VIP1

(automated transcription)

This lecture will be about the general framework behind the concept of hyperfine interactions. We will go first really back to basics, to your first encounters with quantum mechanics. At that time you probably studied the hydrogen atom and a somewhat more complicated atom, the helium atom and so on to real multi-electron atoms. And in doing so, either explicitly or implicitly, you have made some approximations. Let's look at these approximations. I'm quite sure you studied the hydrogen atom in a non-relativistic way. Nowadays, in modern quantum chemistry codes, people can go to any level of relativity you want and for our purpose, the level of relativity will not really be important. So it doesn't matter for us whether we will look relativistically or non-relativistically. If you need it, it can be done. If you studied something that was more complicated than the hydrogen atom, so take helium, then you had a problem, you had to describe the interaction between the two electrons. Electron-electron interaction is absent in hydrogen, is present as soon as you deal with helium. You have introduced methods to deal with this effective electron-electron interaction, probably the Hartree-Fock method. Again in modern quantum chemistry tools, people are using post-Hartree-Fock methods or density functional theory to deal with this electron-electron interaction. Another approximation, which might have been somewhat hidden in your initial course on quantum mechanics, was that you treated the nucleus as an infinitely heavy object. That has one conceptual advantage. You are sure that the nucleus stays at rest. Think about the solar system, you have the sun and the earth, and the solution for their motion is a motion pattern where both evolve around their common center of mass. The same would happen in the hydrogen atom, the nucleus and the electron move around their common center of mass. Unless the nucleus is infinitely heavy, in that case the nucleus will stay at its same position. If you want to drop this approximation, then that's not really complicated, there are classical equations that can take this motion around the common center of mass into account. There is also a quantum aspect to this. An object that is not infinitely heavy can have in quantum mechanics a zero-point motion, and in particular the hydrogen nucleus, which is rather light, might feel this zero-point motion. That is somewhat harder to take into account, but even that can be done. The last approximation which you made is to consider the nucleus as a point nucleus, as really a mathematical point with a given amount of charge. And that is the approximation that we will drop in this course here. In this course we will examine the physics that arises when the nucleus is more than just a point charge. We will drop this last of the four approximations. Let's stick to the hydrogen atom for a while, and let's consider this particular situation which you see at the upper right corner of the screen. You have the hydrogen nucleus, a single proton, at rest, and a single electron at an infinite distance of this nucleus, also at rest. This situation we take as our reference situation, and we give it by convention an energy that is zero. So on this vertical axis here at the left, the dashed line indicates that reference situation. Now I let these two objects, the proton and the electron, come together. And you know what will happen, they will settle down into their most stable configuration, which is the hydrogen atom with the electron in a 1s orbital. That will have an energy that is lower than our reference situation, and the energy difference between that ground state and the reference of electrons and nuclei at infinite distance of each other, that energy is the internal energy of the hydrogen atom, or more generally the internal energy or total energy of my multi-electron atom or of my solid or material. There are many possible solutions in between these two extremes. If you promote the hydrogen electron to a 2p orbital, you have a system with a somewhat higher energy, and you can keep promoting the electron until you reach this infinite distance. That is for the hydrogen atom. You can do the same for more complicated atoms, and here you see a typical diagram from atomic physics, it's a diagram for the sodium atom, where you see the ground state level, here designated as zero, and if you promote electrons you can reach excited solutions. That is exciting electrons inside an atom. Let's now zoom in to the nucleus. The nucleus itself is an object that can be in a ground state or can be excited, and that is something that has been studied in nuclear physics. What you see here at the right is a diagram from a nuclear physics handbook, where you see many possible energy levels of a given nucleus. Mind the energy distance between these levels. This is typically of the order of magnitude of a few kilo electron volts to mega electron volts. And that's quite different from the distance in the atomic diagram, so if we go back to the previous slide to the sodium atom, here you had an energy scale that was in the range of electron volts. So promoting electrons to excited states in an atom takes electron volts, promoting nuclei to a higher excited state requires kilo electron volts to mega electron volts. We can merge these two pictures, so remember the dashed line was the reference state of nuclei and electrons at infinite separation, and here at the lower left of the screen, you see this dashed line again. So for this dashed line, the nucleus was in its ground state, and was at infinite distance from the electrons. If we let them come together, the system settles down in its atomic ground state. If we excite the nucleus to its first excited state, you come at the second dashed level here, which is now the excited nucleus at an infinite distance from the same electrons. Let those interact, and you settle down in a ground state, but with the nucleus in an excited state, and so on. So you can, for every level of the nuclear scheme at the right, you can add this atomic energy levels, which we saw on the previous slide. And that is what we find if we do this in a cartoon-like way. So you have at the left the large energy separations between the nuclear levels, and