same conclusion. The process, actually is one of the kaon decay modes, but proceeds via a weak interaction (draw the quark-line diagram!).

6.5.3 Discrete symmetries

Discrete symmetries that are important for particle physics are

- **Parity** (P): $\boldsymbol{r} \rightarrow -\boldsymbol{r}$ and $t \rightarrow t$,
- **Time-reversal** (T): $\boldsymbol{r} \rightarrow \boldsymbol{r}$ and $t \rightarrow -t$,
- **Charge conjugation** (C): particle $\rightarrow$ antiparticle .

For other quantities the consistent behavior can easily be argued by looking at known relations like $\boldsymbol{p} = m\,\dot{\boldsymbol{r}}$, $\boldsymbol{\ell} = \boldsymbol{r} \times \boldsymbol{p}$, etc. Examples are

quantity	P	T	remark
t	t	$-t$	
$\boldsymbol{r}$	$-\boldsymbol{r}$	$\boldsymbol{r}$	
E	E	E	scalar
$\boldsymbol{p}$	$-\boldsymbol{p}$	$-\boldsymbol{p}$	vector
$\boldsymbol{\ell}$	$\boldsymbol{\ell}$	$-\boldsymbol{\ell}$	axial-vector
$\boldsymbol{s}$	$\boldsymbol{s}$	$-\boldsymbol{s}$	
$\lambda = \boldsymbol{s} \cdot \hat{\boldsymbol{p}}$	$-\lambda$	λ	pseudo-scalar
$\boldsymbol{E}$	$-\boldsymbol{E}$	$\boldsymbol{E}$	
$\boldsymbol{B}$	$\boldsymbol{B}$	$-\boldsymbol{B}$	
$\boldsymbol{A}$	$-\boldsymbol{A}$	$-\boldsymbol{A}$	vector potential!
$\boldsymbol{s} \cdot \boldsymbol{B}$	$\boldsymbol{s} \cdot \boldsymbol{B}$	$\boldsymbol{s} \cdot B$	scalar
$\boldsymbol{s} \cdot \boldsymbol{E}$	$-\boldsymbol{s} \cdot \boldsymbol{E}$	$-\boldsymbol{s} \cdot E$	

In the table we have indicated characteristic behavior of scalars, pseudo-scalars, (polar) vectors and axial vectors. The interaction terms $\boldsymbol{s} \cdot \boldsymbol{E}$ and $\boldsymbol{s} \cdot \boldsymbol{B}$ are given as examples of the implications of the symmetries. If P and/or T are good symmetries any interaction term in the hamiltonian must behave like the energy E. This implies e.g. that a term $\boldsymbol{s} \cdot \boldsymbol{B}$ (magnetic moment in a $\boldsymbol{B}$-field) is allowed, but a term like $\boldsymbol{s} \cdot E$ (electric dipole moment in an $\boldsymbol{E}$-field) is forbidden. To look for T-violating processes one has searched for an electric dipole moment of the neutron, but so far one only has established $d_n < 0.6 \times 10^{-25}$ e cm.

To find the behavior of particle states $|a; \boldsymbol{p}, \lambda\rangle$, one uses the wave function, $\psi(\boldsymbol{r}, t) = \exp\left(-i\,\omega t + i\,\boldsymbol{k} \cdot r\right)$ for a plane wave. The requirement that particles have positive energies, requires for T a transformation of bra's into ket's and vice versa. It is a socalled anti-linear transformation, for which $T(c\,|a\rangle) = c^*\,T|a\rangle$.

	P	T	C
$\lvert a; \boldsymbol{p}, \lambda\rangle$	$\eta_P \lvert a; -\boldsymbol{p}, -\lambda\rangle$	$\eta_T \langle a; -\boldsymbol{p}, \lambda\rvert$	$\eta_C \lvert \overline{a}; \boldsymbol{p}, -\lambda\rangle$

The arbitrary phase η (intrinsic parity, etc.) that is allowed for any quantummechanical state is limited to ± 1 because applying any of these transformations twice must lead to the original state. The intrinsic parities of quarks and leptons are choosen to be positive, that of the antiparticles is -1 the parity of photons (described by a vector field) and similarly gluons is negative,

$$\Pi_q = \Pi_{e^-} = +, \qquad \Pi_{\overline{q}} = \Pi_{e^+} = -, \qquad \Pi_\gamma = -. \tag{6.56}$$

The parity of a fermion-antifermion system, thus, is given by

$$\Pi_{\mathrm{f}\overline{\mathrm{f}}} = (-)^{\ell+1}, \tag{6.57}$$

e.g. $\Pi_\pi = \Pi_\rho = -$.

Time-reversal symmetry becomes important in comparing processes that can run in two directions. Taking into account the kinematic factors (see Eq. 5.16) and the averaging of the polarization possibilities one expects for the processes $a + b \longleftrightarrow c + d$ the relation

$$\sigma(cd \to ab) = \sigma(ab \to cd) \left(\frac{p_{ab}^{\mathrm{cm}}}{p_{cd}^{\mathrm{cm}}}\right)^2 \frac{(2\,s_a + 1)(2\,s_b + 1)}{(2\,s_c + 1)(2\,s_d + 1)}, \tag{6.58}$$

known as the *principle of detailed balance*. Examples exist such as the comparison in $\alpha + {}^{24}\mathrm{Mg} \longleftrightarrow p + {}^{27}\mathrm{Al}$. The appearance of spin factors can also be used to determine the spin of particle. In particular the process $\pi^- + d \longleftrightarrow n + n$, already mentioned as a way to determine the parity of the pion, can also be used to find the spin of the pion ($s_\pi = 0$), given the spins of deuteron ($s_d = 1$) and neutron ($s_n = 1/2$).

Charge conjugation, finally, transforms a particle into its antiparticle. Applying this to a fermion-antifermion system one obtains

$$C_{\mathrm{f}\overline{\mathrm{f}}} = (-)^{\ell+s}, \tag{6.59}$$

i.e. $C_{\pi^0} = C_\eta = +$, while $C_{\rho^0} = C_\omega = -$. A photon is its own antiparticle, but has intrinsic $C_\gamma = -1$ (see exercise 6.9). Since the wave function of N photons must be symmetric one finds that for N_γ photons one has $C = (-)^{N_\gamma}$. The charge-conjugation quantum number is therefore very appropriate to determine the number of photons (or gluons) a (neutral) system can couple to.

> A convenient tool to study decay into many-pion final states is the socalled *G-parity*, which is introduced to include isospin in a consistent way. One finds that a fermion-antifermion system has G-parity $G = (-)^{\ell+s+I}$ and that it can only decay into a system of N_π pions with the same G-parity being $G = (-)^{N_\pi}$. This is not a new quantum number but simply a convenient and consistent combined use of C-parity and isospin.

CONSERVATION RULES			
	Interactions		
quantity	strong	electromagnetic	weak
energy & momentum	yes	yes	yes
baryon number	yes	yes	yes
lepton number	yes	yes	yes
charge	yes	yes	yes
I (isospin)	yes	no	no ($\Delta I = 1/2$, 1)
S (strangeness)	yes	yes	no ($\Delta S =$ 1,0)
C (charm)	yes	yes	no ($\Delta C =$ 1,0)
B (bottomness)	yes	yes	no ($\Delta B =$ 1,0)
T (weak isospin)	no	yes	yes
Y_W	no	yes	yes
P (parity)	yes	yes	no
C (conjugation)	yes	yes	no
CP	yes	yes	almost
T (time reversal)	yes	yes	almost
CPT	yes	yes	yes

Conservation rules (summary)

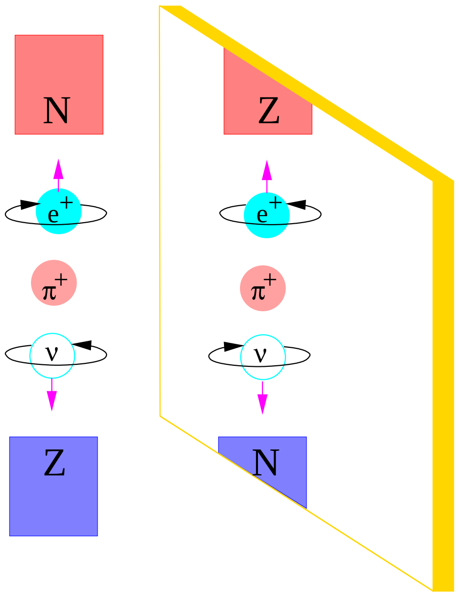
CPT symmetry

All interactions are invariant under the combined action of C, P and T, the socalled *CPT theorem*. It is fundamental in quantum field theories. Some tests involve the equality of masses, lifetimes and magnetic moments of particles and antiparticles:

$$CPT - \text{invariance} \quad \Leftrightarrow \quad \begin{cases} M_a = M_{\overline{a}} \\ \Gamma_a = \Gamma_{\overline{a}} \\ \mu_a = \mu_{\overline{a}} \end{cases} .$$

CP violation

Note that the presence of only a lefthanded neutrino constitutes a maximal violation of parity (P) in the weak interactions. This was suggested by Yang and Lee and discovered in 1957 in an experiment looking at the decay of ^{60}Co.



The decay of a spin zero π^+ into a positron and (lefthanded) neutrino. The helicity of the positron must be negative (angular momentum conservation) and the positrons are attracted towards the northpole of a magnet. The mirror image is the decay into a (righthanded) neutrino and a positron with positive helicity flying towards a southpole of a magnet. In the decay of the pion the positron are seen at the northpole, not at the southpole. Conclusion, the mirror image does not occur in nature, which we attribute to the nonexistence of righthanded neutrinos. The original parity violation experiment by Wu and her collaborators was done by considering the β-decay of ^{60}Co.

The absence of a lefthanded antineutrino also means a maximal violation of charge conjugation symmetry (C). Note, however that the combined operation (CP) transforms ν_L into $\overline{\nu}_R$, hence it is not a priori violated. Actually it turns out that CP is almost a symmetry of the weak interactions. Let us first assume it is a good symmetry and consider the decay of the K^+-particle,

$$\begin{aligned} K^+ &\rightarrow \pi^+\pi^0, \\ &\rightarrow \pi^+\pi^+\pi^-. \end{aligned}$$

From angular momentum conservation one has $J = 0$ for the lefthandside. With spin 0 pions this requires for the first final state $\ell_{\pi^+\pi^0} = 0$ and hence $\Pi_{\pi^+\pi^0} = +$. For the second decay product one has for the two π^+ particles an even value for $\ell_{\pi^+\pi^+}$ (symmetry!). This also implies that the orbital angular momentum of the π^- with respect to the center of mass must be even. Hence one necessarily has $\Pi_{\pi^+\pi^+\pi^-} = -$ for the second decay product. Since parity is not conserved in the weak interactions both processes are allowed and indeed observed.

Next, we turn to the neutral kaon systems, $K^0 = d\overline{s}$ and $\overline{K}^0 = s\overline{d}$. As far as QCD is concerned the two states would be degenerate. They are produced in strong interactions, e.g.

$$\begin{aligned} \pi^- p &\rightarrow \Lambda K^0, \\ \pi^- p &\rightarrow p K^- \overline{K}^0 \end{aligned}$$

(draw quark-line diagrams to convince yourself). The threshold for K^0 production is the lowest and one can thus set up an experiment in which only K^0 particles are produced. Two remarkable observations are made

- When one makes sure that only K^0 are produced (containing an $\overline{s}$-quark), it turns out that depending on the distance to the interaction point $\overline{K}^0$-mesons (containing an s-quark) are found, which initiate e.g. the reaction $\overline{K}^0 p \rightarrow \Lambda\pi^+$. The probabilities of finding K^0 or $\overline{K}^0$ oscillates (see Exercise 6.10).

- In the decay two almost degenerate states are found, decaying into two and three pions, respectively, called K_S (lifetime $\tau \approx 0.9 \times 10^{-10}$ s) and K_L (lifetime $\tau \approx 0.5 \times 10^{-7}$ s), respectively. Their mass difference is extremely small, $M_L - M_S \approx 3.5 \times 10^{-12}$ MeV.

This puzzle is solved if one has physical states that are CP eigenstates. With

$$CP|K^0\rangle = |\overline{K}^0\rangle, \qquad CP|\overline{K}^0\rangle = |K^0\rangle$$

one can construct two such CP eigenstates,

$$|K_1^0\rangle = \frac{1}{\sqrt{2}}\left(|K^0\rangle - |\overline{K}^0\rangle\right), \tag{6.60}$$

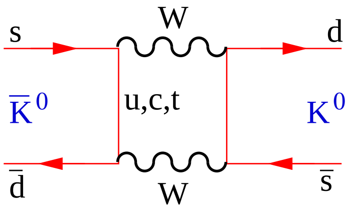
$$|K_2^0\rangle = \frac{1}{\sqrt{2}}\left(|K^0\rangle + |\overline{K}^0\rangle\right), \tag{6.61}$$

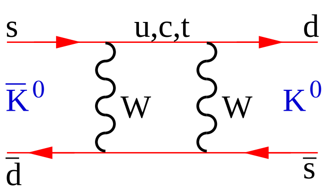
Looking at pion states one has $CP|\pi\pi\rangle = +|\pi\pi\rangle$ for $\pi^+\pi^-$ or $\pi^0\pi^0$ states, while (if the orbital angular momentum between pions is zero) $CP|\pi^+\pi^-\pi^0\rangle = -|\pi^+\pi^-\pi^0\rangle$. If the physical states are CP eigenstates, one expects

$$K_S = K_1^0 \quad \longrightarrow \quad \pi\pi, \tag{6.62}$$

$$K_L = K_2^0 \quad \longrightarrow \quad \pi\pi\pi \tag{6.63}$$

We note that an explanation for the physical states being CP eigenstates simply comes from the fact that a transition $\langle K^0|H|\overline{K}^0\rangle$ exist, e.g. given by the following diagrams,

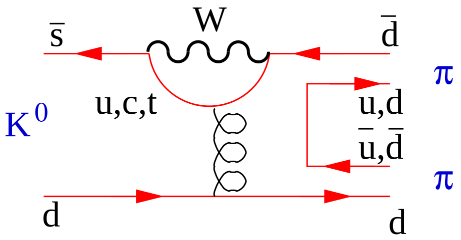




$$\Rightarrow \quad H = \begin{pmatrix} M_0 & \Delta \\ \Delta & M_0 \end{pmatrix}$$

With Δ (requiring twice a weak interaction) being very small, one ends up with two states with a very small mass difference, which nevertheless immediately imply oscillations (Exercise 6.10).

It was discovered in 1964 by Cronin and Fitch that CP actually is violated. Here two effects play a role, the first is a violation because K_S and K_L are not exactly equal to the CP-eigenstates K_1^0 and K_2^0 (mixing); the second is a violation in decay of the CP-eigenstates, e.g. $K_2^0 \to \pi\pi$ (direct CP violation). The mixing comes from complex entries in the CKM matrix, which makes the above (still hermitean) hamiltonian complex. It requires, however, the presence of at least 3 families because otherwise the complex phases can simply be absorbed in the definition of quark states. Direct CP violation comes among others from diagrams like



These type of diagrams, called *Penguin* diagrams and in particular the differences in the diagram for K^0 and $\overline{K}^0$ coming from complex CKM matrix elements, cause direct CP violation.

The incorporation of CP-violation in the standard model via complex entries in the CKM-matrix can of course not really be considered as understanding the origin. To study in more detail CP-violation, experiments in the B-system are underway, where the effects are expected to be much larger. One thing one can explicitly do, is check the unitarity triangle to see if the CKM matrix is unitary.

CP-violation and (assuming CPT a good symmetry) T-violation also is needed to explain in the big bang scenario the surplus of matter over antimatter in the universe. One might wonder it this can be explained because we stated CP-violation was small. Although all visible stuff (atoms) is only matter, this is only about present in a $1 : 10^9$ ratio with invisible stuff such as (self-conjugate) photons (3 K background radiation) and (probably) equal amounts of neutrinos and anti-neutrinos left from the big bang.

6.6 Neutrino's

We already discussed neutrinos and their lefthandedness and we remarked that left- and righthandedness are good properties only for massless particles. Recently indications accumulate that neutrinos are not massless, evidence coming from neutrino oscillations. Oscillations of electron neutrinos from the first family into neutrinos of the other two families could for instance explain the observed shortage of solar neutrinos. The latter is a long-standing problem in astrophysics.

The presence of only lefthanded species of a massive fermion at first sight gives trouble. As discussed in section 6.3, helicity states for a massive fermion are physical (eigenstates of the free hamiltonian), but necessarily both (positive and negative) helicities exist. This is a simple consequence of the fact that helicity depends on the observer (moving slower or faster than the particle).

The solution is the existence of two types of fermions:

- *Dirac fermions.* These are the most well-known ones for which one has both particles and antiparticles. Examples are electrons and quarks. One has two chirality states for the particle (e_R^- and e_L^-) and two for the antiparticle (e_R^+ and e_L^+). The (physical) helicity states are appropriate linear combinations (overlap factors given in section 6.3).

