Hyperfinecourse A: the nucleus

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Abstract

This document is meant for optional background reading when studying www.hyperfinecourse.org. It deals with one of the chapters of this course. The formal course content is defined by the website and videos. The present document does not belong to the formal course content. It covers the same topics, but usually with more mathematical background, more physical background and more examples. Feel free to use it, as long as it helps you mastering the course content in the videos. If you prefer studying from the videos only, this is perfectly fine.

The present text has been prepared by Jeffrey De Rycke (student in this course in the year 2018-2019). He started from a partial syllabus written by Stefaan Cottenier for an earlier version of this course, and cleaned, edited and elaborated upon that material. That syllabus was itself inspired by a course taught by Michel Rots at KU Leuven (roughly 1990-1995).

1 Nuclear Properties

This course will focus on the hyperfine splitting of the energy levels of the atoms, alone or incorperated in molecules or solids. A thorough understanding of different properties of the atom, and in particular about the nucleus, is therefore needed. This part will cover a list of certain nuclear properties. The values of different properties can be found at https://www-nds.iaea.org/nuclearmoments/.

1.1 Z, N, and A

These three numbers were probably the first properties you learned about the nucleus. They are the atomic number, the neutron number, and the mass number. They represent the amount of protons (Z), the amount of neutrons (N), and the total amount of nucleons (A) inside the atom. It follows naturally that Z + N = A. The atomic number uniquely identifies a chemical element. Whilst the neutron number will have an effect on the mass(number), the shape, the stability,... of the nucleus. Nuclei with the same atomic number but with a different amount of neutrons are called isotopes. Nuclei with the same neutron number but with a different amount of protons are called isotones. This word was formed by replacing the **p** (for proton) in isotopes with the letter **n** (for neutron). Nuclei with the same mass number are called isobars. A more exotic term is isodiaphers, which are nuclei with equal neutron excess. The neutron excess is defined as the amount of neutrons minus the amount of protons. Lastly, there are isomers. Which are nuclei with same Z and N, but in a different energy state. Not to be confused with the different energy states of the electron cloud. When representing nuclei, one uses the short notation such as "C" for carbon or "Fe" for iron. In the top left, the mass number is depicted. If one were to plot all known nuclei on a N/Z plot, it would look like the figure on the next page. As the amount of Z grows the amount of N also needs to grow to keep the nuclei stable. This is needed to overcome the electromagnetic force between the protons, using the strong force between the nucleons. There are also nuclei which are more stable than one would expect from a first look. These states can be explained via the nuclear shell model. Much like the atomic shell model, it uses the Pauli exclusion principle to order the nucleons and describe the nucleus. When adding nucleons, there are states with clear jumps and falls in the binding energy. These number of protons and neutrons are called magic numbers. It shouldn't come as a surprise that these numbers are 2, 8, 20... Which are the same amount of electrons giving full shells. If both the amount protons and neutrons are magic numbers, one speaks of "double magic numbers". As the total amount of nucleons grows, it becomes harder and harder to find "stable" nuclei. It becomes harder to overcome the electromagnetic repulsion. The most stable nucleus (highest binding energy per nucleon) is Nickel-62. Not to be confused with Iron-56, which has the lowest mass per nucleon. Therefore, fission of elements heavier than Nickel-62 will release energy, whilst one needs fusion of elements lighter than Nickel-62 to release energy. In nature, only elements up to Uranium are found. The lightest elements were created during the Big Bang and the following Big Bang nucleosynthesis. Heavier elements (up to Nickel) can be created via fusion during the latest stages of stars, when the pressure (due to gravity) is high enough to let said fusion take place. Heavier elements are created during events such as supernovae.