for each of these nuclear levels, we add electrons, let the system settle down in its ground state, and so we have the atomic energy levels with the typical electron volt energy scale. Let's now look to details. We take one of these energy levels, this one here, and describe the properties of the atom for that situation. That atom might have a total orbital angular momentum L, and a total spin angular momentum S. You have seen in courses on atomic physics or quantum physics before, that the energy of an atom depends on how this L angular momentum is oriented with respect to this S angular momentum, that is the spin-orbit coupling effect. By the effect of spin-orbit coupling, the energy of the system will be slightly different depending on the orientation of L with respect to S, and the energy difference between these different situations will not be of the order of magnitude of electron volts, but rather of the order of magnitude of millielectron volts. That is called the fine structure of an atom. It's usually not represented in terms of L and S separately, but in terms of the total angular momentum J, so every fine structure level corresponds to a different value of the total angular momentum J, but that is nothing else than expressing a different orientation of L with respect to S. Let's look at a specific example to understand this a little bit better. We have again our atomic energy level scheme for the sodium atom, and we will focus on these solutions here which are circled in red, where we have promoted an electron to the 3p orbitals. How do we describe the situation, the electron configuration of the sodium atom after that excitation, that is given by the term symbols that are encircled here at the top, 2p one half and 2p three halves. The p means that this is an L equals one situation, so orbital angular momentum is one. The 2S plus one is two, so that means that the spin angular momentum is one half, and how many orientations can you have for L equals one with respect to S equals one half? The angular momentum rules in quantum physics tell you that every value between L plus S and absolute value of L minus S are possible. So in this case three halves and one halves, so that's the subscript J which you see there. So these two situations have 2p one half, 2p three halves, same spin angular momentum, same orbital angular momentum, but two different values of J, so two different orientations of L with respect to S. And if you watch closely on the diagram you would see indeed that these two energy levels are not completely identical, there is a difference of a few millielectron volts between both. That is the fine structure for in this case the sodium. That is well known in quantum physics, I'm sure you have seen this in your bachelor courses before. That will not be the topic of this course, in this course we will look at even larger detail and we will look to something what is called the hyperfine structure. If we zoom in to one of these fine structure levels and if you watch closely enough with high enough resolution you will see that these levels correspond to several levels again, now with a separation of typically microelectron volts. These are fine structure levels and what is their physical origin? They depend on how the nucleus is oriented with respect to that total electron cloud. The total electron cloud which in one of the fine structure levels has a precise value of J, but now you can orient that J vector with respect to the nucleus and different orientations will give rise to different hyperfine levels. You can wonder how can you orient the electron cloud with respect to the nucleus, if the nucleus is a point there is no way of doing that, but a nucleus is more than a point, a nucleus can have a magnetic moment which gives it a preferential direction in space so it makes sense to ask how is the angular momentum vector J of the electron cloud oriented with respect to the nuclear dipole moment of the nucleus. The nuclear magnetic moment is a vector, the total angular momentum is a vector as well and we will see that this total angular momentum of the electron cloud gives rise to a magnetic field at the position of the nucleus, a magnetic field that is a vector as well. So this energy separation, this hyperfine splitting due to this interaction can be described as a dot product between two vectors. The details will follow later. Similarly a nucleus can have a preferred direction in space due to its shape. If the nucleus is an ellipsoid then again it makes sense to ask how the electron cloud is oriented with respect to this ellipsoid. The ellipsoid property of the nucleus, the deformation of the nucleus is described by the quadrupole moment tensor, a spherical tensor of rank two and the electron cloud with its given angular momentum J will give rise to an electric field that is non-constant at the position of the nucleus, an electric field that has a gradient. That gradient of the electric field is itself a tensor quantity and that will interact with the non-spherical shape of the nucleus. So again these hyperfine structure levels will be described by a dot product between two tensors, two tensors of rank two. The details of this description will again follow later. In this course there will be two VIPs, very important pictures, pictures that summarize a lot about the content of the course and now in this first session we have just constructed the first of these two very important pictures. It's this one, it's repeated here, it's the picture that describes all possible energy scales that arise in discussing atoms or solids. It starts from the kilo electron volt to mega electron volt separation between the nuclear levels. If you zoom into this you see electron volt levels, you see levels separated by typically electron volts which describe the interaction between electrons and this nuclei. If you zoom into this you see that there are details on a millielectron volt scale which is the fine structure and which depends on subtle properties of the electron cloud, spin orbit coupling for instance, and if you zoom into one of these fine structure levels you find the hyperfine structure which depends on how the nucleus, which is not a point like object any longer, how the nucleus is oriented with respect to that electron cloud.