- *Majorana fermions.* These are fermions for which particle $\equiv$ antiparticle, similar as e.g. for photons. In that case the states which we up to now called ν_L and $\overline{\nu}_R$ are actually the left- and righthanded components of one (Majorana) neutrino. The (physical) helicity states now are just linear combinations of these two components. This of course can only work for a neutral fermion.

Note that with the neutrinos being Majorana fermions, the particle-antiparticle arrows which we assigned to fermion lines in diagrams no longer should be used for neutrinos. Lepton number can be violated by two units $\Delta L_e = 2$, etc. With a mass term one also has the possibility of neutrino oscillations between neutrinos belonging to different families. This simply depends on the fact if the mass eigenstates are the same or different as the states entering the interactions. In the case the mass eigenstates are different lepton numbers of different families can change.

Let us illustrate the phenomenon of oscillations for two (instead of three) neutrinos. Assume that the quantum mechanical state at production (say a muon neutrino arising from pion decay) is not an eigenstate of the hamiltonian. Assuming two relevant neutrino species, these eigenstates of the hamiltonian are two orthogonal states $|\nu_1\rangle$ and $|\nu_2\rangle$ which are used as our basis. They are eigenstates with definite energies corresponding to slightly different masses m_1 and m_2, i.e. $E_1 = \sqrt{p^2 + m_1^2}$ and $E_2 = \sqrt{p^2 + m_2^2}$. Thus we have in general

$$|\psi(t)\rangle = c_1\,|\nu_1(t)\rangle + c_2\,|\nu_2(t)\rangle = c_1\,e^{-i\,E_1 t}\,|\nu_1(0)\rangle + c_2\,e^{-i\,E_2 t}\,|\nu_2(0)\rangle. \tag{6.64}$$

Assuming that a muon-neutrino produced in the atmosphere is a linear superposition of the two mass eigenstates ν_1 and ν_2, i.e. at time $t = 0$,

$$|\nu(0)\rangle = \cos\theta\,|\nu_1(0)\rangle + \sin\theta\,|\nu_2(0)\rangle,$$

one has at time t

$$|\nu(t)\rangle = \cos\theta\; e^{-i\,E_1 t}\,|\nu_1(0)\rangle + \sin\theta\; e^{-i\,E_2 t}\,|\nu_2(0)\rangle,$$

and the probability to find at time t again a muon-neutrino is

$$|\langle\nu_\mu|\nu(t)\rangle|^2 = 1 - \sin^2 2\theta\,\sin^2\left(\frac{E_1 - E_2}{2}\,t\right). \tag{6.65}$$

For the situation that $m_1,\, m_2 \ll p$ one has $E_1 \approx E_2$, both roughly equal to $E = p$. The (tiny) energy difference is

$$E_1 - E_2 \approx \frac{m_1^2 - m_2^2}{2E} \equiv \frac{\Delta m^2}{2E},$$

After travelling a distance L with approximately the speed of light c (time is L/c) one then has a survival probability

$$P(\nu_\mu) = 1 - \sin^2 2\theta\,\sin^2\left(\frac{\Delta m^2\,L}{4E}\right) \equiv 1 - \sin^2 2\theta\,\sin^2\left(\pi\,\frac{L}{\lambda_V}\right) \tag{6.66}$$

with

$$\lambda_V = 4\pi\,\frac{E}{\Delta m^2}. \tag{6.67}$$

or for numerical purposes

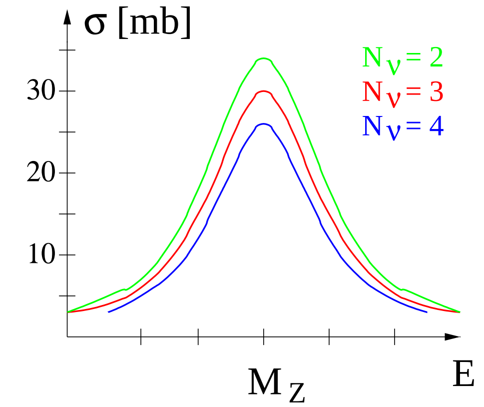
$$\lambda_V\ [\mathrm{km}] = 2.5\,\frac{E\ [\mathrm{GeV}]}{\Delta m^2\ [\mathrm{eV}^2]}. \tag{6.68}$$

Numerically a wavelength $\lambda_V = 1000$ km corresponds for a neutrino with a typical energy of 1 GeV to a mass squared difference of $\Delta m^2 c^4 = (0.05\ \mathrm{eV})^2$.

Neutrino oscillations have been observed for atmospheric (predominantly μ-type) neutrinos over distances of order thousands of kilometers, and for solar neutrinos with indications that the deficit of electron-type neutrinos (expectation based on solar models) appears as other type of neutrinos.

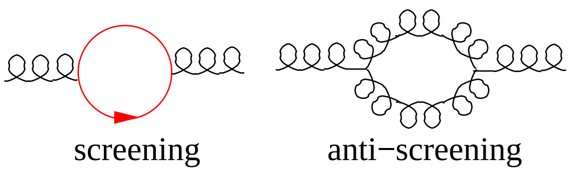
6.7 Unification

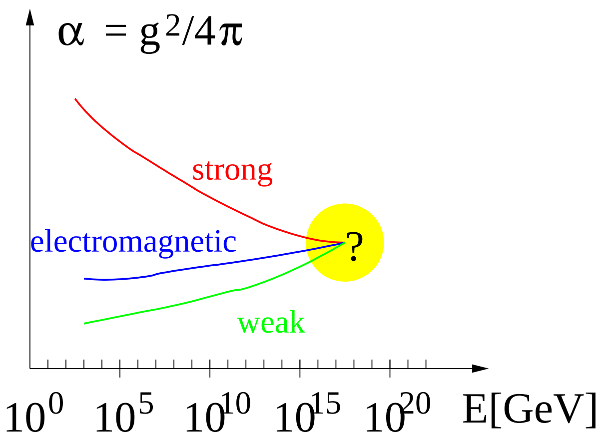
Many questions remain on the foundation of the Standard Model. For instance, one has found that there are not more than 3 families of quarks and leptons, at least families with the same structure, i.e. in essence massless neutrinos.



The Z^0 resonance shapes shown here are based on all (visible) decay modes into quarks ($q\bar{q}$) for five of the six quarks, leptons ($\ell^+\ell^-$), and (invisible) decay modes for 2, 3 or 4 neutrino's. The experimental shape measured with the LEP accelerator at CERN points with very small errors to $N_\nu = 3$.

But why three families? Other questions are those about the origin of the quark CKM mixing matrix and the *small* violation of CP-invariance, do neutrinos have a mass, and what is precisely the nature of the Higgs mechanism. Within the Standard Model also several questions remain on the structure of hadrons, that can not be answered within perturbative quantum field theory.





Using methods from quantum field theory one can study the strength of the coupling constants of the various interactions. For instance for QCD the higher order Feynman diagrams, shown left, lead to screening and anti-screening of the, in this case color, charge. The anti-screening wins and the strength of the interactions increases for larger distances and decreases for smaller distances (or via Fourier transform) higher momenta/energies (known as *asymptotic freedom*). For QED the second diagram is absent and the coupling constant increases for higher energies. It has been argued that they may meet at some high scale, referred to as the GUT (*grand unification theory*) scale around 10^{16} GeV, i.e. distances of the order of 10^{-32} m.

Many (theoretical) attempts are being undertaken to embed the Standard Model in more elegant theories built for instance on a single symmetry group in order to have only one coupling constant, or incorporate fermion-boson symmetry (*supersymmetry*). Also the incorporation of gravity in the unification is an important goal. Attempts include consideration of more than 3 space dimensions as required for setting up a consistent theory in which particles are no longer points in space-time, but (open or closed) strings moving along a world-sheet instead of a worldline. With the increase of the energy scale one also goes back to the first instants after the big bang.

6.8 Exercises

Exercise 6.1

Express for two particles (masses m_1 and m_2) in the center of mass the momentum in terms of the energy $E^{cm} \equiv \sqrt{s}$. Determine the center of mass momentum in the decay processes

$$
\begin{array}{ll}
\rho^0 \longrightarrow \pi^+\pi^- & (M_\rho = 770 \text{ MeV}, M_{\pi^\pm} = 140 \text{ MeV}), \\
\pi^- \longrightarrow \mu^-\overline{\nu}_\mu & (M_\mu = 106 \text{ MeV}, M_\nu \approx 0), \\
\pi^- \longrightarrow e^-\overline{\nu}_e & (M_e = 0.5 \text{ MeV}), \\
Z^0 \longrightarrow e^+e^- & (M_Z \approx 91 \text{ GeV}), \\
\gamma \longrightarrow e^+e^- & (M_\gamma = 0).
\end{array}
$$

Note: details on kinematics can be found in the appendix on kinematics.

Exercise 6.2

Consider the following two decay modes of a pion,

$$
\begin{array}{rcl}
\pi^- & \rightarrow & e^-\overline{\nu}_e \\
 & \rightarrow & \mu^-\overline{\nu}_\mu
\end{array}
$$

The underlying process is quite similar, and for both processes sufficient energy is available. Use the calculated energy and momentum of the electron and muon to calculate the overlap between chirality states (lefthanded and righthanded) and helicity states. Indicate how lefthandedness of the weak interactions can explain the extremely small ratio $\Gamma(\pi \to e\nu_e)/\Gamma(\pi \to \mu\nu_\mu) \sim 10^{-4}$.

Exercise 6.3

Check that the Wolfenstein parametrization of the CKM matrix respects unitarity (in an expansion in λ). Show that the unitarity condition for the first and third rows of the matrix can be represented as a triangle in the complex (ρ, η) plane.

Exercise 6.4

Construct the explicit wave functions of the proton (Eq. 6.37) and neutron. There are several ways to proceed. One can construct in several ways (starting first with an *ud*-configuration or a *uu*-configuration) a state with the appropriate quantum numbers. After imposing the right symmetry for the full system (think of all parts of the wave function, color, spin and isospin) always the same state will emerge.

Exercise 6.5

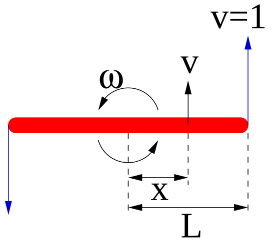
Use the explicit wave functions of proton and neutron to evaluate the expectation value of the magnetic moment operator. Use the experimental proton and neutron magnetic moments to determine a nonstrange quark magnetic moment.

Exercise 6.6

In this exercise we will illustrate how a linear potential leads to a linear relation between the total angular momentum J of a system and the mass squared M^2 for large values of J. This leads to the socalled Regge trajectories for excited $q\overline{q}$ states, for which one has found relations

$$J = \alpha_0 + \alpha' M^2,$$

with $\alpha' = 1/2\pi\, T_0$ being a universal slope, while α_0 depends on the kind of mesons (pions, rho-mesons, K-mesons, etc.). Show this relation. For this, realize that for large J one can use semi-classical arguments (like Bohr quantization in Hydrogen atom). For a linear potential between light quarks one can use the picture of a rotating rod with constant (linear) energy density T_0 with the (in essence massless) quarks at the ends moving with the velocity of light.



$$M = \int_{-L}^{L} dx\, \frac{T_0}{\sqrt{1-v^2}},$$

$$J = \int_{-L}^{L} dx\, \frac{T_0\, x\, v}{\sqrt{1-v^2}}$$

Exercise 6.7

Explicitly writing the sum in the deep-inelastic cross section for electron-proton scattering (Eq. 6.48) gives

$$\sigma^{ep} \;\propto\; \frac{4}{9}\left(u(x)+\overline{u}(x)\right) + \frac{1}{9}\left(d(x)+\overline{d}(x)\right) + \frac{1}{9}\left(s(x)+\overline{s}(x)\right)$$

(assuming the probability for finding heavier quarks to be zero). In fact the distributions refer to the proton, $u(x) = u^p(x)$, etc. To find the expression for electron-neutron deep inelastic scattering we use isospin symmetry, $d^n(x) = u^p(x) = u(x)$, $u^n(x) = d^p(x) = d(x)$ and $s^n(x) = s^p(x) = s(x)$. Show that one finds

$$\sigma^{en} \;\propto\; \frac{1}{9}\left(u(x)+\overline{u}(x)\right) + \frac{4}{9}\left(d(x)+\overline{d}(x)\right) + \frac{1}{9}\left(s(x)+\overline{s}(x)\right)$$

Use weak interaction vertices to write down to which combinations of quark distributions the following (charged current) cross sections are proportional, $\sigma^{\nu p}$, $\sigma^{\overline{\nu} p}$, $\sigma^{\nu n}$, and $\sigma^{\overline{\nu} n}$. The experiment can be done for the charged weak current because one needs a final state lepton that can be detected. In this way one can determine the quark distributions for separate flavors and distinguish quarks and antiquarks.

Exercise 6.8

Construct the $Y - I_z$ diagrams for mesons containing a $\overline{c}$-quark, and those for the B- and $\overline{B}$-mesons containing a $\overline{b}$ and b-quark respectively. Give names and charge-assignments.

Exercise 6.9

Determine for the decay of a $J^P = 1^-$ particle, e.g. $\rho^0 \longrightarrow \mathrm{f}\bar{\mathrm{f}}$ the ${}^{2s+1}\ell_J$ state of the fermion-antifermion system. What implies the observation of $\rho^0 \to e^+e^-$ thus about the C quantum number of the ρ^0? The same argument shows that a photon has $J^{PC} = 1^{--}$.

Exercise 6.10

The time evolution for an unstable particle in its rest frame is given by

$$\psi(t) = \psi(0)\, \exp(-i\, Mt - \Gamma\, t/2)$$

with correspondingly the probability of finding the particle

$$I(t) = I(0)\, \exp(-\Gamma\, t) = I(0)\, \exp(-t/\tau).$$

Starting with a beam of K^0 mesons (produced in strong interactions), expand in the physical states K_L and K_S which have masses M_L and M_S and widths Γ_L and Γ_S, and write down the wave function at time t. Show that the intensities of finding K^0 or $\overline{K}^0$ states (which via $\overline{K}^0 + p \to \Lambda + \pi^+$ can be identified) vary as a function of time. For instance, show that

$$I(K^0) = \frac{1}{4}\left[e^{-\Gamma_L\, t} + e^{-\Gamma_S\, t} + 2\, e^{-\frac{1}{2}(\Gamma_L+\Gamma_S)\, t}\, \cos\left(\Delta M\, t\right)\right],$$

where $\Delta M = |M_L - M_S|$. What is $I(\overline{K}^0)$. Plot the intensities as a function of $t/\tau_S = \Gamma_S\, t$ using $\tau_L/\tau_S \approx 580$ and $\Delta M\, \tau_S \approx 0.5$.

Chapter 7

Astrophysics and Cosmology

Chapter 8

Concepts, skills and questions

8.1 The structure of Matter

8.1.1 Introduction

1. Construct characteristic quantities for quantummechanical and/or relativistic systems bound by or subject to particular type of interactions.

8.1.2 Units

1. Ability to estimate order of magnitudes of related physical quantities given one of them, such as energy $\leftrightarrow$ frequency $\leftrightarrow$ wavelength for a photon.

8.1.3 Physics and Mathematics

1. Construct dimensionless differential equations and deduce characteristic energy and length scales.

2. What are spherical harmonics, Laguerre polynomials, Legendre polynomials, Hermite polynomials? How is their behavior. Where can one find these functions, recursion relations, etc.?

8.1.4 The constituents of Matter

1. What are the constituents of matter. What are the characteristic scales at the various layers? What are the characteristic (excitation) energies? What are the binding forces?

2. What underlies the structure of atoms? Discuss the Periodic Table?

3. Give a few reasons why atomic nuclei cannot be built from protons and electrons?

4. How many forces do we distinguish in nature? Compare their strengths. What are the corresponding force-carrying particles?

5. What is the composition of baryons and mesons? Are these fermions or bosons?

8.2 Atoms

section in notes	section(s) in Brehm and Mullin
2.1	3.1 - 3.9
2.2	7.1 - 7.4
2.3	5.8, 7.5,
2.4	8.9, 8.10, 8.12
2.5	9.1 - 9.3, 9.5 - 9.9
2.6	8.1 - 8.5, 8.11

8.2.1 Introduction

1. What is wrong with the Thomson model of the atom?

2. What is the structure of the spectrum of hydrogen and what does it teach us on the energy spectrum of hydrogen?

3. Application of Bohr quantization to the hydrogen atom and other potentials.

8.2.2 The Schrödinger equation for the hydrogen atom

1. The different steps in getting to the simple radial Schrödinger equation for the hydrogen atom: reduction to center of mass (use of reduced electron mass); looking for stationary states; separating radial and angular parts for a central potential; making equations dimensionless.