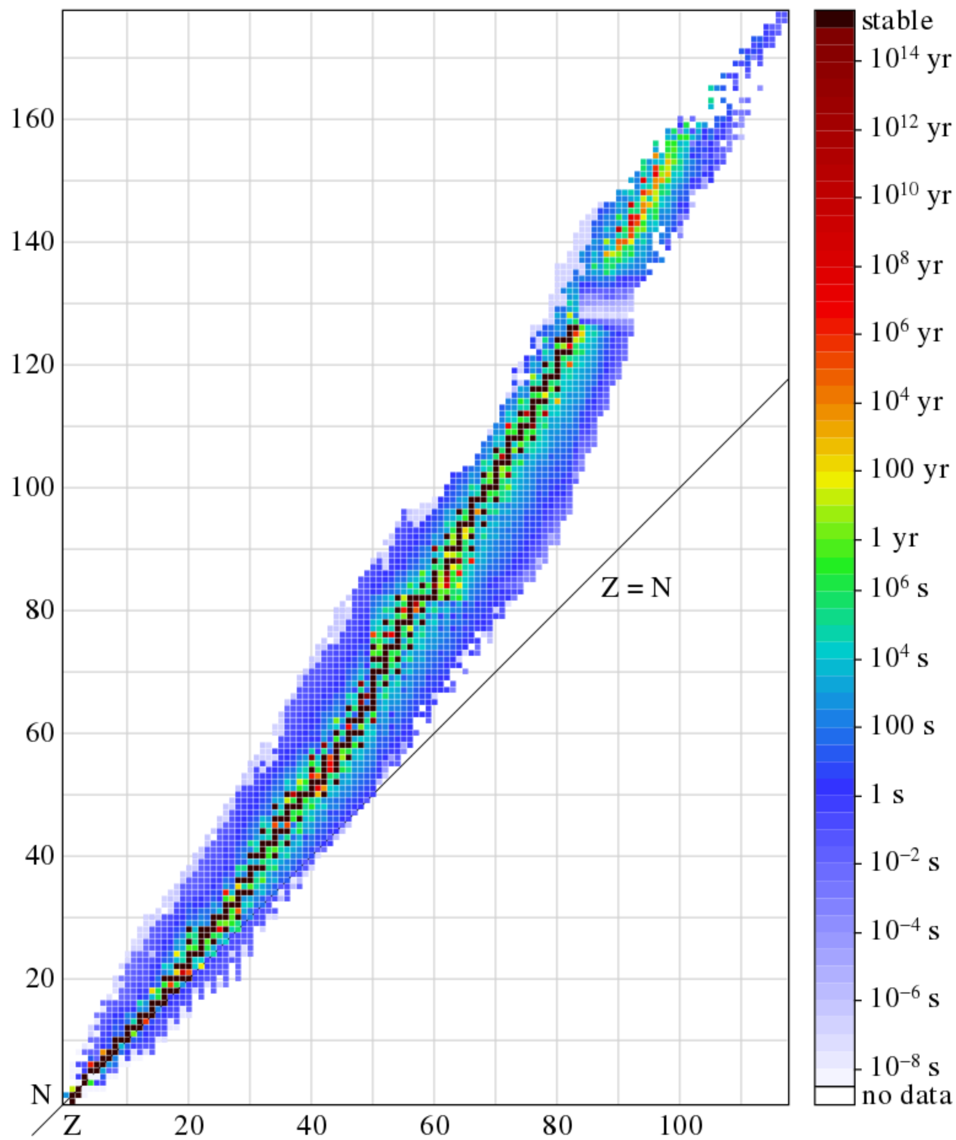

Figure 1: Plot of all known nuclei. N i.f.o. Z.

1.2 Mass

The mass of a proton, as wall as a neutron, is about 1 GeV[1]. The mass of a nucleus is not simply the sum of all nucleon masses. When nucleons come together to form a nucleus, some mass is lost as "binding energy". As discussed before, this binding energy can serve as a measure for how tight the nucleons hold together. To correct for the amount of nucleons, the binding energy is often expressed as binding energy per nucleon. The mass of a nucleus is also often expressed in a.m.u.'s, which is the same as 1 gram per mole. Which is, by definition, 1/12th of the mass of a Carbon-12 atom[2], or $1.66 \cdot 10^{-27} kg$.

1.3 Lifetime

Not all nuclei are stable. Some can decay to other nuclei (or pairs of nuclei). The lifetime can range from yoctoseconds to infinity. But more typical values are femtoseconds to 10^{10} seconds. The experimentally verified lifetime of the proton (Hydrogen nucleus) is, as for now, longer than the age of the universe. It is therefore accepted to be a stable particle. This is needed to conserve baryon number. Some new physics theorems propose proton decay and therefore violation of baryon number. This violation is needed to explain e.g. the matter anti-matter discrepancy in the universe. Observing the decay of a proton would therefore have interesting consequences in our understanding of the universe.

