magnetic hyperfine interaction: overlap contribution

(automated transcription)

In some of the previous sessions we have studied the monopole contribution in the charge-charge interaction, and we have noticed that if there is overlap, if the condition R1 smaller than R2 is not fulfilled, that in these situations extra effects can appear. In the present session we will examine exactly the same phenomenon, but now for the dipole term in the current-current interaction. Let us quickly remember what exactly we did for the monopole term in the charge-charge interaction. So we had the regular monopole contribution in the charge-charge interaction, and if there is overlap, if R1 is not always smaller than R2, then we could have first order corrections due to this overlap. And here we see the equation of this first order overlap correction to the energy. It depends on the mean square radius of the nucleus, so this extra contribution vanishes if the nucleus becomes a point where the radius is zero, and it depends on the charge density at the center of the nucleus, the electron charge density at the center of the nucleus, so this contribution vanishes as well if there are no electrons inside the nucleus. This is a correction term, so it is small compared to the regular monopole interaction. Keep these points in mind and we will compare this now to the situation of the magnetic dipole term. What was our perturbing Hamiltonian for the dipole term in the current-current interaction? That was minus mu dot B, mu being the nuclear magnetic moment, B the hyperfine field, the magnetic field created by the electrons at the position of the nucleus. And the regular dipole terms, the ones that appear if you do the multipole expansion with the condition R1 always smaller than R2, these are the ones where the hyperfine field corresponds to the orbital hyperfine field and the spin-dipolar hyperfine field. We didn't mention that explicitly when we discussed these two hyperfine fields, but this is effectively the case. The overlap correction, corrections to this regular dipole contribution when electrons enter the nucleus, these are twofold and one of them we have seen before, that was this Fermi contact contribution. There is an extra hyperfine field when electrons enter the nucleus with the additional condition that the hyperfine field is only there if there is a spin imbalance inside the nucleus, if there are more electrons from one spin type inside the nucleus than electrons from another spin type. In this Fermi contact contribution we immediately see a difference with the overlap contribution to the charge-charge monopole term. This Fermi contact contribution does not vanish if the nucleus becomes a mathematical point. There is no size information of the nucleus in this term, so that's one difference. Another difference is that, as we have seen in the case of BCC iron, this Fermi contact hyperfine field is often the dominant hyperfine field, larger than the orbital and spin-dipolar contributions. So although it is an overlap correction, in magnitude it is more important than the regular dipole contribution. There is another contribution due to overlap that does depend on the size of the nucleus, and that is what is called the Bohr-Weisskopf effect. So let's have a look on what the Bohr-Weisskopf effect really is, and that will be a small contribution. Let's imagine a real nucleus, so a collection of protons and neutrons, and let's try to imagine where does the magnetic moment of this nucleus comes from. The nucleus as a whole has a magnetic moment, but the nucleus is now not a point, it's a distribution of protons and neutrons, protons that have their own intrinsic magnetic moment, neutrons have also their intrinsic magnetic moment, so the sum of these intrinsic magnetic moments will certainly contribute to the magnetic moment of the nucleus, but these charged protons and neutrons, they are also orbiting inside the nucleus that generates currents, and currents generate magnetic moments, so part of the nuclear magnetic moment will also be due to this orbital motions of the neutrons and the protons. That indicates that this magnetic moment of the nucleus is a property that originates from different regions in space. Some volume regions of the nucleus will contribute more to the nuclear magnetic moment than others. That means if we try to express exactly the energy due to the interaction of some magnetic field with the nuclear magnetic moment, if we try to express that exactly, we have to write an integral expression. We have to consider an infinitesimal part of the nucleus, look what is the contribution of that point in space to the nuclear magnetic moment, that will be an infinitesimal part of the nuclear magnetic moment, that will interact with the local value of the magnetic field, and then we have to integrate this expression over the entire nuclear volume to find the total interaction energy. If we now take two isotopes of the same element, these will, in general, have two different magnetic moments, two different nuclear magnetic moments, and these two different magnetic moments will be distributed in, in principle, very different ways over space. Well, let's do an experiment with two such isotopes, we will bring these two nuclei inside an external magnetic field, and only the nuclei, so these are not nuclei part of atoms, these are naked nuclei, stripped of all their electrons. We bring them into an external magnetic field, and that external magnetic field, if it is a homogeneous magnetic field, its value will be the same everywhere inside a nuclear volume. So if we express the magnetic interaction energy between these two nuclear moments and that external field, we can bring the external field outside of the integral, and we have only the integral over d mu, so we find the total magnetic moment. If we now could measure this interaction energy, and we see in the second half of this course methods, experimental methods to do so, so we can measure that energy, so if we measure that energy for the first isotope, and we measure that energy for the second isotope, and we make the ratio of these two energies, then this ratio will be exactly identical to the ratio of the two nuclear magnetic moments, because the external magnetic field that is present in both cases will cancel if we make that ratio. Now we repeat that experiment, but instead of bringing these two isotopes in an external magnetic field, we bring them in the same atom, so we give the same number of electrons to both of these nuclei, these electrons will generate a magnetic hyperfine field, and we measure the interaction energy between these nuclear magnetic moments and the hyperfine field. If we do that, then we cannot guarantee at all that these hyperfine fields will have exactly the same values at every point in the two nuclei. So we cannot take the hyperfine fields out of the integration. If we would know how the hyperfine field depends on space, we can work out the first integral, we can work out the second integral, and make the ratio, and this ratio will be very close to the ratio of the nuclear magnetic moments, but will not be exactly identical to that ratio. The difference between both can be expressed as some multiplication factor 1 plus a small number, and that is what we call the Bohr-Weisskopf effect. The Bohr-Weisskopf effect means that this second ratio here is not exactly identical to that first ratio here. The deviation between these two ratios, this quantity delta, is called the hyperfine anomaly. And this is often a very small number, it's in the range of at most a few percent. So the fact that it is small means that what we have discussed here is a small effect, but it is definitely there and can be experimentally observed. So if we go back to our overview slide, we can summarize that we have seen the regular dipole contribution, where the hyperfine field is generated by the orbital and the spin-dipolar contributions, and then corrections due to electrons that enter the nucleus. One correction that in many cases is actually the dominant contribution, and that does not depend on the size of the nucleus, it only depends on the spin imbalance inside the nucleus, and a second correction, the Bohr-Weisskopf effect, that does depend on the size of the nucleus. And one would vanish if the nucleus becomes a point.