2. Discuss the structure of the spectrum for hydrogen, levels, quantum numbers, degeneracy.

3. Look at the typical sizes of orbits, e.g. by making a table of $\langle r/a_0 \rangle$, $\sqrt{\langle (r/a_0)^2 \rangle}$, etc.

8.2.3 Radiative transitions

1. Discuss the time dependence of the occupation number of two levels in a heat bath with energy density u_ν. What are the Einstein coefficients. What is essential for a laser (principle) and how can it be achieved (principle).

2. The electric dipole transition for photons with polarization $\boldsymbol{\epsilon}$ is described with via the dipole operator. Its matrix elements determine the Einstein coefficients.

3. The Einstein coefficients for spontaneous emission determine the lifetime of an excited state. What is the order of magnitude of this lifetime.

4. Discuss the various selection rules for electric dipole transitions and quadrupole transitions.

8.2.4 Refinements in the spectrum of hydrogen

1. Give the steps that are necessary to treat the spin-orbit interaction in hydrogen. Explain why it is necessary to couple ℓ and s to total angular momentum j.

2. Discuss the hyperfine splitting for the groundstate of hydrogen. What are the possible total angular momentum values? Is this truely the total angular momentum?

8.2.5 Many electron atoms

1. Symmetry of wave functions under permutations. Do not confuse permutation symmetry with space inversion (parity)!

2. Bosons and fermions have symmetric and antisymmetric wave functions, respectively.

3. The Pauli exclusion principle.

4. Discuss in detail the quantum numbers of ground state and excited state configurations in helium, orbital angular momentum, spin multiplicities, parity, total angular momentum, degeneracy, permutation symmetry of the states.

5. Calculate the effect of the electron repulsion in helium using perturbation theory.

6. Argue which spin states have lowest energy in helium. Why is for ortho-helium the groundstate configuration absent?

7. Give radiative (electric dipole) transitions between levels in the spectrum.

8. Use the variational principle to get an improved wave function for the helium ground state configuration.

9. What are ionization energies and electron affinities.

10. Hydrogen has a (small) positive electron affinity, i.e. H^- is bound.

11. What is the centrla field approximation. Argue within this approximation that higher ℓ-values have higher energies because they have a smaller Z_{eff}.

12. Discuss the structure of the periodic table. What are noble gases?

13. Construct for given groundstate or excited state configurations the allowed multiplets and indicate the electric dipole transitions. Give the energy ordering using the Hund rules.

14. Give te fine structure of a multiplet in the LS-scheme and/or the jj-scheme.

8.2.6 Magnetic effects in atoms

1. Discuss the effects of spin in an external magnetic field.
2. Discuss the effects of orbital angular momentum in an external field.
3. Discuss the structure of energy levels in a realistic atom, i.e. including the fine structure, in an external magnetic field and discuss the various limits (Zeeman effect and Paschen-Back limit; small B-field, what is actually small?). What is the Landé factor.
4. Discuss the splitting of lines in the spectrum in the limiting cases (small and large B-field) for a particular multiplet.

8.3 Molecules and chemical binding

section in notes	section(s) in Brehm and Mullin
3.1	10

8.3.1 The quantum structure of molecules

8.5 Nuclei

See also the items on nuclei in chapter 1.

section in notes	section(s) in Brehm and Mullin
5.1	14.1, 14.2, 14.3, 14.4
5.2	14.5, 14.6
5.3	
5.4	14.7, 14.8, 14.12
5.5	14.9, 14.10, 14.11
5.6	15

8.5.1 Properties of nuclei

1. What are isotopes and isobars? Give a few examples.
2. What is nuclear binding energy? What is roughly the order of magnitude? How is its variation as a function of the mass number A?
3. Estimate the amounts of energy released in fusion and fission reactions.
4. How large are nuclei (order of magnitude)? How does the size vary with mass number A? What does this imply for the density?
5. Why are spins of nuclei with even mass number A integer and those with odd mass number half-integer?
6. What are characteristic orders of magnitude of nuclear magnetic moments?
7. Explain why the magnetic moment of ^{3}H is close to that of the proton, while that of ^{3}He is close to that of the neutron.

8.5.2 Semi-empirical mass formula

1. Give qualitative discussions for the various terms in the semi-empirical mass formula?
2. Estimate the magnitude of the electrostatic self-energy by calculating $e^2/4\pi\epsilon_0 R$ for $R = 1$ fm.
3. Explain via the semi-empirical mass formula why $N > Z$ for heavy nuclei.
4. Explain why some nuclei have more than one stable isotope?

8.5.3 Scattering theory

1. In the socalled Born approximation, cross sections are proportional to the square of the absolute value of the potential in momentum space.
2. The effect of an extended charge distribution in an electromagnetic scattering process is the replacement $Z \rightarrow Z\,F(\boldsymbol{q})$, where $F(\boldsymbol{q})$ is the form factor.
3. The form factor $F(\boldsymbol{q})$ is the Fourier transform of the charge distribution, satisfying $F(0) = Q$.
4. What determines how fast the form factor goes to zero as a function of q?

8.5.4 The nucleon-nucleon force

1. Discuss the main features of the nucleon-nucleon potential.
2. Deduce the possible J^Π values that one can have for *pp*-, *nn*- and *pn*-pairs. Which isospin states are allowed for these J^Π values?
3. Derive the relations between depth and size (without and with hard-core) of the nucleon-nucleon potential in the zero-binding approximation for the deuteron using a square well (without and with hard-core).
4. What is the behavior of the tail of the nucleon-nucleon potential and which mechanism is responsible for this behavior?

8.5.5 The nuclear shell-model

1. What are magic numbers for nuclei and why are these different from the Z-values for noble gases in atoms?
2. Determine the J^Π-values for ground states and excited states of nuclei using the level structure of the nuclear shell-model.

8.5.6 Nuclear reactions and decay

1. Give some examples of β-decay? Discuss for the case of an even A nucleus with several stable isotopes the β-decay scheme.

2. In atoms, the radiative transitions are dominantly $E1$-transitions. Explain why in nuclei also higher multipoles are important.

3. Given a groundstate and excited state of a nucleus, determine which electric or magnetic transitions can occur.

4. Why do alpha-decay lifetimes cover such a tremendous large range?

8.6 Particles

See also the items on particles in chapter 1

section in notes	section(s) in Brehm and Mullin
6.1	16.1
6.2	16.2, 16.3
6.3.1	16.6, 16.7, 16.14
6.3.2	16.13, 16.16
6.4	16.15, 16.10, 16.11, 16.12
6.5.1	
6.5.2	
6.5.3	16.6, 16.9
6.6	
6.7	16.17

8.6.1 Introduction

1. What are baryons and mesons? What are their possible spins?

2. Discuss ways to find the lifetime of unstable particles? In particular, how can one measure lifetimes much smaller than 10^{-15} s?

3. What is the criterium for a decay process following from energy and momentum conservation?

4. What is the criterium that determines if a scattering process is allowed from energy and momentum conservation?

8.6.2 Forces between elementary particles

1. Discuss the basic forces in nature? Which ones are responsible for binding particles and give examples.

2. Explain why the weak interactions are so weak. What is their range?

3. In gauge theories based on symmetry groups, the important consequence is the presence of just *one* coupling constant. All relative couplings are determined by the charge operators (in general matrices).

4. Explain the qualitative behavior that is expected for the cross section in e^+e^- scattering and in particular the ratio of the cross section into hadrons and that into $\mu^+\mu^-$.

8.6.3 Electroweak interactions

1. Explain why the decay of a π^+ into $\mu^+\nu_\mu$ is much more probable than the decay into $e^+\nu_e$.

2. Draw diagrams for the decay of the τ^--lepton into leptonic final states.

3. Draw the diagram for the weak decay of the neutron.

8.6.4 Hadrons

1. Express the tension T_0 in the linear potential in Newtons.

2. Discuss the microscopic structure of a baryon-baryon-meson vertex, such as the $NN\pi$ vertex needed in the nucleon-nucleon potential.

3. Discuss the 'light' baryon and meson multiplets (u, d, and s-quarks).

4. Give the quarkline diagram for particular processes, e.g. $\pi^-p \to \Lambda K^0$ and also for the subsequent decay modes of the Λ (see table in section 6.1).

5. Use the N-Δ mass difference and the color hyperfine splitting for six quarks to estimate the height of the repulsive core expected in the NN-potential.

6. Explain the ratio of magnetic moments for proton and neutron.

7. Give the various decay modes of, for instance, the D^+-meson (see table in section 6.1).

8.6.5 Symmetries and conservation laws

1. Which symmetries are related to conservation of energy, momentum, angular momentum and parity?

2. Use conservation rules (or violation thereof) to determine which interaction is responsible for a specific decay/process, e.g. like in the case of $K^+ \to \pi^+\pi^0$.

3. Discuss parity violation in pion decay.

4. Why are K^0 and $\overline{K}^0$ degenerate as far as strong interactions is concerned?

5. Discuss the phenomenon of K^0-$\overline{K}^0$ oscillations.

8.6.6 Neutrinos

1. What type of neutrinos would one expect to be produced in the Sun?

2. Discuss neutrino oscillations and calculate the oscillation wavelength in the case of mixing between two neutrino species with a mass difference of 0.05 eV.

3. If a neutrino is of the Majorana type one expects neutrinoless double β-decay. Draw the diagram for this.

Appendix A

Angular momentum eigenfunctions

The angular momentum operators are best studied in polar coordinates

$$\begin{aligned} x &= r\,\sin\theta\,\cos\varphi, \\ y &= r\,\sin\theta\,\sin\varphi, \\ z &= r\,\cos\theta \end{aligned}$$

from which one gets

$$\begin{pmatrix} \frac{\partial}{\partial r} \\ \\ \frac{\partial}{\partial \theta} \\ \\ \frac{\partial}{\partial \varphi} \end{pmatrix} = \begin{pmatrix} x/r & y/r & z/r \\ \\ x\,\cot\theta & y\,\cot\theta & -r\,\sin\theta \\ \\ -y & x & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \\ \frac{\partial}{\partial y} \\ \\ \frac{\partial}{\partial z} \end{pmatrix}.$$

The $\boldsymbol{\ell}$ operators are given by

$$\begin{aligned} \ell_x &= -i\hbar\left(y\,\frac{\partial}{\partial z} - z\,\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\varphi\,\frac{\partial}{\partial\theta} + \cot\theta\,\cos\varphi\,\frac{\partial}{\partial\varphi}\right), \\ \ell_y &= -i\hbar\left(z\,\frac{\partial}{\partial x} - x\,\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\varphi\,\frac{\partial}{\partial\theta} + \cot\theta\,\sin\varphi\,\frac{\partial}{\partial\varphi}\right), \\ \ell_z &= -i\hbar\left(x\,\frac{\partial}{\partial y} - y\,\frac{\partial}{\partial x}\right) = -i\hbar\,\frac{\partial}{\partial\varphi}. \end{aligned}$$

Searching eigenfunctions becomes easy if one realizes that the operators only affect the angular dependence. One has

$$\ell_z\left(\frac{x}{r}\right) = -\left(\frac{y}{r}\right), \qquad \ell_z\left(\frac{y}{r}\right) = +\left(\frac{x}{r}\right), \qquad \ell_z\left(\frac{z}{r}\right) = 0,$$

which shows that the $\boldsymbol{\ell}$ operators acting on polynomials of the form

$$\left(\frac{x}{r}\right)^{n_1}\left(\frac{y}{r}\right)^{n_2}\left(\frac{z}{r}\right)^{n_3}$$

do not change the total degree $n_1 + n_2 + n_3 \equiv \ell$. They only change the degrees of the different terms in the expressions. Simple statistics is sufficient to see that for a particular degree ℓ, there are $2\ell+1$ functions. These are the eigenfunctions of $\boldsymbol{\ell}^2$, the spherical harmonics, which can be distinguished by also considering the operator ℓ_z, commuting with $\boldsymbol{\ell}^2$,

$$\begin{aligned}\boldsymbol{\ell}^2\, Y_\ell^m(\theta,\varphi) &= \ell(\ell+1)\hbar^2\, Y_\ell^m(\theta,\varphi),\\ \ell_z\, Y_\ell^m(\theta,\varphi) &= m\hbar\, Y_\ell^m(\theta,\varphi).\end{aligned}$$

Realizing the polynomial structure one e.g. immediately sees that the parity of the Y_ℓ^m's is $(-)^\ell$. Instead of the combinations x/r, y/r and z/r, it is convenient to use eigenfunctions of ℓ_z, which are proportional to $e^{im\varphi}$,

$$\begin{aligned}Y_1^1(\theta,\varphi) &= -\sqrt{\frac{3}{8\pi}}\,\frac{x+iy}{r} = -\sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{i\varphi},\\ Y_1^0(\theta,\varphi) &= \sqrt{\frac{3}{4\pi}}\,\frac{z}{r} = \sqrt{\frac{3}{4\pi}}\,\cos\,\theta,\\ Y_1^{-1}(\theta,\varphi) &= \sqrt{\frac{3}{8\pi}}\,\frac{x-iy}{r} = \sqrt{\frac{3}{8\pi}}\,\sin\theta\, e^{-i\varphi}.\end{aligned}$$

which are the $\ell=1$ functions. Useful relations are the following,

$$Y_\ell^m(\theta,\varphi) = (-)^{(m+|m|)/2}\sqrt{\frac{2\ell+1}{4\pi}\,\frac{(\ell-|m|)!}{(\ell+|m|)!}}\,P_\ell^{|m|}(\cos\,\theta)\, e^{im\varphi},$$

where $\ell = 0,1,2,\ldots$ and $m = \ell,\ell-1,\ldots,-\ell$, and the associated Legendre polynomials are given by

$$P_\ell^{|m|}(x) = \frac{1}{2^\ell\,\ell!}\,(1-x^2)^{|m|/2}\,\frac{d^{\ell+|m|}}{dx^{\ell+|m|}}\,\left[(x^2-1)^\ell\right].$$

The $m=0$ states are related to the (orthogonal) Legendre polynomials, $P_\ell = P_\ell^0$, given by

$$P_\ell(\cos\,\theta) = \sqrt{\frac{4\pi}{2\ell+1}}\,Y_\ell^0(\theta).$$

They are defined on the $[0,1]$ interval and the lowest ones are

$$P_0(x) = 1, \qquad P_1(x) = x, \qquad P_2(x) = \frac{1}{2}(3x^2-1).$$

The $\ell=2$ spherical harmonics are the five(!) quadratic polynomials of degree two,

$$\begin{aligned}Y_2^{\pm 2}(\theta,\varphi) &= \sqrt{\frac{15}{32\pi}}\,\frac{(x^2-y^2)\pm 2i\,xy}{r^2} = \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\, e^{\pm 2i\varphi},\\ Y_1^{\pm 1}(\theta,\varphi) &= \mp\sqrt{\frac{15}{8\pi}}\,\frac{z(x\pm iy)}{r^2} = \mp\sqrt{\frac{15}{8\pi}}\,\sin\theta\,\cos\,\theta\, e^{\pm i\varphi}.\\ Y_2^0(\theta,\varphi) &= \sqrt{\frac{5}{16\pi}}\,\frac{3\,z^2-r^2}{r^2} = \sqrt{\frac{5}{16\pi}}\,\left(3\cos^2\theta-1\right),\end{aligned}$$

The spherical harmonics form a complete set of functions on the sphere, satisfying the orthonormality relations

$$\int d\Omega\; Y_\ell^{m*}(\theta,\varphi)\, Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\,\delta_{mm'}.$$

Appendix B

Some differential equations

B.1 Generalized Laguerre polynomials

For the solution of a dimensionless equation such as that for the Hydrogen atom, Eq. 1.12, we can turn to an algebraic manipulation program or a mathematical handbook. The solutions of the equation

$$y'' + g_0(x)\, y = 0 \qquad \text{with} \quad g_0(x) = \left[\frac{2p+a+1}{2x} + \frac{1-a^2}{4x^2} - \frac{1}{4}\right], \tag{B.1}$$

are given by

$$y(x) = e^{-x/2}\, x^{(a+1)/2}\, L_p^a(x). \tag{B.2}$$

where L_p^a are polynomials of degree p. They are normalized as

$$\int_0^\infty dx\; x^{a+1}\, e^{-x}\, \left[L_p^a(x)\right]^2 = (2p+a+1)\,\frac{(p+a)!}{p!}, \tag{B.3}$$

and also satisfy the differential equation

$$\left[x\,\frac{d^2}{dx^2} + (a+1-x)\,\frac{d}{dx} + p\right] L_p^a(x) = 0. \tag{B.4}$$