There are different kinds of decay. For example: a neutron can decay to a proton and an electron (and an anti-electronneutrino). Therefore shifting to Z+1 and N-1. This is called beta decay. A proton can decay to a neutron, a positron (and an electronneutrino). This process is called inverse beta decay. This can not be confused with "pure" proton decay. An isolated proton can not decay (as far as we have observed). But when inside a nucleus, the daughter nucleus can have a greater binding energy, therefore allowing said decay. A proton can also absorb an electron, creating a neutron (and an electronneutrino). Therefore shifting to Z-1 and N+1. When this happens, we talk about electron capture. A nucleus can emit an entire Helium nucleus, this is called alpha-decay (and the Helium nucleus an alpha particle). A nucleus can also break apart in other pairs of nuclei, this is certainly true for really heavy elements. Lastly, the internal distribution of protons and neutrons can change, resulting in a configuration with exactly the same particles, yet with a lower overall energy (i.e. a lower energy level). With this process, photons (gamma-rays) are emitted.

[1] In nuclear physics, as well as particle physics, mass is oftentimes expressed in terms of energy. Which can be found via Einstein's energy-mass relation.

[2] Therefore, the masses of the electrons are included.

1.4 Size

The size of a nucleus is in the order of femtometre. Where the proton has a diameter of 1.6 fm, while more heavier atoms such as uranium can have a diameter of 15 fm. The radius (and therefore the diameter) is often defined as the rms (root-mean-square) of the radius.

1.5 Spin and Parity

Two other properties are the spin and parity of a nucleus. The parity is either even or odd. It is a rather quantum mechanical property. When the wave function of the nucleus changes sign upon spatial coordinates reflection, one has odd parity. When the sign stays the same, one has even parity. When representing parity, "+" is used for even parity and "-" for odd parity. A nucleus (in its ground state or excited) always has a well defined parity. This is also true for the parity of the entire wave function of an atom. A well defined parity of a quantum system is not something one usually has. More information regarding the parity of nuclei and atoms can be found at section 5 of https://en.wikipedia.org/wiki/Parity_(physics).

The spin of a nucleus is the resulting effect of the alignment of the spins of the nucleons, and how they orbit around each other. A single proton or neutron has spin 1/2. When combining nucleons into a nuclei, these nucleons will pair together following the shell model. A ground level nucleus with 2 protons and 2 neutrons and no orbital momentum will have spin 0. As the two protons and the two neutrons will be paired up, thus each pair having zero spin. When we only have one proton and one neutron, they will not pair together (we fill the shells separate for protons and neutrons). Thus resulting in a spin 1 particle if the orbital momentum is zero. For ground level nuclei and no orbital momentum, the spins can only be 0, 1/2, or 1. Corresponding to all paired nucleons, 1 unpaired nucleon, or both protons and neutrons being unpaired. When exciting the nucleons, much as in the atomic shell model, more unaligned spins are possible. Therefore resulting in higher nuclear spins. Gaining orbital momentum between the nucleons will also result in a higher nuclear spin. The spin can easily go up to spin 10.

1.6 Deformation Parameter and Magnetic Moment

These are the two new properties which will get much attention in this course. As they are directly related to the hyperfine splitting. The magnetic moment arises from the spin of the nuclei and is often expressed in nuclear magneton units $= \frac{e\hbar}{2m_p} = 5.05 \cdot 10^{-27} J/T$. The value in this unit can range from 0 to about 10. The deformation parameter is used to describe the deviation from spherical symmetry. It is often denoted as β_2 and is directly linked to the electric quadrupole moment. It has unit of Coulomb times square meter, and is often denoted in units $e \cdot 10^{-24}cm^2$. This last surface value is called a "barn", therefore the quadrupole moment is often written as "eb" for electron-barn, sometimes even shortened to simply "b". The value in this unit can range from 0 to about 5, but has been measured as high as 8 (for Lutetium-176). A broader description and use of these parameters will follow in the course of this course.