Note that depending on books, different conventions are around, differing in the indices of the polynomials, the normalization, etc. Some useful properties are

$$L_p(x) \equiv L_p^0(x) = \frac{e^x}{p!}\,\frac{d^p}{dx^p}\left[x^p\, e^{-x}\right] = \frac{1}{p!}\left(\frac{d}{dx} - 1\right)^p x^p, \tag{B.5}$$

$$L_p^a(x) = (-)^a\,\frac{d^a}{dx^a}\left[L_{p+a}(x)\right]. \tag{B.6}$$

Some general expressions are

$$L_0^a(x) = 1, \qquad L_1^a(x) = 1 + a - x.$$

Some recursion relations are

$$(p+1)\, L_{p+1}^a(x) = (2p+a+1-x)\, L_p^a(x) - (p+a)\, L_{p-1}^a(x), \tag{B.7}$$

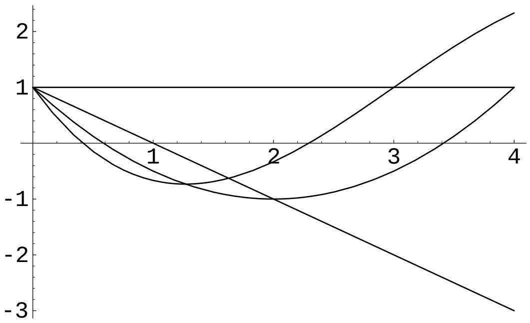
$$x\, L_p^{a+1}(x) = (x-p)\, L_p^a(x) + (p+a)\, L_{p-1}^a(x), \tag{B.8}$$

$$L_p^a(x) = L_p^{a-1}(x) + L_{p-1}^a(x). \tag{B.9}$$

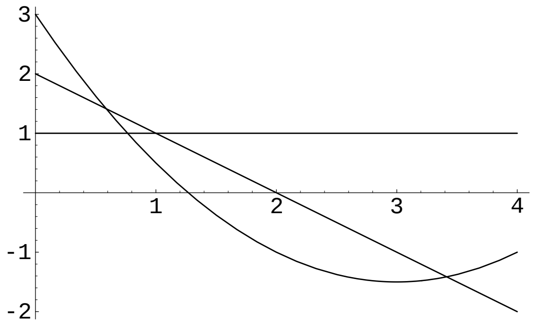
Some explicit polynomials are

$$
\begin{aligned}
L_0(x) &= 1, \\
L_1(x) &= 1 - x, \\
L_2(x) &= 1 - 2x + \frac{1}{2}\,x^2, \\
L_3(x) &= 1 - 3x + \frac{3}{2}\,x^2 - \frac{1}{6}\,x^3,
\end{aligned}
$$

$$
\begin{aligned}
L_0^1(x) &= 1, \\
L_1^1 &= 2\left(1 - \frac{1}{2}\,x\right), \\
L_2^1(x) &= 3\left(1 - x + \frac{1}{6}\,x^2\right).
\end{aligned}
$$



The $L_p(x)$ or `LaguerreL[p,x]` functions for $p = 0$, 1, 2, and 3.



The $L_p^a(x)$ or `LaguerreL[p,a,x]` functions for $a = 1$ and $p = 0$, 1, and 2.

B.2 Hermite polynomials

The problem of the one-dimensional harmonic oscillator in essence reduces to the differential equation

$$y'' + g_0(x)\,y = 0 \qquad \text{with} \quad g_0(x) = 2n + 1 - x^2 \tag{B.10}$$

for which the solutions are given by

$$y(x) = e^{-x^2/2}\,H_n(x). \tag{B.11}$$

where H_n are polynomials of degree n. They are normalized as

$$\int_{-\infty}^{\infty} dx\; e^{-x^2}\,[H_n(x)]^2 = 2^n\,n!\sqrt{\pi}, \tag{B.12}$$

and satisfy the differential equation

$$\left[\frac{d^2}{dx^2} - 2x\,\frac{d}{dx} + 2n\right] H_n(x) = 0. \tag{B.13}$$

Some useful properties are

$$H_n(x) = (-)^n\,e^{x^2}\,\frac{d^n}{dx^n}\,e^{-x^2}, \tag{B.14}$$

$$x\,H_n(x) = \frac{1}{2}\,H_{n+1}(x) + n\,H_{n-1}(x), \tag{B.15}$$

$$\frac{d}{dx}\,H_n(x) = 2n\,H_{n-1}(x). \tag{B.16}$$

Some explicit polynomials are

$$\begin{aligned} H_0(x) &= 1, \\ H_1(x) &= 2x, \\ H_2(x) &= 4x^2 - 2, \\ H_3(x) &= 8x^3 - 12x. \end{aligned}$$

B.3 Creation and annihilation operators

The harmonic oscillator can be solved in a representation independent way. Starting with the hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}\, m\omega^2\, x^2, \tag{B.17}$$

with noncommuting operators

$$[x, p] = i\hbar, \tag{B.18}$$

one introduces

$$a = x\,\sqrt{\frac{m\omega}{2\,\hbar}} + i\,p\,\sqrt{\frac{\hbar}{2\,m\omega}} \tag{B.19}$$

$$a^\dagger = x\,\sqrt{\frac{m\omega}{2\,\hbar}} - i\,p\,\sqrt{\frac{\hbar}{2\,m\omega}} \tag{B.20}$$

satisfying

$$[a, a^\dagger] = 1. \tag{B.21}$$

The hamiltonian can be expressed in the number operator $N = a^\dagger a$,

$$\begin{aligned} H &= \hbar\omega \left\{ \left(x\,\sqrt{\frac{m\omega}{2\,\hbar}} - i\,p\,\sqrt{\frac{\hbar}{2\,m\omega}} \right) \left(x\,\sqrt{\frac{m\omega}{2\,\hbar}} + i\,p\,\sqrt{\frac{\hbar}{2\,m\omega}} \right) - \frac{i}{2}\,[x, p] \right\} \\ &= \hbar\omega \left\{ a^\dagger a + \frac{1}{2} \right\} = \hbar\omega \left\{ N + \frac{1}{2} \right\}. \end{aligned} \tag{B.22}$$

It is straightforward to find the commutation relations between N and a and $a^\dagger$,

$$[N, a^\dagger] = a^\dagger, \quad \text{and} \quad [N, a] = -a. \tag{B.23}$$

Defining states $|n\rangle$ as eigenstates of N with eigenvalue n, $N|n\rangle = n|n\rangle$ one finds

$$\begin{aligned} N\, a^\dagger |n\rangle &= (n+1)\, a^\dagger |n\rangle, \\ N\, a|n\rangle &= (n-1)\, a|n\rangle \end{aligned}$$

i.e. $a^\dagger$ and a act as raising and lowering operators. From the normalizations one obtains $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$ and $a|n\rangle = \sqrt{n}\,|n-1\rangle$, and we see that a state $|0\rangle$ must exist for which $N|0\rangle = a|0\rangle = 0$. In this way one has found for the harmonic oscillator the spectrum of eigenstates $|n\rangle$ (with n a non-negative integer) with $E_n = (n + 1/2)\omega$.

Appendix C

Angular momentum

Definitions

The angular momentum operator for a particle is $\boldsymbol{\ell} = \boldsymbol{r} \times \boldsymbol{p}$. They satisfy the commutation relations

$$[\ell_i, \ell_j] = i\hbar\, \epsilon_{ijk}\, \ell_k, \tag{C.1}$$

Eigenstates in the Hilbert space of functions (in this case only depending on angles) have been discussed in the appendix on spherical harmonics. In addition particles may have a spin. This observable corresponds with a vector operator $\boldsymbol{s}$. These (three) hermitean operators also satisfy the commutation relations

$$[s_i, s_j] = i\hbar\, \epsilon_{ijk}\, s_k, \tag{C.2}$$

similar to the ones for the angular momentum operator. The spin operators $\boldsymbol{s}$, however, commute with the operators $\boldsymbol{r}$ and $\boldsymbol{p}$ and thus also with $\boldsymbol{\ell}$. The space in which they act will be deduced from the commutation relations, which is the full starting point for spin.

Rotation invariance

Without spin, rotation invariance required specific commutation relations with $\boldsymbol{\ell}$. In fact *scalar* quantities S and *vectors* $\boldsymbol{V}$ under rotations behaved like

$$[\ell_i, S] = 0, \tag{C.3}$$

$$[\ell_i, V_j] = i\hbar\, \epsilon_{ijk}\, V_k, \tag{C.4}$$

e.g. scalars $S = \boldsymbol{r}^2$, $\boldsymbol{p}^2$, $\boldsymbol{r} \cdot \boldsymbol{p}$ or $\boldsymbol{\ell}^2$ and vectors $\boldsymbol{V} = \boldsymbol{r}$, $\boldsymbol{p}$ or $\boldsymbol{\ell}$.

Including spin vectors $\boldsymbol{s}$, the notion of behavior under rotations has to be generalized. Although $\boldsymbol{s}$ is a vector and $\boldsymbol{\ell} \cdot \boldsymbol{s}$ a scalar one has $[\ell_i, s_j] = 0$ and $[\ell_i, \boldsymbol{\ell} \cdot \boldsymbol{s}] = -i\hbar\, (\boldsymbol{\ell} \times \boldsymbol{s})_i$. Only the operator

$$\boldsymbol{j} \equiv \boldsymbol{\ell} + \boldsymbol{s}, \tag{C.5}$$

satisfies

$$[j_i, S] = 0, \tag{C.6}$$

$$[j_i, V_j] = i\hbar\, \epsilon_{ijk}\, V_k, \tag{C.7}$$

for all vectors, including $\boldsymbol{s}$ and $\boldsymbol{j}$ itself and all scalars including $\boldsymbol{s}^2$ and $\boldsymbol{\ell}\cdot\boldsymbol{s}$.

For a system of many particles the operators $\boldsymbol{r}$, $\boldsymbol{p}$ and $\boldsymbol{s}$ for different particles commute. The sum operators

$$\boldsymbol{L} = \sum_{n=1}^{N} \boldsymbol{\ell}_n, \qquad \boldsymbol{S} = \sum_{n=1}^{N} \boldsymbol{s}_n, \qquad \boldsymbol{J} = \sum_{n=1}^{N} \boldsymbol{j}_n = \boldsymbol{L} + \boldsymbol{S}, \tag{C.8}$$

satisfy commutation relations $[L_i, L_j] = i\hbar\,\epsilon_{ijk}\,L_k$, $[S_i, S_j] = i\hbar\,\epsilon_{ijk}\,S_k$, and $[J_i, J_j] = i\hbar\,\epsilon_{ijk}\,J_k$. Only the operator $\boldsymbol{J}$ satisfies

$$[J_i, S] = 0, \tag{C.9}$$
$$[J_i, V_j] = i\hbar\,\epsilon_{ijk}\,V_k, \tag{C.10}$$

for any scalar S or vector $\boldsymbol{V}$. Rotation invariance for a system of particles requires $[\boldsymbol{J}, H] = 0$.

Spin states

As mentioned above, the commutation relations are all that defines spin. An operator that commutes with all three spin operators (a socalled Casimir operator) is $\boldsymbol{s}^2 = s_x^2 + s_y^2 + s_z^2$,

$$[s_i, s_j] = i\hbar\,\epsilon_{ijk}\,s_k, \tag{C.11}$$
$$[\boldsymbol{s}^2, s_i] = 0. \tag{C.12}$$

Only one of the three spin operators can be used to label states, for which without loss of generality s_z can be choosen. In addition we can use $\boldsymbol{s}^2$, which commutes with s_z. One writes states $\chi_m^{(s)} = |s,m\rangle$ satisfying

$$\boldsymbol{s}^2|s,m\rangle = \hbar^2\,s(s+1)|s,m\rangle, \tag{C.13}$$
$$\boldsymbol{s}_z|s,m\rangle = m\hbar\,|s,m\rangle. \tag{C.14}$$

It is of course a bit premature to take $\hbar^2\,s(s+1)$ as eigenvalue. One needs to prove that the eigenvalue of $\boldsymbol{s}^2$ is positive, but this is straightforward as it is the sum of three squared operators. Since the spin operators are hermitean each term is not just a square but also the product of the operator and its hermitean conjugate. In the next step, the operators s_x and s_y are recombined into

$$s_\pm \equiv s_x \pm i\,s_y. \tag{C.15}$$

The commutation relations for these operators are,

$$[\boldsymbol{s}^2, s_\pm] = 0, \tag{C.16}$$
$$[s_z, s_\pm] = \pm\hbar\,s_\pm, \tag{C.17}$$
$$[s_+, s_-] = 2\hbar\,s_z, \tag{C.18}$$

The first two can be used to show that

$$\begin{aligned}\boldsymbol{s}^2\,s_\pm|s,m\rangle &= s_\pm\boldsymbol{s}^2|s,m\rangle = \hbar^2\,s(s+1)\,s_\pm|s,m\rangle,\\ s_z\,s_\pm|s,m\rangle &= (s_\pm s_z \pm \hbar\,s_\pm)\,|s,m\rangle = (m\pm 1)\hbar\,s_\pm|s,m\rangle,\end{aligned}$$

hence the name step-operators (raising and lowering operator) which achieve

$$s_\pm|s,m\rangle = c_\pm|s,m\pm 1\rangle.$$

Furthermore we have $s_\pm^\dagger = s_\mp$ and $\boldsymbol{s}^2 = s_z^2 + (s_+s_- + s_-s_+)/2$, from which one finds that

$$\begin{aligned} |c_\pm|^2 = \langle s,m|s_\pm^\dagger s_\pm|s,m\rangle &= \langle s,m|\boldsymbol{s}^2 - s_z^2 - [s_\pm, s_\mp]/2|s,m\rangle \\ &= \langle s,m|\boldsymbol{s}^2 - s_z^2 \mp \hbar\, s_z|s,m\rangle = s(s+1) - m(m\pm 1). \end{aligned}$$

It is convention to use the positive (real) root in

$$\begin{aligned} s_+|s,m\rangle &= \hbar\sqrt{s(s+1)-m(m+1)}\,|s,m+1\rangle \\ &= = \hbar\sqrt{(s-m)(s+m+1)}\,|s,m+1\rangle \qquad \text{(C.19)} \\ s_-|s,m\rangle &= \hbar\sqrt{s(s+1)-m(m-1)}\,|s,m-1\rangle \\ &= \hbar\sqrt{(s+m)(s-m+1)}\,|s,m-1\rangle. \qquad \text{(C.20)} \end{aligned}$$

This shows that given a state $|s,m\rangle$, we have a whole series of states

$$\ldots|s,m-1\rangle,\ |s,m\rangle,\ |s,m+1\rangle,\ldots$$

But, we can also easily see that since $\boldsymbol{s}^2 - s_z^2 = s_x^2 + s_y^2$ must be an operator with positive definite eigenstates that $s(s+1) - m^2 \geq 0$, i.e. $|m| \leq \sqrt{s(s+1)}$ or strictly $|m| < s+1$. From the second expressions in Eqs C.19 and C.20 one sees that this inequality requires $m_{max} = s$ as one necessary state to achieve a cutoff of the series of states on the upper side, while $m_{min} = -s$ is required as a necessary state to achieve a cutoff of the series of states on the lower side. Moreover to have both cutoffs the step operators require that the difference $m_{max} - m_{min} = 2\,s$ must be an integer, i.e. the only allowed values of spin quantum numbers are

$$\begin{aligned} &s = 0,\ 1/2,\ 1,\ 3/2,\ldots, \\ &m = s, s-1,\ldots,-s. \end{aligned}$$

Thus for spin states with a given quantum number s, there exist $2s+1$ states.

Matrix representations of spin operators

In the space of spin states with a given quantum number s, we can write the spin operators as $(2s+1)\times(2s+1)$ matrices. Let us illustrate this first for spin $s = 1/2$. Define the states

$$\begin{aligned} &\chi_{+1/2}^{(1/2)} \quad \text{or} \quad \chi_\uparrow \quad \text{or} \quad |\uparrow\rangle \quad \text{or} \quad |1/2,+1/2\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \\ &\chi_{-1/2}^{(1/2)} \quad \text{or} \quad \chi_\downarrow \quad \text{or} \quad |\downarrow\rangle \quad \text{or} \quad |1/2,-1/2\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned}$$

Using the definition of the quantum numbers in Eq. C.14 one finds that

$$s_z = \hbar\begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}, \quad s_+ = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad s_- = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

For spin 1/2 we find the familiar spin matrices, $\boldsymbol{s} = \hbar\boldsymbol{\sigma}/2$,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For spin 1 we may define the basis states,

$$\chi^{(1)}_{+1} = |1,+1\rangle \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \chi^{(1)}_{0} = |1,0\rangle \equiv \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \chi^{(1)}_{-1} = |1,0\rangle \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The spin matrices are then easily written down

$$s_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \; s_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}, \; s_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix},$$

from which also s_x and s_y can be constructed.

Combining angular momenta

We consider situations in which two sets of angular momentum operators play a role, e.g.

- An electron with spin in an atomic $(n\ell)$-orbit (spin $\boldsymbol{s}$ and orbital angular momentum $\boldsymbol{\ell}$ combined into a total angular momentum $\boldsymbol{j} = \boldsymbol{\ell} + \boldsymbol{s}$).
- Two electrons with spin (spin operators $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$, combined into $\boldsymbol{S} = \boldsymbol{s}_1 + \boldsymbol{s}_2$).
- Two electrons in atomic orbits (orbital angular momenta $\boldsymbol{\ell}_1$ and $\boldsymbol{\ell}_2$ combined into total orbital angular momentum $\boldsymbol{L} = \boldsymbol{\ell}_1 + \boldsymbol{\ell}_2$).
- Combining the total orbital angular momentum of electrons in an atom ($\boldsymbol{L}$) and the total spin ($\boldsymbol{S}$) into the total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$.

Let us discuss as the generic example

$$\boldsymbol{J} = \boldsymbol{j}_1 + \boldsymbol{j}_2. \tag{C.21}$$

We have states characterized by the direct product of two states,

$$|j_1, m_1\rangle \otimes |j_2, m_2\rangle, \tag{C.22}$$

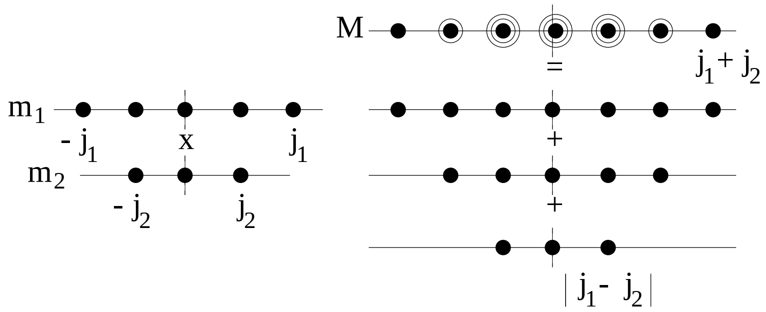
which we can write down since not only $[\boldsymbol{j}_1^2, j_{1z}] = [\boldsymbol{j}_2^2, j_{2z}] = 0$, but also $[j_{1m}, j_{2n}] = 0$. The sum-operator $\boldsymbol{J}$ obviously is not independent, but since the $\boldsymbol{J}$-operators again satisfy the well-known angular momentum commutation relations we can look for states characterized by the commuting operators $\boldsymbol{J}^2$ and J_z, $|\ldots; J, M\rangle$. It is easy to verify that of the four operators characterizing the states in Eq. C.22, $[\boldsymbol{J}^2, j_{1z}] \neq 0$ and $[\boldsymbol{J}^2, j_{2z}] \neq 0$ (Note that $\boldsymbol{J}^2$ contains the operator combination $2\boldsymbol{j}_1 \cdot j_2$, which contains operators like j_{1x}, which do not commute with j_{1z}). It is easy to verify that one does have

$$[\boldsymbol{J}^2, \boldsymbol{j}_1^2] = [\boldsymbol{J}^2, \boldsymbol{j}_2^2] = 0,$$
$$[J_z, \boldsymbol{j}_1^2] = [J_z, \boldsymbol{j}_2^2] = 0,$$

and thus we can relabel the $(2j_1+1)(2j_2+1)$ states in Eq. C.22 into states characterized with the quantum numbers

$$|j_1, j_2; J, M\rangle. \tag{C.23}$$

The basic observation in the relabeling is that $J_z = j_{1z} + j_{2z}$ and hence $M = m_1 + m_2$. This leads to the following scheme, in which in the left part the possible m_1 and m_2-values are given and the upper right part the possible sum-values for M including their degeneracy.



1. Since $|m_1| \le j_1$ and $|m_2| \le j_2$, the maximum value for M is $j_1 + j_2$. This state is unique.

2. Since $J_+ = j_{1+} + j_{2+}$ acting on this state is zero, it corresponds to a state with $J = j_1 + j_2$. Then, there must exist other states (in total $2J+1$), which can be constructed via $J_- = j_{1-} + j_{2-}$ (in the scheme indicated as the first set of states in the right part below the equal sign).

3. In general the state with $M = j_1 + j_2 - 1$ is twofold degenerate. One combination must be the state obtained with J_- from the state with $M = j_1 + j_2$, the other must be orthogonal to this state and again represents a 'maximum M'-value corresponding to $J = j_1 + j_2 - 1$.

4. This procedure goes on till we have reached $M = |j_1 - j_2|$, after which the degeneracy is equal to the $\min\{2j_1+1, 2j_2+1\}$, and stays constant till the M-value reaches the corresponding negative value.

Summarizing, when combining two angular momenta j_1 and j_2 one finds resulting angular momenta J with values

$$J = j_1 + j_2,\ j_1 + j_2 - 1, \ldots, |j_1 - j_2|,$$

going down in steps of one. Note that the total number of states is (as expected)

$$\sum_{J=|j_1-j_2|}^{j_1+j_2} (2J+1) = (2j_1+1)(2j_2+1). \tag{C.24}$$

Furthermore we have in combining angular momenta:

half-integer with half-integer $\longrightarrow$ integer
integer with half-integer $\longrightarrow$ half-integer
integer with integer $\longrightarrow$ integer

Clebsch-Gordon coefficients

The actual construction of states just follows the steps outlined above. Let us illustrate it for the case of combining two spin 1/2 states. We have four states according to labeling in Eq. C.22,

$$|s_1, m_1\rangle \otimes |s_2, m_2\rangle : \qquad \begin{aligned} &|1/2,+1/2\rangle \otimes |1/2,+1/2\rangle \equiv |\uparrow\uparrow\rangle, \\ &|1/2,+1/2\rangle \otimes |1/2,-1/2\rangle \equiv |\uparrow\downarrow\rangle, \\ &|1/2,-1/2\rangle \otimes |1/2,+1/2\rangle \equiv |\downarrow\uparrow\rangle, \\ &|1/2,-1/2\rangle \otimes |1/2,-1/2\rangle \equiv |\downarrow\downarrow\rangle. \end{aligned}$$

1. The highest state has $M = 1$ and must be the first of the four states above. Thus for the labeling $|s_1, s_2; S, M\rangle$

$$|1/2, 1/2; 1, +1\rangle = |\uparrow\uparrow\rangle. \tag{C.25}$$

2. Using $S_- = s_{1-} + s_{2-}$ we can construct the other $S + 1$ states.

$$\begin{aligned} &S_-|1/2, 1/2; 1, +1\rangle = \hbar\sqrt{2}\,|1/2, 1/2; 1, 0\rangle, \\ &(s_{1-} + s_{2-})|\uparrow\uparrow\rangle = \hbar(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \end{aligned}$$

and thus

$$|1/2, 1/2; 1, 0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\Big). \tag{C.26}$$

Continuing with S_- (or in this case using the fact that we have the lowest nondegenerate M-state) we find

$$|1/2, 1/2; 1, -1\rangle = |\downarrow\downarrow\rangle. \tag{C.27}$$

3. The state with $M = 0$ is twofold degenerate. One combination is already found in the above procedure. The other is made up of the same two states appearing on the right hand side in Eq. C.26. Up to a phase, it is found by requiring it to be orthogonal to the state $|1/2, 1/2; 1, 0\rangle$ or by requiring that $S_+ = s_{1+} + s_{2+}$ gives zero. The result is

$$|1/2, 1/2; 0, 0\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\Big). \tag{C.28}$$

The convention for the phase is that the higher m_1-value appears with a positive sign.

It is easy to summarize the results in a table, where one puts the states $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ in the different rows and the states $|j_1, j_2; J, M\rangle$ in the different columns, i.e.

$$\begin{array}{c|ccc} j_1 \times j_2 & \vdots & \text{J} & \vdots \\ & \vdots & \text{M} & \vdots \\ \hline \cdots\ \cdots & & & \\ m_1\ m_2 & & & \\ \cdots\ \cdots & & & \end{array}$$

For the above case we have

$1/2 \times 1/2$		1	1	0	1
		1	0	0	-1
$+1/2$	$+1/2$	1			
$+1/2$	$-1/2$		$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	
$-1/2$	$+1/2$		$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	
$-1/2$	$-1/2$				1

Note that the recoupling matrix is block-diagonal because of the constraint $M = m_1 + m_2$. The coefficients appearing in the matrix are the socalled Clebsch-Gordan coefficients. We thus have

$$|j_1, j_2; J, M\rangle = \sum_{m_1, m_2} C(j_1, m_1, j_2, m_2; J, M)\, |j_1, m_1\rangle \otimes |j_2, m_2\rangle. \tag{C.29}$$

Represented as a matrix as done above, it is unitary (because both sets of states are normed). Since the Clebsch-Gordan coefficients are choosen real, the inverse is just the transposed matrix, or

$$|j_1, m_2\rangle \otimes |j_2, m_2\rangle = \sum_{J,M} C(j_1, m_1, j_2, m_2; J, M)\, |j_1, j_2; J, M\rangle. \tag{C.30}$$

In some cases (like combining two spin 1/2 states) one can make use of symmetry arguments. If a particular state has a well-defined symmetry under permutation of states 1 and 2, then all M-states belonging to a particular J-value have the same symmetry (because $j_{1\pm} + j_{2\pm}$ does not alter the symmetry. This could have been used for the $1/2 \times 1/2$ case, as the highest total M is symmetric, all $S = 1$ states are symmetric. This is in this case sufficient to get the state in Eq. C.26.

We will give two other examples. The first example is

$1 \times 1/2$		$3/2$	$3/2$	$1/2$	$3/2$	$1/2$	$3/2$
		$+3/2$	$+1/2$	$+1/2$	$-1/2$	$-1/2$	$-3/2$
$+1$	$+1/2$	1					
$+1$	$-1/2$		$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$			
0	$+1/2$		$\sqrt{\frac{2}{3}}$	$-\sqrt{\frac{1}{3}}$			
0	$-1/2$				$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$	
-1	$+1/2$				$\sqrt{\frac{1}{3}}$	$-\sqrt{\frac{2}{3}}$	
-1	$-1/2$						1

for instance needed to obtain the explicit states for an electron with spin in an (2p)-orbit coupled to a total angular momentum $j = 3/2$ (indicated as $2p_{3/2}$) with $m = 1/2$ is (depending on choice of notation)

$$\begin{aligned}
\phi(\boldsymbol{r}, t) &= \frac{u_{2p}(r)}{r} \left(\sqrt{\frac{1}{3}}\, Y_1^1(\theta, \phi)\, \chi_\downarrow + \sqrt{\frac{2}{3}}\, Y_1^0(\theta, \phi)\, \chi_\uparrow \right) \\
&= \frac{u_{2p}(r)}{r} \begin{pmatrix} \sqrt{\frac{2}{3}}\, Y_1^0(\theta, \phi) \\ \\ \sqrt{\frac{1}{3}}\, Y_1^1(\theta, \phi) \end{pmatrix}.
\end{aligned}$$

The second example is

1×1		2	2	1	2	1	0	2	1	2
		$+2$	$+1$	$+1$	0	0	0	-1	-1	-2
$+1$	$+1$	1								
$+1$	0		$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$						
0	$+1$		$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$						
$+1$	-1				$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{3}}$			
0	0				$\sqrt{\frac{2}{3}}$	0	$-\sqrt{\frac{1}{3}}$			
$+1$	-1				$\sqrt{\frac{1}{6}}$	$-\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{3}}$			
0	-1							$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	
-1	0							$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	
-1	-1									1

This example, useful in the combination of two spin 1 particles or two electrons in p-waves, illustrates the symmetry of the resulting wave functions when combining two identical angular momenta (or spins). The highest angular momentum is symmetric, the next lower antisymmetric, etc.

Appendix D

Plane wave states

Plane wave states

Plane wave states are the eigenstates of the hermitean operator $\hat{\boldsymbol{p}}$ (in this chapter we use hats to indicate operators) Denoting the eigenstates as $|\boldsymbol{p}\rangle$ or $|\boldsymbol{k}\rangle$ and the eigenvalues as $\boldsymbol{p} = \hbar\boldsymbol{k}$,

$$\hat{\boldsymbol{p}}|\boldsymbol{k}\rangle = \hbar\boldsymbol{k}|\boldsymbol{k}\rangle. \tag{D.1}$$

In the Hilbert space of wave functions ($\psi(\boldsymbol{r}) = \langle\boldsymbol{r}|\psi\rangle$) we have, consistent with the commutation relation $[r_i, p_j] = i\hbar\delta_{ij}$

$$\hat{\boldsymbol{p}}\,\psi(\boldsymbol{r}) = -i\hbar\,\boldsymbol{\nabla}\psi(\boldsymbol{r}). \tag{D.2}$$

The eigenstates of the momentum operator are

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \langle\boldsymbol{r}|\boldsymbol{k}\rangle = \sqrt{\rho}\,\exp\left(i\,\boldsymbol{k}\cdot\boldsymbol{r}\right) \tag{D.3}$$

(This defines ρ as an arbitrary normalization). A convenient regularization is obtained by using box normalization, in which case one finds that for one particle in a box with sides L, i.e. $0 \le x \le L$, $0 \le y \le L$ and $0 \le z \le L$ (i.e. density $\rho = 1/L^3$), the wave function is found after imposing periodic boundary conditions[1],

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{L^{3/2}}\,\exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}), \tag{D.4}$$

with $\boldsymbol{k} = (2\pi/L)\,(n_x, n_y, n_z)$, showing a density of states in k-space given by $(L/2\pi)^3$.

We have the following properties for plane waves (given in discrete and in continuous form):

$$\langle\boldsymbol{k}|\boldsymbol{k}'\rangle = \delta_{\boldsymbol{k},\boldsymbol{k}'} = \rho\,(2\pi)^3\,\delta^3(\boldsymbol{k}-\boldsymbol{k}') \qquad \text{(orthogonality)},$$

$$|\psi\rangle = \sum_{\boldsymbol{k}}|\boldsymbol{k}\rangle\langle\boldsymbol{k}|\psi\rangle = \int\frac{d^3k}{(2\pi)^3\,\rho}\;|\boldsymbol{k}\rangle\,\underbrace{\langle\boldsymbol{k}|\psi\rangle}_{\tilde{\psi}(\boldsymbol{k})} \qquad \text{(completeness)},$$

$$I = \sum_{\boldsymbol{k}}|\boldsymbol{k}\rangle\langle\boldsymbol{k}| = \int\frac{d^3k}{(2\pi)^3\,\rho}\;|\boldsymbol{k}\rangle\langle\boldsymbol{k}| \qquad \text{(Identity)},$$

$$\hat{\boldsymbol{p}} = \sum_{\boldsymbol{k}}|\boldsymbol{k}\rangle\,\hbar\boldsymbol{k}\,\langle\boldsymbol{k}| = \int\frac{d^3k}{(2\pi)^3\,\rho}\;|\boldsymbol{k}\rangle\,\hbar\boldsymbol{k}\,\langle\boldsymbol{k}|.$$

[1] Periodic boundary conditions must be imposed to avoid getting an overcomplete set of states. For instance, hermiticity of the momentum operator requires that $\psi^*\psi|_{-L}^{L} = 0$

The momentum eigenstates can be conveniently used when switching from coordinate to momentum representation,

$$\begin{aligned}
\psi(\boldsymbol{r}) = \langle \boldsymbol{r}|\psi\rangle &= \int \frac{d^3\boldsymbol{k}}{(2\pi)^3\,\rho}\,\langle \boldsymbol{r}|\boldsymbol{k}\rangle\langle \boldsymbol{k}|\psi\rangle \\
&= \int \frac{d^3\boldsymbol{k}}{(2\pi)^3\,\sqrt{\rho}}\,\exp\left(i\,\boldsymbol{k}\cdot\boldsymbol{r}\right)\tilde{\psi}(\boldsymbol{k}), \qquad \text{(D.5)} \\
\tilde{\psi}(\boldsymbol{k}) = \langle \boldsymbol{k}|\psi\rangle &= \int d^3\boldsymbol{r}\,\langle \boldsymbol{k}|\boldsymbol{r}\rangle\langle \boldsymbol{r}|\psi\rangle \\
&= \int d^3\boldsymbol{r}\,\sqrt{\rho}\,\exp\left(-i\,\boldsymbol{k}\cdot\boldsymbol{r}\right)\psi(\boldsymbol{r}), \qquad \text{(D.6)}
\end{aligned}$$

which is of course just Fourier transforming. Common choices for the normalization of plane waves are $\rho = 1$ or $\rho = (2\pi)^{-3}$ (non-relativistic) or $\rho = E/M$ or $\rho = 2E$ (relativistic).