2 Multipole Moments

2.1 mathematical description

When describing the orbit of a satellite around the Earth, we concentrate all the mass of the sphere inside the centre of the Earth. This gives quite decent solutions within a certain precision, due to the Earth being sort off equal to a sphere[3]. Treating the Earth as a point like particle is the same as treating it as a "gravitational monopole". If one would take said assumed perfectly round Earth and stretch it along one axis, one would need more information to accurately describe the mass distribution. One could introduce a dipole term to accomplish that. The more we deform said distribution of mass, the more terms one would need to describe the mass distribution up to a (self) desired precision. This is precisely how a multipole expansion works. You take a random general distribution of mass or charge, and calculated the multipole terms needed for your calculations, as illustrated in the image below.

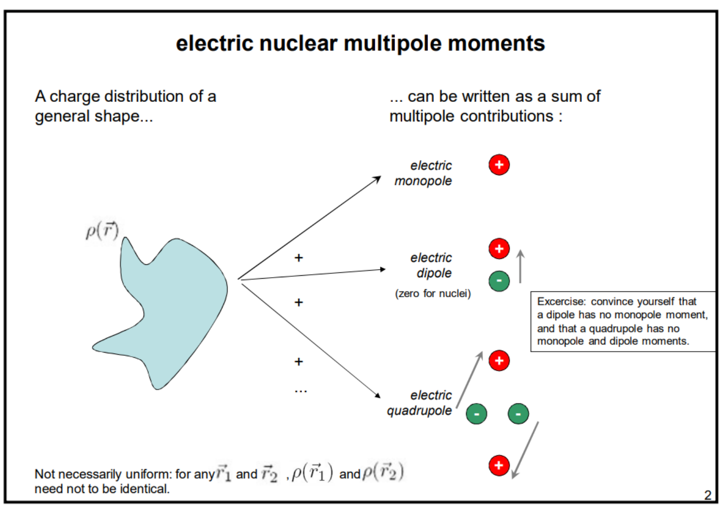

Figure 2: Visual representation of a multipole expansion of a random charge distribution.

[3]For a perfect spheroidal Earth, concentrating all the mass within a point would no longer be an approximation, but would give an exact solution.

If the distribution is really far away or rather spherical symmetric, you might only need the monopole term. If you want more precision on the forces and energy effects, you need a more precise description of the distribution, thus needing more multipole terms.

We all know an electric monopole. The electron, for example, is an electric monopole. A dipole is two monopoles with opposite charge, separated by a certain distance. A quadrupole is two dipoles seperated by a certain distance, and so forth. It is clear that the higher order terms consist of more and more charges, thus closer mimicking the original charge distribution. We will list the first 3 multipole moments: what they are, and how to calculate them.

- The monopole term. This is just one charge. It will translate itself mathematically to the total charge of the distribution, therefore a scalar[4]. It is the same as treating a planet as a point mass. With the change that we can also have negative charges (and no negative masses). Translating this to a formula gives us for a continuous distribution:

$$Q = \int \rho(\mathbf{r}')d\mathbf{r}'$$

And for a discrete distribution:

$$Q = \sum_{i=1}^{i=N} q_i$$

- The dipole term. This is no longer a scalar, but a vector[5]. It has three components k = x, y, z. One for each spatial coordinate. We will need to multiply each charge with the spatial coordinate of said charge. Translating this to a formula gives us for a continuous distribution for one of the three components:

$$Q_k = \int r'_k \rho(\mathbf{r}')d\mathbf{r}'$$

And for a discrete distribution:

$$Q_k = \sum_{i=1}^{i=N} q_i d_{ik}$$

- The quadrupole term. This component has 9 terms, corresponding to all possible matches between x, y, z and x, y, z. This term can not be represented by a vector but needs a 3x3 traceless symmetric matrix. Or, in other words, a tensor of rank two. Again, we let k range from x to y to z. The same goes for l. These formulas may seem rather ad hoc, but

[4]This is the same as a rank-0 tensor.
[5]This is the same as a rank-1 tensor.

they are rather difficult to derive purely from searching for a mathematical analogue to the physical representation. It is best to accept them at face value and try to understand them. The symbol δ_{kl} is called a "Kronecker delta". It is zero when $k \neq l$ and 1 when $k = l$. Due to the fact that it is a traceless symmetric matrix, one can check your answers, making sure $Q_{xx} + Q_{yy} + Q_{zz} = 0$ and $Q_{kl} = Q_{lk}$ for all k's and l's. Translating this to a formula gives us for a continuous distribution for one of the nine components:

$$Q_{kl} = \int (3r'_k r'_l - r'^2 \delta_{kl}) \rho(\mathbf{r}') d\mathbf{r}'$$

And for a discrete distribution:

$$Q_{kl} = \sum_{i=1}^{i=N} (3d_{ik} d_{il} - ||\mathbf{d}_i||^2 \delta_{kl}) q_i$$

Higher order formulas will not be given but can be found via the general expression in spherical coordinates:

$$f(\theta, \phi) = \sum_{0}^{\infty} \sum_{m=-l}^{m=l} C_l^m Y_l^m(\theta, \phi)$$

Where the $Y_l^m(\theta, \phi)$'s are the standard spherical harmonics, and the C_l^m's are coefficients which depend on the function.

2.2 The Nucleus

Let us now apply this knowledge to the nucleus. The electric monopole term of the nucleus will simply be the charge of the nucleus. Representing the nucleus as a point charge. This is the representation that we are used to. When dealing with hyperfine interactions, we no longer represent the nucleus as a point charge, but as an object with a shape and size. Higher order multipole terms are therefore needed. As seen in the course video "Why are odd electric moments zero?", the electric dipole moment does not exist. The electric quadrupole term represents, as discussed before, the deviation from spherical symmetry. You will find the electric quadrupole term as a single number β_2[6]. However, in the future we will see that there will be no contradiction between using this one number, or the 5 components in the rank-2 tensor. Higher terms such as the hexadecapole will be labeled as β_4. It is important to note that the multipole expansion only gives info about the shape of the distribution, not the size of the distribution. For the size, we have the rms of the radius.

The electric quadrupole moment is large when the nucleus is heavy, and when the nucleus is strongly deformed. Explained by needing higher order multipole terms to accurately describe said type of nuclei. The rms of r increases as well with increasing mass.

Until now, we used the multipole expansion to describe a static charge distribution, the same can be done for a static current distribution. The words "static" and "current" might seem as an oxymoron, but just imagine an electron revolving around the same point in space indefinitely. The electron is moving, but the current (the electronloop) stays in the same position. Regarding magnetic multipole terms, the opposite for electric multipole terms is true. The odd terms survive while the even terms vanish. This represents itself e.g. into a magnet splitting into two other magnets when breaking in two. Instead of splitting into a monopole magnetic southpole and a monopole magnetic northpole[7]. The first non-zero term therefore is the magnetic dipole moment. The second non-zero term is the magnetic octopole moment. Which is often more than we need for our hyperfine interactions, but can be used to further accurately describe the energy levels. As said before, the magnetic dipole moment is represented by one number, often in terms of nuclear magnetons. This number is the magnitude of the dipole vector.

[6] It is now clear what this two represents, it is the "second" multipole term. Zero being the monopole term.

[7] Magnetic monopoles are predicted in new advanced theories within particle physics, there is ongoing search for them. So far, none have been found.

2.3 Multipole Radiation

This section will be rather short, as a more in-depth description of the video would soon derail too much.

Classical multipole radiation is created when an oscillating charge distribution is present. To be clear, it is the position of the charges that oscillate, not the charges itself. This would break charge conservation, and one would rather not like breaking physics. The gravitational equivalence of multipole (EM) radiation, are gravitational waves. Just as in gravitational waves, energy is lost from the system when multipole radiation is created. One needs to fed the system energy to let it oscillate and create multipole radiation. An oscillating multipole can therefore not be used to represent a decaying nucleus emitting radiation, as a nucleus is not powered. A nucleus is not an oscillating multipole moment, yet it can still emit multipole radiation. How does this work? Each exited state of the same nucleus can be represented via a multipole expansion, unique to each state. When the nucleus decays, it changes from one multipole to another multipole. This transition between multipoles will be the multipole radiation, and can be unshockingly expressed as a multipole expansion. It is important to note that the nucleus is not allowed to have e.g. an electric dipole moment, but the transition expansion can perfectly have said moment.