Consistency of Eq. D.2 with the properties of momentum states can be checked, e.g.

$$\begin{aligned}
\langle \boldsymbol{r}|\hat{\boldsymbol{p}}|\psi\rangle &= \int \frac{d^3\boldsymbol{k}}{(2\pi)^3\,\rho}\,\langle \boldsymbol{r}|\boldsymbol{k}\rangle\,\hbar\boldsymbol{k}\langle \boldsymbol{k}|\psi\rangle = \int \frac{d^3\boldsymbol{k}}{(2\pi)^3\sqrt{\rho}}\,\hbar\boldsymbol{k}\,\exp\left(i\,\boldsymbol{k}\cdot\boldsymbol{r}\right)\tilde{\psi}(\boldsymbol{k}) \\
&= -i\hbar\boldsymbol{\nabla}\int \frac{d^3\boldsymbol{k}}{(2\pi)^3\sqrt{\rho}}\,\exp\left(i\,\boldsymbol{k}\cdot\boldsymbol{r}\right)\tilde{\psi}(\boldsymbol{k}) = -i\hbar\boldsymbol{\nabla}\psi(\boldsymbol{r})
\end{aligned}$$

Flux corresponding to plane waves

The flux is obtained from the wave function via the expression for the current,

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{\hbar}{2i\,m}\left(\psi^*\,\boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi)^*\psi\right) = \rho\,\frac{\boldsymbol{p}}{m} = \rho\,\boldsymbol{v}. \tag{D.7}$$

The flux corresponding to a plane wave thus is along $\boldsymbol{p}$ and its magnitude is $\rho\,v$.

Density of states for plane waves

Plane waves are characterized by a vector $\boldsymbol{p} = \hbar\boldsymbol{k}$. The density of plane waves is

$$\rho(\boldsymbol{p})\,d^3p = \frac{d^3p}{(2\pi\hbar)^3\,\rho}. \tag{D.8}$$

We have here left free the normalization of the plane waves.

Rewriting the final state density $\rho(\boldsymbol{p})$ in terms of E and Ω we find for the nonrelativistic case with $E = \boldsymbol{p}^2/2m$

$$\rho(\boldsymbol{p})\,d^3p = \frac{\boldsymbol{p}^2}{(2\pi\hbar)^3\,\rho}\,d|\boldsymbol{p}|\,d\Omega_p = \frac{m\,|\boldsymbol{p}|}{(2\pi\hbar)^3\,\rho}\,dE\,d\Omega_p = \rho(E)\,dE\,\frac{d\Omega_p}{4\pi}, \tag{D.9}$$

or

$$\rho(E) = \frac{m\,|\boldsymbol{p}|}{2\pi^2\,\hbar^3\,\rho} = \frac{1}{(2\pi)^2\,\rho}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}. \tag{D.10}$$

(spin degeneracy factor has not yet been included).

For the relativistic case with $E^2 = \boldsymbol{p}^2 + m^2$ (using $\hbar = c = 1$) one has with normalization $\rho = (E/m)\,\rho_0$,

$$\frac{2m\,d^3p}{(2\pi)^3\,2E\,\rho_0} = \frac{2m\,\boldsymbol{p}^2}{(2\pi)^3\,2E\,\rho_0}\,d|\boldsymbol{p}|\,d\Omega_p = \frac{m\,|\boldsymbol{p}|}{(2\pi)^3\,\rho_0}\,dE\,d\Omega_p = \rho(E)\,dE\,\frac{d\Omega_p}{4\pi}, \tag{D.11}$$

or

$$\rho(E) = \frac{m\,|\boldsymbol{p}|}{2\pi^2\,\rho_0} = \frac{m\sqrt{E^2 - m^2}}{2\pi^2\,\rho_0}. \tag{D.12}$$

The first way of expressing thus has the advantage of being valid both in the nonrelativistic and relativistic situation.

Appendix E

Time-dependent perturbations and Fermi's golden rule

For a hamiltonian without explicit time-dependence, i.e. $H = H(\boldsymbol{r}, \boldsymbol{p}, \ldots)$ one has stationary state solutions of the form $|\phi\rangle\, e^{-iEt/\hbar}$, where $|\phi\rangle$ is time-independent and is a solution of the eigenvalue equation $H|\phi\rangle = E|\phi\rangle$. Given an initial state, there are two possibilities

1. One starts (e.g. after a measurement) with $\psi(0) = |\phi_i\rangle$, where ϕ_i is one of the eigenstates of H with eigenvalue/energy E_i. In that case $|\psi(t)\rangle = |\phi_i\rangle\, e^{-iE_it/\hbar}$ and all expectation values of operators (that do not explicitly depend on time) are time-independent.

2. One starts in a mixed state, say $|\psi(0)\rangle = |\phi_1\rangle + |\phi_2\rangle$. In that case one has $|\psi(t)\rangle = |\phi_1\rangle\, e^{-iE_1t/\hbar} + |\phi_2\rangle\, e^{-iE_2t/\hbar}$ or $|\psi(t)\rangle \propto |\phi_1\rangle + |\phi_2\rangle\, e^{-i(E_2-E_1)t/\hbar}$, which leads to oscillations in expectation values with frequency $\sim (E_2 - E_1)/\hbar$.

In the situation that the hamiltonian of a system contains explicit time dependence, i.e. $H = H(\boldsymbol{r}, \boldsymbol{p}, \ldots, t)$ one no longer has stationary state solutions of the form $|\phi\rangle\, e^{-iEt/\hbar}$, but is left with $|\phi\rangle = |\phi(t)\rangle$.

Treatment of time-dependent perturbations

Consider the case $H = H_0 + \lambda\, V(t)$, with a known (time-independent) part for which the eigenstates and eigen-energies satisfy $H_0|\phi_n\rangle = E_n|\phi_n\rangle$. Using completeness of the states $|\phi_n\rangle$ one writes

$$|\psi(t)\rangle = \sum_n c_n(t)\, |\phi_n\rangle\, e^{-iE_nt/\hbar}. \tag{E.1}$$

Note that one could have absorbed the exponential time-dependence in $c_n(t)$, but not doing so is more appropriate in perturbation theory, because the time-dependence of c_n is then solely due to $\lambda\, V$.

By substituting the expression for $|\psi(t)\rangle$ in the Schrödinger equation, one finds

$$i\hbar\, \dot{c}_p(t) = \sum_n \lambda\, V_{pn}(t)\, c_n(t)\, e^{+i\,\omega_{pn}t}, \tag{E.2}$$

where $V_{pn} = \langle\phi_p|V|\phi_n\rangle$ and $\omega_{pn} = (E_p - E_n)/\hbar$. As expected, if $\lambda V = 0$, the coefficients are time-independent.

In perturbation theory, one tries a solution of the form

$$c_p(t) = c_p^{(0)}(t) + \lambda\, c_p^{(1)}(t) + \ldots, \tag{E.3}$$

and find that the time-dependence of a specific order is determined by the the lower order,

$$i\hbar\, \dot{c}_p^{(m+1)} = \sum_n V_{pn}(t)\, c_n^{(m)}(t)\, e^{+i\,\omega_{pn}t}. \tag{E.4}$$

Starting with $c_p(0) = \delta_{pi}$ one immediately sees that the first two orders are given by

$$c_p^{(0)}(\tau) = \delta_{pi}, \tag{E.5}$$

$$c_p^{(1)}(\tau) = \frac{1}{i\hbar}\int_0^\tau dt\; V_{pi}(t)\, e^{+i\,\omega_{pi}t}. \tag{E.6}$$

This can straightforwardly been extended and leads to the socalled 'time-ordered' exponential, which we will not discuss here.

The quantity $|c_p(\tau)|^2$ is the probability to find the system in the state $|\phi_p\rangle$, which means the probability for a transition $i \to p$. The first order result is valid if $|c_p^{(0)}(\tau)+c_p^{(1)}(\tau)|^2 \approx 1$.

Fermi's golden rule

We now return to the perturbative treatment of time-dependence and note that also for a time-independent interaction V, transitions occur, if the initial state is not an eigenstate of the full Hamiltonian, but only of H_0. If V is sufficiently weak, we find the result in first order perturbation theory,

$$\begin{aligned} c_p^{(1)}(\tau) &= \frac{V_{pi}}{i\hbar}\int_0^\tau dt\; e^{+i\,\omega_{pi}t} = -\frac{V_{pi}}{\hbar\omega_{pi}}\, e^{+i\,\omega_{pi}t}\Big|_0^\tau \\ &= \frac{V_{pi}}{\hbar\omega_{pi}}\left(1 - e^{+i\,\omega_{pi}\tau}\right) = -\frac{2\,V_{pi}}{\hbar\omega_{pi}}\,\sin(\omega_{pi}\tau/2)\, e^{+i\,\omega_{pi}\tau/2}, \end{aligned} \tag{E.7}$$

and thus for $p \neq i$,

$$P_{i\to p}^{(1)}(\tau) = \frac{4\,|V_{pi}|^2}{\hbar^2}\,\frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2}. \tag{E.8}$$

The function

$$f(\omega_{pi}) = \frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2}$$

is for increasing times τ ever more strongly peaked around $\omega_{pi} = 0$. The value at zero is $f(0) = \tau^2/4$, the first zeros are at $|\omega_{pi}| = 2\pi/\tau$. Since

$$\int d\omega_{pi}\;\frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2} = \frac{\pi\,\tau}{2}, \tag{E.9}$$

we approximate

$$\frac{\sin^2(\omega_{pi}\tau/2)}{\omega_{pi}^2} = \frac{\pi\,\tau}{2}\,\delta(\omega_{pi}). \tag{E.10}$$

Then we find[1]

$$P^{(1)}_{i\to p}(\tau) = \tau\,\frac{2\pi}{\hbar}\,|V_{pi}|^2\,\delta(E_p - E_i) \tag{E.11}$$

or for the transition probability per unit time,

$$\dot{P}^{(1)}_{i\to p} = \frac{2\pi}{\hbar}\,|V_{pi}|^2\,\delta(E_p - E_i) \qquad \text{Fermi's Golden Rule.} \tag{E.12}$$

Although the allowed final state is selected via the energy delta function, it is often possible that the system can go to many final states, because we are dealing with a continuum. In that case one needs the *density of states* $\rho(E)$, where $\rho(E)\,dE$ is the number of states in an energy interval dE around E. The transition probability per unit time is then given by

$$\dot{P}^{(1)}_{i\to p} = \int dE_f\,\rho(E_f)\,\frac{2\pi}{\hbar}\,|V_{fi}|^2\,\delta(E_f - E_i) = \frac{2\pi}{\hbar}\,|V_{pi}|^2\,\rho(E_p)\Big|_{E_p=E_i} \tag{E.13}$$

(Fermi's Golden Rule No. 2).

[1] $\delta(ax) = \frac{1}{|a|}\,\delta(x)$

Appendix F

Electromagnetic interactions

F.1 Interactions of matter with electromagnetic fields

We give here a simplified treatment to see the origin of the simplest interactions terms with electric and magnetic fields. We consider plane waves for the scalar and vector potential,

$$\phi = \tilde{\phi}(\boldsymbol{k},\omega)\ \exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)], \tag{F.1}$$
$$\boldsymbol{A} = \tilde{\boldsymbol{A}}(\boldsymbol{k},\omega)\ \exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)], \tag{F.2}$$

with $\omega = |\boldsymbol{k}|c$, corresponding with the energy and momentum relation, $E = |\boldsymbol{p}|c$, for a massless photon. Although the physical fields are real, we can work with the plane waves by always taking also the complex conjugate solution into account. The corresponding behavior for the electric and magnetic fields can be obtained from the potentials[1]

$$\boldsymbol{E} = \tilde{\boldsymbol{E}}(\boldsymbol{k},\omega)\ \exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)], \tag{F.3}$$
$$\boldsymbol{B} = \tilde{\boldsymbol{B}}(\boldsymbol{k},\omega)\ \exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)]. \tag{F.4}$$

with $\tilde{\boldsymbol{E}} = -i\,\boldsymbol{k}\,\tilde{\phi} + (\omega/c)\,\tilde{\boldsymbol{A}}$ and $\tilde{\boldsymbol{B}} = i\,\boldsymbol{k}\times\tilde{\boldsymbol{A}}$. The interaction of matter with an electromagnetic field is given by

$$H_{int} = \int d^3r\ \ [\rho(\boldsymbol{r})\,\phi(\boldsymbol{r}) - \boldsymbol{j}(\boldsymbol{r})\cdot\boldsymbol{A}(\boldsymbol{r})]\,, \tag{F.5}$$

where ρ and $\boldsymbol{j}$ are the charge and current distribution. The dipole approximation is valid when the wave length $\lambda = 2\pi/|\boldsymbol{k}|$ is much larger than the typical size of the system, e.g. for light ($\lambda \approx 6000\mathring{A}$) and atoms (size $\approx 1-10\mathring{A}$). In that case one can restrict oneself to the first nontrivial term in

$$\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)] = e^{-i\,\omega t}\,(1 + i\,\boldsymbol{k}\cdot\boldsymbol{r} + \ldots). \tag{F.6}$$

[1] Recall that

$$\boldsymbol{E} = -\boldsymbol{\nabla}\Phi - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t},$$
$$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$$

One obtains

$$\begin{aligned}
H_{int} &= \int d^3r \; \Big[(1+i\,\boldsymbol{k}\cdot\boldsymbol{r})\,\rho(\boldsymbol{r})\,\tilde{\phi}(\boldsymbol{k},\omega) - (1+i\,\boldsymbol{k}\cdot\boldsymbol{r})\,\boldsymbol{j}(\boldsymbol{r})\cdot\tilde{\boldsymbol{A}}(\boldsymbol{k},\omega) + \ldots\Big] && \text{(F.7)}\\
&= \int d^3r \; \Big[\rho(\boldsymbol{r})\,\tilde{\phi}(\boldsymbol{k},\omega) + i\,\boldsymbol{k}\cdot\boldsymbol{r}\,\rho(\boldsymbol{r})\,\tilde{\phi}(\boldsymbol{k},\omega) \\
&\qquad\qquad + (\boldsymbol{r}\times\boldsymbol{j}(\boldsymbol{r}))\cdot(i\boldsymbol{k}\times\tilde{\boldsymbol{A}}(\boldsymbol{k},\omega)) + \ldots\Big] && \text{(F.8)}\\
&= Q\,\tilde{\phi}(\boldsymbol{k},\omega) - \boldsymbol{D}\cdot\tilde{\boldsymbol{E}}(\boldsymbol{k},\omega) - \boldsymbol{\mu}\cdot\tilde{\boldsymbol{B}}(\boldsymbol{k},\omega) + \ldots, && \text{(F.9)}
\end{aligned}$$

where we have used that $i\,\boldsymbol{k}\,\tilde{\phi} = -\tilde{\boldsymbol{E}} + (\omega/c)\,\tilde{\boldsymbol{A}}$ and $i\,\boldsymbol{k}\times\tilde{\boldsymbol{A}} = \tilde{\boldsymbol{B}}$. The charge and current distributions give rise to charge, electric and magnetic dipole moments,

$$Q = \int d^3r \; \rho(\boldsymbol{r}) \Longrightarrow \sum_i q_i, \qquad \text{(F.10)}$$

$$\boldsymbol{D} = \int d^3r \; \boldsymbol{r}\,\rho(\boldsymbol{r}) \Longrightarrow \sum_i q_i\,\boldsymbol{r}_i, \qquad \text{(F.11)}$$

$$\boldsymbol{\mu} = \int d^3r \; \boldsymbol{r}\times\boldsymbol{j}(\boldsymbol{r}) \Longrightarrow \sum_i \frac{q_i}{m_i}\,\boldsymbol{\ell}_i, \qquad \text{(F.12)}$$

The results after the arrow in the above equations indicate the results for a number of charges q_i at position $\boldsymbol{r}_i$, i.e. $\rho(\boldsymbol{r}) = \sum_i q_i\,\delta^3(\boldsymbol{r}-\boldsymbol{r}_i)$. For a neutral system the first interaction term disappears and the next important one is the interaction with the electric dipole moment ($\boldsymbol{D}$).

F.2 Emission and absorption of radiation by atoms

The radiation fields can be described with just a vector potential

$$\boldsymbol{A} = \boldsymbol{\epsilon}(\boldsymbol{k},\omega)\,\frac{c\,\tilde{E}_0(\boldsymbol{k},\omega)}{i\,\omega}\,\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)] \qquad \text{(F.13)}$$

and $\phi = 0$. The vector $\boldsymbol{\epsilon}$ is called the polarization. One has

$$\boldsymbol{E} = \boldsymbol{\epsilon}\,\tilde{E}_0\,\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)], \qquad \text{(F.14)}$$

$$\boldsymbol{B} = \frac{\boldsymbol{k}\times\boldsymbol{\epsilon}}{|\boldsymbol{k}|}\,\tilde{E}_0\,\exp[i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)]. \qquad \text{(F.15)}$$

In the dipole approximation the interaction with matter is given by

$$V(t) = -\boldsymbol{D}\cdot\boldsymbol{E}(t) = -\boldsymbol{D}\cdot\boldsymbol{\epsilon}\,\tilde{E}_0\,e^{-i\,\omega t}. \qquad \text{(F.16)}$$

Although we have a time-dependent interaction, we can proceed as in the derivation of Fermi's golden rule. We obtain now

$$c_p^{(1)}(\tau) = \frac{\langle\phi_p|\boldsymbol{D}\cdot\boldsymbol{\epsilon}|\phi_i\rangle\,\tilde{E}_0}{i\hbar}\,\frac{e^{i\,(\omega_{pi}-\omega)\tau}-1}{i\,(\omega_{pi}-\omega)}, \qquad \text{(F.17)}$$

which gives as before rise to a delta function $\delta(\omega-\omega_{pi})$. With ω being the positive photon frequency, this can only describe *absorption* of a photon, $\hbar\omega = E_p - E_i > 0$. As discussed before, also the complex conjugate solution must be considered, which gives the same result with $\omega \to -\omega$. This gives rise to a delta function $\delta(\omega + \omega_{pi})$ and describes the *emission* of a photon, $\hbar\omega = -\hbar\omega_{pi} = E_i - E_p > 0$. The transition probability can be summarized by

$$P^{(1)}_{i\to p}(\tau) = \frac{\tilde{E}_0^2(\omega)}{\hbar^2} \, |\langle\phi_p|\boldsymbol{D}\cdot\boldsymbol{\epsilon}|\phi_i\rangle|^2 \, \frac{\pi\,\tau}{2} \, \delta(\omega - |\omega_{pi}|). \tag{F.18}$$

If one is not working with monochromatic light one has an integral over different frequencies ω. Instead of the intensity of the field $\tilde{E}_0$ one can use the number of incident photons $N(\omega)$ (number/(area$\times$time)). This number is determined by equating the energy densities in a frequency interval $d\omega$,

$$u_\omega \, d\omega = \frac{1}{2}\,\epsilon_0 \, E_0^2(\omega)\, d\omega = \frac{N(\omega)\,\hbar\omega}{c}\, d\omega. \tag{F.19}$$

Integrating over the photon frequencies, one sees that the atom absorps or emits photons of the right frequency leading to a transition rate

$$\dot{P}^{(1)}_{i\to p} = \frac{\pi}{\epsilon_0\,\hbar c}\, |\omega_{pi}| \, N(|\omega_{pi}|) \, |\langle\phi_p|\boldsymbol{D}\cdot\boldsymbol{\epsilon}|\phi_i\rangle|^2. \tag{F.20}$$

For electrons $\boldsymbol{D} = -\sum_i e\,\boldsymbol{r}_i = -e\,\boldsymbol{R}$. For unpolarized light $\boldsymbol{\epsilon}$ is arbitrary and averaging gives a factor 1/3. In terms of the fine structure constant $\alpha = e^2/4\pi\,\epsilon_0\,\hbar c$ the averaged transition rate is

$$W_{i\to p} = \overline{\dot{P}^{(1)}_{i\to p}} = \frac{4}{3}\,\pi^2\,\alpha\,|\omega_{pi}|\,N(|\omega_{pi}|)\,|\langle\phi_p|\boldsymbol{R}|\phi_i\rangle|^2. \tag{F.21}$$

Note that by treating also the electromagnetic field quantummechanically one finds in addition to the *stimulated absorption or emission* rate a *spontaneous emission* rate

$$W^{\text{spont.}}_{i\to p} = \frac{4}{3}\,\alpha\,\frac{\omega_{ip}^3}{c^2}\,|\langle\phi_p|\boldsymbol{R}|\phi_i\rangle|^2, \tag{F.22}$$

governed by the same transition matrix element and thus obeying the same selection rules.

Appendix G

Aspects of scattering theory

Scattering theory

Finding an appropriate solution of the Schrödinger equation for positive energies is just the 3-dimensional analogue of the 1-dimensional problem of transmission and reflection. The time-independent Schrödinger equation (for one particle in an external potential or two interacting particles in the CM system) is

$$\left(\boldsymbol{\nabla}^2 + k^2\right)\psi(\boldsymbol{r}) = \frac{2m}{\hbar^2}\,V(\boldsymbol{r})\,\psi(\boldsymbol{r}), \tag{G.1}$$

where $E = \hbar^2 k^2/2m$. This is a linear equation with on the righthand a *source* term. There is a whole family of solutions of such an equation. Given a solution of the above *inhomogeneous* equation, one can obtain all solutions by adding any of the possible solutions of the *homogeneous* equation,

$$\left(\boldsymbol{\nabla}^2 + k^2\right)\psi_{\rm hom}(\boldsymbol{r}) = 0. \tag{G.2}$$

The solutions of the homogeneous equation are well-known, namely the plane waves,

$$\phi_k(\boldsymbol{r}) = \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}), \tag{G.3}$$

characterized by a wave vector $\boldsymbol{k}$.

Another systematic way of obtaining the solutions of the homogeneous equation is by considering the radial Schrödinger equation, i.e. writing

$$\psi(\boldsymbol{r}) = \frac{u(r)}{r}\,Y_\ell^m(\theta,\phi), \tag{G.4}$$

the radial wave function $u(r)$ satisfies for the homogeneous equation

$$\left(\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + k^2\right)u(r) = 0. \tag{G.5}$$

There are two type of solutions of this equation

- Regular solutions: spherical Bessel functions of the first kind: $u(r) = kr\,j_\ell(kr)$. Properties:

$$j_0(z) = \frac{\sin z}{z},$$

$$
\begin{aligned}
j_\ell(z) &= z^\ell \left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{\sin z}{z} \quad \stackrel{z\to 0}{\longrightarrow} \quad z^\ell, \\
& \qquad\qquad\qquad\qquad\quad \stackrel{z\to\infty}{\longrightarrow} \quad \frac{\sin(z-\ell\pi/2)}{z}.
\end{aligned}
$$

- Irregular solutions: spherical Bessel functions of the second kind: $u(r) = kr\, n_\ell(kr)$. Properties:

$$
\begin{aligned}
n_0(z) &= -\frac{\cos z}{z}, \\
n_\ell(z) &= -z^\ell \left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{\cos z}{z} \quad \stackrel{z\to 0}{\longrightarrow} \quad z^{-(\ell+1)}, \\
& \qquad\qquad\qquad\qquad\quad \stackrel{z\to\infty}{\longrightarrow} \quad -\frac{\cos(z-\ell\pi/2)}{z}.
\end{aligned}
$$

Equivalently one can use linear combinations, known as Hankel functions,

$$
\begin{aligned}
kr\, h_\ell^{(1)}(kr) = kr\,(j_\ell(kr) + i\, n_\ell(kr)) &\quad \stackrel{z\to\infty}{\longrightarrow} \quad (-i)^{\ell+1}\, e^{i\,kr}, \\
kr\, h_\ell^{(2)}(kr) = kr\,(j_\ell(kr) - i\, n_\ell(kr)) &\quad \stackrel{z\to\infty}{\longrightarrow} \quad (i)^{\ell+1}\, e^{-i\,kr}.
\end{aligned}
$$

A specific example of an expansion into these spherical solutions, is the expansion of the plane wave,

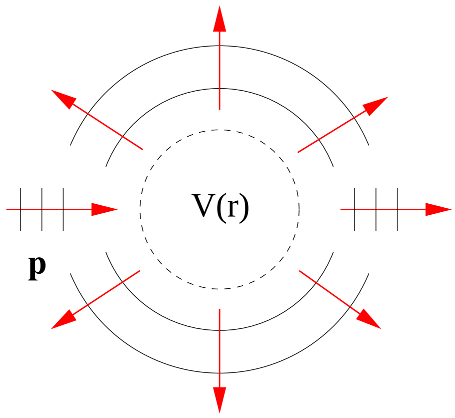
$$
\exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) = e^{i\,kz} = e^{i\,kr\,\cos\theta} = \sum_{\ell=0}^{\infty}(2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\cos\theta), \qquad \text{(G.6)}
$$

where the Legendre polynomials P_ℓ can be also expressed in Y_ℓ^0,

$$
P_\ell(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^0(\theta).
$$

Asymptotic solution and connection to cross sections

In order to construct solutions of the Schrödinger equation that describe a scattering process, one wants the appropriate asymptotic behavior, which includes a plane wave part, describing the incoming part and outgoing spherical waves, describing the scattering part, pictorially represented below



We thus require the following asymptotic form,

$$\psi(\boldsymbol{r}) \quad \stackrel{r\rightarrow\infty}{\longrightarrow} \quad \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) + \frac{e^{i\,kr}}{r}\,f(k;\theta,\phi). \tag{G.7}$$

We have seen in the previous chapter that for $r \to \infty$, this is a solution of the homogeneous equation.

> It can also simply be checked that the above represents a solution if $r \to \infty$, by inserting it into the homogeneous equation. In order to select the leading part for large r one needs to use that $\boldsymbol{\nabla} f(k;\theta,\phi) \propto 1/r$ and $\boldsymbol{\nabla}^2 f(k;\theta,\phi) \propto 1/r^2$.

For the asymptotic solution the current corresponding to the first part is given by

$$\boldsymbol{j}_{in} = \frac{\hbar\boldsymbol{k}}{m}, \tag{G.8}$$

while the second part up to $\mathcal{O}(1/r)$ corresponds with a radially outward directed flux of magnitude

$$j_r = -\frac{i\hbar}{2m}\left[\psi^*\frac{d}{dr}\psi - \left(\frac{d}{dr}\psi^*\right)\psi\right] = \frac{\hbar k}{m}\,\frac{|f(k;\theta,\phi)|^2}{r^2}. \tag{G.9}$$

From it, one derives the cross section using that

$$|j_{in}|\,d\sigma(\theta,\phi) = n(\theta,\phi)\,d\Omega = j_r\,r^2\,d\Omega, \tag{G.10}$$

i.e.

$$\frac{d\sigma}{d\Omega} = |f(k;\theta,\phi)|^2. \tag{G.11}$$

The above considerations require a careful analysis of the forward direction ($\theta = 0$), where the interference term becomes important. For an acceptable asymptotic scattering solution one must have that $\int d\Omega\ j_r|_{r=R} = 0$ for large R, i.e. that there is no loss of probability. This leads to the *optical theorem* or Bohr-Peierls-Placzek relation,

$$\mathcal{I}m\,f_{el}(\theta = 0) = \frac{k}{4\pi}\,\sigma_T, \tag{G.12}$$

where σ_T is the total cross section and f_{el} is the scattering amplitude for elastic scattering.

> In order to derive this result, one must consider the full current. Keeping only the dominant contributions when $r \to \infty$, this is given by
>
> $$j_r = \frac{\hbar k}{m}\left\{\cos\theta + \frac{|f|^2}{r^2} + \mathcal{R}e\left[(1+\cos\theta)\,\frac{e^{ikr(1-\cos\theta)}}{r}\,f\right]\right\}$$
>
> Integrating over the polar angle (writing $\cos\theta \equiv X$) gives for the interference term:
>
> $$\begin{aligned}\mathcal{R}e\int_{-1}^{1} dX\ (1+X)\,\frac{e^{i\,kr(1-X)}}{r}\,f \\ &= \mathcal{R}e\int_{-1}^{1} d\left(e^{i\,kr(1-X)}\right)\ \frac{(1+X)f}{-i\,kr^2} \\ &= \mathcal{R}e\left(\frac{2\,f(k;\theta=0)}{-i\,kr^2}\right) - 2\mathcal{R}e\int_{-1}^{1} dX\ \frac{e^{i\,kr(1-X)}}{-i\,kr^2}\,\frac{d}{dX}\,[(1+X)f] \\ &= -\frac{2\,\mathcal{I}m\,f(k;\theta=0)}{kr^2} + \mathcal{O}\left(\frac{1}{r^3}\right).\end{aligned}$$

The interference term thus actually only contributes at forward angles if $r \to \infty$. Neglecting any contribution disappearing faster than $1/r^2$ the integral over the angles gives

$$\int d\Omega\; j_r\Big|_{r=R} = \frac{1}{R^2}\left[\int d\Omega\; |f|^2 - \frac{4\pi}{k}\,\mathcal{I}m\, f(k;\theta=0)\right],$$

yielding the optical theorem. In fact the result is only derived if the total cross section is given by the integration over $|f|^2$, but it should be clear that flux conservation needs only to hold if we integrate over elastic and inelastic channels, while the interference only occurs for the elastic channel. We will encounter the result again in the section on partial wave expansions.

The integral equation for the scattering amplitude

In order to solve the inhomogeneous equation, we first solve the Green's function equation

$$\left(\boldsymbol{\nabla}^2 + k^2\right) G(\boldsymbol{r},\boldsymbol{r}') = -\delta^3(\boldsymbol{r}-\boldsymbol{r}'). \tag{G.13}$$

With the help of the Green's function an inhomogeneous solution for

$$\left(\boldsymbol{\nabla}^2 + k^2\right)\psi(\boldsymbol{r}) = \rho(\boldsymbol{r}),$$

can be written down, namely

$$\psi(\boldsymbol{r}) = -\int d^3r'\; G(\boldsymbol{r},\boldsymbol{r}')\,\rho(\boldsymbol{r}').$$

By choosing an 'appropriate' Green's function one can built in boundary conditions. Note that the difference between any two Green's function is a solution of the homogeneous equation.

It is not difficult to check that two particular Green's functions in this case are

$$G^{(\pm)}(\boldsymbol{r}-\boldsymbol{r}') = -\frac{\exp\left(\pm i\,k|\boldsymbol{r}-\boldsymbol{r}'|\right)}{4\pi\,|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{G.14}$$

In particular $G^{(+)}$ has the correct asymptotic behavior as discussed in the previous section. As an *exact* solution valid for all r, we can write

$$\psi(\boldsymbol{r}) = \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{m}{2\pi\,\hbar^2}\int d^3r'\;\frac{\exp\left(\pm i\,k|\boldsymbol{r}-\boldsymbol{r}'|\right)}{|\boldsymbol{r}-\boldsymbol{r}'|}\,V(\boldsymbol{r}')\,\psi(\boldsymbol{r}'). \tag{G.15}$$

This result is the desired integral representation of the inhomogenous Schrödinger equation, which has the advantages that the boundary conditions for interpretation as a scattering solution have been built in. It is therefore a good starting point for approximations

The result for $f(k;\theta,\phi)$ is obtained by taking the limit for $r \to \infty$ in the integral equation, in particular

$$|\boldsymbol{r}-\boldsymbol{r}'| = r\sqrt{1 - 2\,\frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{r^2} + \frac{r'^2}{r^2}} \;\approx\; r\left[1 - \frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{r^2} + \ldots\right],$$

$$\frac{\exp\left(\pm i\,k|\boldsymbol{r}-\boldsymbol{r}'|\right)}{|\boldsymbol{r}-\boldsymbol{r}'|} \;\approx\; \frac{e^{i\,kr}}{r}\,\exp\left(i\,\boldsymbol{k}'\cdot\boldsymbol{r}'\right) + \ldots,$$

where $\boldsymbol{k}' \equiv k\hat{\boldsymbol{r}}$. This gives

$$\psi(\boldsymbol{r}) \quad \stackrel{r\to\infty}{\longrightarrow} \quad \exp(i\,\boldsymbol{k}\cdot\boldsymbol{r}) - \frac{e^{i\,kr}}{r}\,\frac{m}{2\pi\,\hbar^2}\int d^3r'\;\exp\left(-i\,\boldsymbol{k}'\cdot\boldsymbol{r}'\right)\,V(\boldsymbol{r}')\,\psi(\boldsymbol{r}'). \tag{G.16}$$

and thus the exact expression is

$$f(k;\theta,\phi) = -\frac{m}{2\pi\,\hbar^2}\int d^3r'\;\exp\left(-i\,\boldsymbol{k}'\cdot\boldsymbol{r}'\right)\,V(\boldsymbol{r}')\,\psi(\boldsymbol{r}'). \tag{G.17}$$

The Born approximation and beyond

The Born approximation is obtained by using perturbation methods, namely to approximate in the above expression $\psi(\boldsymbol{r}') = \exp\left(i\,\boldsymbol{k}\cdot\boldsymbol{r}'\right)$, yielding the result

$$f(k;\theta,\phi) = -\frac{m}{2\pi\,\hbar^2}\int d^3r'\;\exp\left(i\,\boldsymbol{q}\cdot\boldsymbol{r}'\right)\,V(\boldsymbol{r}'), \tag{G.18}$$

where $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$. This gives for the cross section the same result as obtained using Fermi's golden rule.

We can go beyond the first order result by introducing the scattering amplitude T. It is defined by

$$V\psi \equiv T\phi,$$

where ψ is the scattering solution and ϕ the incoming plane wave part of it. One then finds that the integral equation, $V\psi = V\phi + V\,\tilde{G}\,V\psi$ turns into $T\phi = V\phi + V\,\tilde{G}\,T\phi$, i.e. an equation for T,

$$T = V + V\,\tilde{G}\,T, \tag{G.19}$$

the socalled *Lippmann-Schwinger* equation. Here $\tilde{G}$ is the Green's function with factor $-2m/\hbar^2$ absorbed, which is the inverse of $E - H_0$. The exact expression for the scattering amplitude f thus is

$$f(k;\theta,\phi) = -\frac{m}{2\pi\,\hbar^2}\,\langle\boldsymbol{p}'|T|\boldsymbol{p}\rangle. \tag{G.20}$$

The lowest order (Born) result is the first term in the expansion of Eq. G.19,

$$T = V + V\,\tilde{G}\,V + V\,\tilde{G}\,V\,\tilde{G}\,V + \ldots.$$

To judge the validity of the Born approximation one checks if the scattering term in the wave function is small,

$$\frac{m}{2\pi\,\hbar^2}\left|\int d^3r'\;\frac{\exp\left(i\,k|\boldsymbol{r}-\boldsymbol{r}'|\right)}{|\boldsymbol{r}-\boldsymbol{r}'|}\,V(\boldsymbol{r}')\,\psi(\boldsymbol{r}')\right| \ll 1. \tag{G.21}$$

The disturbance of the plane wave is near $r \approx 0$, while for selfconsistency $\psi(\boldsymbol{r})$ should be dominantly plane wave, thus

$$\left|\int d^3r'\;\frac{\exp\left(i\,kr' + i\,\boldsymbol{k}\cdot\boldsymbol{r}'\right)}{r'}\,V(\boldsymbol{r}')\right| \ll \frac{2\pi\,\hbar^2}{m}$$

$$\left|2\pi\int_{-1}^{1} dX\int dr'\;r'\,e^{i\,kr'(1+X)}\,V(r')\right| \ll \frac{2\pi\,\hbar^2}{m},$$

$$\left|\int dr'\;\left(e^{2i\,kr'} - 1\right)V(r')\right| \ll \frac{\hbar^2 k}{m} = \hbar v.$$

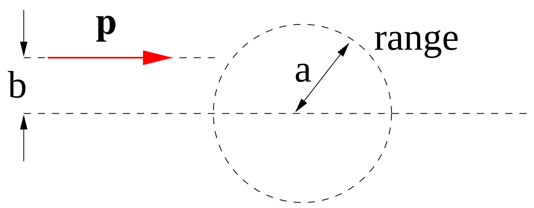
We see two limits in which the Born approximation is applicable

- Weak potentials with a finite range.
  Starting with the second of the above estimates, we see for a potential with average depth V_0 and range a one has after bringing the absolute value under the integral $V_0\, a^2 \ll \hbar^2/m$, i.e.
$$V_0 \ll \frac{\hbar^2}{m\, a^2}, \tag{G.22}$$
  a condition where an approximately equal sign usually is already ok.

- High energies (but nonrelativistic!).
  In the last of the three expressions the exponential is fast-varying for high momenta k and can be neglected, so $V_0\, a \ll \hbar^2\, k/m$, i.e.
$$ka \gg \frac{m\, V_0\, a^2}{\hbar^2} \qquad \text{or} \qquad E \gg \frac{m\, V_0^2\, a^2}{\hbar^2}. \tag{G.23}$$

Partial wave expansion

At low energies a particle scattering off a target with impact parameter b has an angular momentum $\hbar\sqrt{\ell(\ell+1)} = p\, b$,



If the potential has a finite range a the angular momenta that are important correspond to $b \leq a$. From this we obtain $\hbar\ell \leq pa = \hbar ka$ or $\ell \leq ka$. Therefore it is especially at low energies convenient to expand into different partial waves, eigenstates of angular momentum, because the lower partial waves dominate. Also for central potentials, which satisfy $[\boldsymbol{L}, V(r)] = 0$, it is useful to expand in partial waves, since each angular momentum state in that case is a proper scattering solution.

Starting off with the plane wave, we have
$$e^{ikz} = \sum_\ell (2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\cos\theta). \tag{G.24}$$

It only contains the ϕ-independent spherical harmonics, namely $Y_\ell^0(\theta) = \sqrt{(2\ell+1)/4\pi}\, P_\ell(\cos\theta)$. Assuming azimuthal symmetry the scattering amplitude only depends on θ and also can be expanded in Legendre polynomials,
$$f(k;\theta) = \sum_\ell (2\ell+1)\, f_\ell(k)\, P_\ell(\cos\theta). \tag{G.25}$$

Thus one obtains
$$\psi_{sc}(\boldsymbol{r}) \quad \stackrel{r\to\infty}{\longrightarrow} \quad \sum_\ell (2\ell+1)\, P_\ell(\cos\theta)\, i^\ell \underbrace{\left[j_\ell(kr) + (-i)^\ell\, \frac{e^{i\,kr}}{r}\, f_\ell(k) \right]}_{\psi_{sc}^{(\ell)}(r)}. \tag{G.26}$$

Rewriting the scattering wave in the following way,

$$\begin{aligned}\psi_{sc}^{(\ell)}(\boldsymbol{r}) \quad &\stackrel{r\to\infty}{\longrightarrow} \quad \frac{\sin(kr - \ell\pi/2)}{kr} + (-i)^\ell\,\frac{e^{i\,kr}}{r}\,f_\ell(k)\\ &= \quad \frac{1}{2i\,k}\left[-\frac{e^{-i(kr-\ell\pi/2)}}{r} + \frac{e^{i(kr-\ell\pi/2)}}{r}\,(1+2i\,kf_\ell(k))\right],\end{aligned} \tag{G.27}$$

Conservation of flux tells us that the incoming and outgoing fluxes should be equal in magnitude, i.e.

$$1 + 2i\,kf_\ell(k) \equiv e^{2i\,\delta_\ell(k)}, \tag{G.28}$$

where $\delta_\ell(k)$ is called the *phase shift*. Going back and expressing $f_\ell(k)$ in the phase shift one finds

$$f_\ell(k) = \frac{e^{2i\,\delta_\ell(k)} - 1}{2i\,k} = \frac{e^{i\,\delta_\ell(k)}\,\sin\delta_\ell(k)}{k}, \tag{G.29}$$

and

$$\psi_{sc}^{(\ell)}(\boldsymbol{r}) \quad \stackrel{r\to\infty}{\longrightarrow} \quad e^{i\,\delta_\ell(k)}\,\frac{\sin(kr - \ell\pi/2 + \delta_\ell(k))}{kr}. \tag{G.30}$$

Cross sections and partial waves

At this point it is useful to slightly generalize the result of the previous section. If also inelastic scattering is possible a particular ℓ-wave amplitude is parametrized

$$1 + 2i\,kf_\ell(k) \equiv \eta_\ell\,e^{2i\,\delta_\ell(k)}, \tag{G.31}$$

where η_ℓ is called the *elasticity.* One then has for the elastic cross section

$$\frac{d\sigma_{el}}{d\Omega} = |f(k;\theta)|^2 = 4\pi\sum_{\ell,\ell'}\sqrt{(2\ell+1)(2\ell'+1)}\,f_\ell(k)\,f_{\ell'}(k)\,Y_\ell^{0*}(\theta)\,Y_{\ell'}^0(\theta). \tag{G.32}$$

Integrating over angles the orthonormality of the Y_ℓ^m's can be used to get

$$\sigma_{el} = \frac{4\pi}{k^2}\sum_\ell(2\ell+1)\,\sin^2\delta_\ell(k) \tag{G.33}$$

The optical theorem, which relates the forward scattering amplitude to the total cross section gives

$$\sigma_T = \frac{2\pi}{k^2}\sum_\ell(2\ell+1)\,(1-\eta_\ell\,\cos 2\delta_\ell), \tag{G.34}$$

which indeed is identical for purely elastic scattering ($\eta_\ell = 1$). The difference is the inelastic cross section,

$$\sigma_{inel} = \frac{\pi}{k^2}\sum_\ell(2\ell+1)\,(1-\eta_\ell^2). \tag{G.35}$$

Appendix H

kinematics in scattering processes

Phase space

The 1-particle state is denoted $|p\rangle$. It is determined by the energy-momentum four vector $p = (E, \boldsymbol{p})$ which satisfies $p^2 = E^2 - \boldsymbol{p}^2 = m^2$. A physical state has positive energy. The phase space is determined by the weight factors assigned to each state in the summation or integration over states, i.e. the 1-particle phase space is

$$\int \frac{d^3p}{(2\pi)^3\, 2E} = \int \frac{d^4p}{(2\pi)^4}\, \theta(p^0)\, (2\pi)\delta(p^2 - m^2), \tag{H.1}$$

(proven in Chapter 2). This is generalized to the multi-particle phase space

$$d\mathcal{R}(p_1, \ldots, p_n) = \prod_{i=1}^{n} \frac{d^3p_i}{(2\pi)^3\, 2E_i}, \tag{H.2}$$

and the *reduced phase space element* by

$$d\mathcal{R}(s, p_1, \ldots, p_n) = (2\pi)^4\, \delta^4(P - \sum_i p_i)\, d\mathcal{R}(p_1, \ldots, p_n), \tag{H.3}$$

which is useful because the total 4-momentum of the final state usually is fixed by overall momentum conservation. Here s is the invariant mass of the n-particle system, $s = (p_1 + \ldots + p_n)^2$. It is a useful quantity, for instance for determining the threshold energy for the production of a final state $1 + 2 + \ldots + n$. In the CM frame the threshold value for s obviously is

$$s_{\text{threshold}} = \left(\sum_{i=1}^{n} m_i\right)^2. \tag{H.4}$$

For two particle states $|p_a, p_b\rangle$ we start with the four vectors $p_a = (E_a, \boldsymbol{p}_a)$ and $p_b = (E_b, \boldsymbol{p}_b)$ satisfying $p_a^2 = m_a^2$ and $p_b^2 = m_b^2$, and the total momentum four-vector $P = p_a + p_b$. For two particles, the quantity

$$s = P^2 = (p_a + p_b)^2, \tag{H.5}$$

is referred to as the invariant mass squared. Its square root, $\sqrt{s}$ is for obvious reasons known as the center of mass (CM) energy.

To be specific let us consider two frequently used frames. The first is the CM system. In that case

$$p_a = (E_a^{\mathrm{cm}}, \boldsymbol{q}), \tag{H.6}$$

$$p_b = (E_b^{\mathrm{cm}}, -\boldsymbol{q}), \tag{H.7}$$

It is straightforward to prove that the unknowns in this particular system can be expressed in the invariants (m_a, m_b and s). Prove that in the CM system

$$|\boldsymbol{q}| = \sqrt{\frac{(s - m_a^2 - m_b^2)^2 - 4\, m_a^2 m_b^2}{4s}} = \sqrt{\frac{\lambda(s, m_a^2, m_b^2)}{4s}}, \tag{H.8}$$

$$E_a^{\mathrm{cm}} = \frac{s + m_a^2 - m_b^2}{2\sqrt{s}}, \tag{H.9}$$

$$E_b^{\mathrm{cm}} = \frac{s - m_a^2 + m_b^2}{2\sqrt{s}}. \tag{H.10}$$

The function $\lambda(s, m_a^2, m_b^2)$ is a function symmetric in its three arguments, which in the specific case also can be expressed as $\lambda(s, m_a^2, m_b^2) = 4(p_a \cdot p_b)^2 - 4p_a^2\, p_b^2$.

The second frame considered explicitly is the socalled target rest frame in which one of the particles (called the target) is at rest. In that case

$$p_a = (E_a^{\mathrm{trf}}, \boldsymbol{p}_a^{\mathrm{trf}}), \tag{H.11}$$

$$p_b = (m_b, \boldsymbol{0}), \tag{H.12}$$

Also in this case one can express the energy and momentum in the invariants. Prove that

$$E_a^{\mathrm{trf}} = \frac{s - m_a^2 - m_b^2}{2m_b}, \tag{H.13}$$

$$|\boldsymbol{p}_a^{\mathrm{trf}}| = \frac{\sqrt{\lambda(s, m_a^2, m_b^2)}}{2m_b}. \tag{H.14}$$

One can, for instance, use the first relation and the abovementioned threshold value for s to calculate the threshold for a specific n-particle final state in the target rest frame,

$$E_a^{\mathrm{lab}}(\text{threshold}) = \frac{1}{2\, m_b}\left((\sum_i m_i)^2 - m_a^2 - m_b^2\right). \tag{H.15}$$

Explicit calculation of the reduced two-body phase space element gives

$$\begin{aligned}
d\mathcal{R}(s, p_1, p_2) &= \frac{1}{(2\pi)^2}\frac{d^3p_1}{2E_1}\frac{d^3p_2}{2E_2}\delta^4(P - p_1 - p_2) \\
&\overset{CM}{=} \frac{1}{(2\pi)^2}\frac{d^3q}{4\, E_1\, E_2}\delta(\sqrt{s} - E_1 - E_2) \\
&= \frac{1}{(2\pi)^2}\, d\Omega(\hat{q})\frac{\boldsymbol{q}^2\, d|\boldsymbol{q}|}{4\, E_1\, E_2}\delta(\sqrt{s} - E_1 - E_2)
\end{aligned}$$

which using $|\boldsymbol{q}|\, d|\boldsymbol{q}| = E_1\, dE_1 = E_2\, dE_2$ gives

$$\begin{aligned}
d\mathcal{R}(s, p_1, p_2) &= \frac{|\boldsymbol{q}|}{(2\pi)^2}\, d\Omega(\hat{q})\frac{d(E_1 + E_2)}{4(E_1 + E_2)}\delta(\sqrt{s} - E_1 - E_2) \\
&= \frac{|\boldsymbol{q}|}{4\pi\sqrt{s}}\,\frac{d\Omega(\hat{q})}{4\pi} = \frac{\sqrt{\lambda_{12}}}{8\pi\, s}\,\frac{d\Omega(\hat{q})}{4\pi},
\end{aligned} \tag{H.16}$$

where λ_{12} denotes $\lambda(s, m_1^2, m_2^2)$.

Kinematics of 2 → 2 scattering processes

The simplest scattering process is 2 particles in and 2 particles out. Examples appear in

$$\begin{aligned}
\pi^- + p &\rightarrow \pi^- + p && \text{(H.17)}\\
&\rightarrow \pi^0 + n && \text{(H.18)}\\
&\rightarrow \pi^+ + \pi^- + n && \text{(H.19)}\\
&\rightarrow \ldots . && \text{(H.20)}
\end{aligned}$$

The various possibilities are referred to as different reaction channels, where the first is referred to as elastic channel and the set of all other channels as the inelastic channels. Of course there are not only 2-particle channels. The initial state, however, usually is a 2-particle state, while the final state often arises from a series of 2-particle processes combined with the decay of an intermediate particle (resonance).

Consider the process $a+b \rightarrow c+d$. An often used set of invariants are the Mandelstam variables,

$$\begin{aligned}
s &= (p_a + p_b)^2 = (p_c + p_d)^2 && \text{(H.21)}\\
t &= (p_a - p_c)^2 = (p_b - p_d)^2 && \text{(H.22)}\\
u &= (p_a - p_d)^2 = (p_b - p_c)^2 && \text{(H.23)}
\end{aligned}$$

which are not independent as $s + t + u = m_a^2 + m_b^2 + m_c^2 + m_d^2$. The variable s is always larger than the minimal value $(m_a + m_b)^2$. A specific reaction channel starts contributing at the threshold value $s^{thr} = (\sum_i m_i)^2$. Instead of the scattering angle, which for the above $2 \rightarrow 2$ process in the case of azimuthal symmetry is defined as $\hat{\boldsymbol{p}}_a \cdot \hat{\boldsymbol{p}}_c = \cos\theta$ one can use in the CM the invariant

$$t \equiv (p_a - p_c)^2 \stackrel{CM}{=} m_a^2 + m_c^2 - 2\,E_a E_c + 2\,qq'\,\cos\theta^{\text{cm}},$$

with $q = \sqrt{\lambda_{ab}}/2\sqrt{s}$ and $q' = \sqrt{\lambda_{cd}}/2\sqrt{s}$. The minimum and maximum values for t correspond to θ^{cm} being 0 or 180 degrees,

$$\begin{aligned}
t_{min}^{max} &= m_a^2 + m_c^2 - 2\,E_a E_c \pm 2\,qq'\\
&= m_a^2 + m_c^2 - \frac{(s + m_a^2 - m_b^2)(s + m_c^2 - m_d^2)}{2\,s} \pm \frac{\sqrt{\lambda\lambda'}}{2\,s}. && \text{(H.24)}
\end{aligned}$$

Using the relation between t and $\cos\theta^{\text{cm}}$ it is straightforward to express $d\Omega^{\text{cm}}$ in dt, $dt = 2\,qq'\,d\cos\theta^{\text{cm}}$ and obtain for the two-body phase space element

$$\begin{aligned}
d\mathcal{R}(s, p_c, p_d) &= \frac{q'}{4\pi\sqrt{s}}\,\frac{d\Omega^{\text{cm}}}{4\pi} = \frac{\sqrt{\lambda_{cd}}}{8\pi\,s}\,\frac{d\Omega^{\text{pp}}}{4\pi} && \text{(H.25)}\\
&= \frac{dt}{8\pi\,\sqrt{\lambda_{ab}}} = \frac{dt}{16\pi\,q\,\sqrt{s}}. && \text{(H.26)}
\end{aligned}$$