the monopole shift

(automated transcription)

The first multipole correction that we will explicitly examine is something which we will call the electric monopole shift. Where does it fit in the table we saw in a previous session? Let's first look at a situation which you knew already, which is the interaction here in the upper left corner, the interaction between the monopole moment of a nucleus and the electric potential due to the electrons at the position of the nucleus. Just to fix the ideas, let's see what this expression would be for the well-known case of the hydrogen atom. We have to write the monopole moment of the hydrogen nucleus, and I just literally fill out the general expressions we have seen before, and we find that the monopole moment of the hydrogen nucleus is the charge of the nucleus, it would be with z equals one. The monopole field, I fill out the general expression, and what does appear in the last line? That is the electric potential due to the electron distribution, and at which point do you want to know this electric potential? Well this is the electric potential at the position of the nucleus. So how do you find then the monopole energy? You make the dot product between this monopole moment and monopole field, and in this case both are scalars, so the dot product becomes a normal product, and this is then finally the electrostatic energy of a point nucleus interacting with an electron distribution. If this would be for hydrogen, you would have in this way for the different electron states, you would have the different energy levels of the non-relativistic hydrogen atom. What we stressed in the gravitational example was what changes to this picture if the nucleus gets a different shape, in particular if the nucleus deviates from spherical symmetry. That would mean going down in this list. That will be a topic for next sessions, today we will concentrate on what will change if the condition which we could apply, that all nuclear coordinates are smaller than all the electron coordinates, if this condition is not fulfilled any longer. So that means staying on the monopole line in the matrix, but going to the right. So that is what we call in general terms the influence of overlap. The electron charge distribution and nuclear charge distributions will be allowed to overlap in some sense, and these overlap contributions are series expansions themselves, so you can describe them as a first order overlap contribution, second order overlap contribution, and we will not really use the term overlap contribution, but rather the term shift. So you will have a first order monopole shift, first order quadrupole shift, first order hexadecapole shift, the latter one is way too small, we will not discuss them, second order monopole shift, second order quadrupole shift, which is very small again, will not be discussed. So how does this first order monopole shift look like? This is again the expression for a general atom, some terms that come from the nucleus and the kinetic energy of the electrons, and then something that depends on the monopole moment of the nucleus, E times Z, multiplied by the potential due to the electron cloud at the position of the nucleus. That is the regular monopole term. In the gravitational example we saw that if we use this Taylor expansion, solving the multipole expansion in a Cartesian approach, then we could identify a term that was due to this overlap, and that term was actually that first order monopole shift. We will not re-derive it here, just remember how it looked like, so we had some constants multiplied by the mass density of mass distribution 2 at the origin of the axis system, which means at the center of mass of mass distribution 1, and this multiplied with something as the mean square radius of mass distribution 1. If we would translate this expression for the gravitational problem into operators in order to apply it to a quantum situation, then we have identified the term we need. So we have to wonder what is the operator that would give us the charge density of the electron cloud at the center of the nucleus. You after some thinking you will realize that you can express this in this way. You take the electron wave function, and now take the matrix element of this wave function with a Dirac delta operator at the origin. So this operator will take out from this integral, from this dot product, only the contribution at the origin at the center of mass of the nucleus. So that's a straightforward operator translation of this classical property. For the mean square radius of the nucleus it is even more straightforward, so the charge density of the nucleus you can write as wave function complex conjugated times the wave function, and with the R square operator in between. So this is this diagonal matrix element. So our perturbing Hamiltonian for the monopole shift, for the first order monopole shift will be this delta operator times the R squared operator. And this has to be evaluated in the eigenfunctions of the unperturbed system. So that would lead to this energy correction, so this third term is an energy correction due to the overlap between nuclear and electron charge distributions. It's useful to ponder the structure of this term for a while. So this second term here, the regular monopole interaction, you could write it as Q tilde, and I temporarily use this symbol Q tilde as the monopole moment of the nucleus, so E times Z, multiplied by whatever is left, and if you inspect the dimensions you will recognize what we had before, the potential at the position of the nucleus due to the electron cloud. Well this correction term, the first order monopole shift, you could force it in the same structure, you could isolate the monopole moment of the nucleus, Q tilde, multiplied by everything else, and this must have, again, the dimensions of a potential. This is an extra contribution to the electric potential at the position of the nucleus. But whereas the monopole field depends entirely on the properties of the electron cloud, in these brackets here there is nothing that does not depend on the electrons, whereas this term depends only on the electron cloud, this additional potential at the position of the nucleus depends on properties of the electron cloud, namely how many electrons are present in the center of the nucleus, but also on a property of the nucleus, the mean square radius of the nucleus. So it's a potential that is nucleus dependent and electron dependent. When does this potential disappear, so when do we not see the presence of this additional interaction, well when there are no electrons inside the nucleus, so when this rho e is zero or when the nucleus is exactly a mathematical point and not something spherical with an average radius. Are there electrons inside the nucleus, because if that isn't the case then we don't have to care about that term at all. In order to examine that, let us go back to the hydrogen atom. If you go to this link here at the top, you would find the mathematical expressions for the radial part of the different eigenstates of the hydrogen atom. What we will need is the difference between the S functions, radial part of the S functions and anything else, and that has been summarized in this picture here. So the radial part of in this case a 2S wavefunction of hydrogen is drawn in red, the radial part of a 2P wavefunction of hydrogen is drawn in blue. The horizontal axis starts at the left at zero, which is the center of the nucleus and goes up to infinity. And what do you see, the S wavefunctions and only the S wavefunctions will have a non-zero value at the origin of the nucleus. At least in a non-relativistic picture, if you would solve the hydrogen atom relativistically, then you would see that a particular kind of p-electrons, the p-one-half electrons with relativistic quantum number kappa being one-half, these p-electrons also have a non-zero probability to be inside the nucleus. But even in the relativistic picture, nothing more than the S and the p-one-half electrons. Anyway there are electrons that can be inside the nuclear volume, so these will give rise to such a first order electric monopole shift. That electric monopole shift is always positive, if you inspect the expressions you have a minus sign in the expression, but the charge density of the electrons is negative as well, so that gives a positive contribution. And this positive contribution will depend first of all on how many electrons are inside the nucleus, and second on the radius of the nucleus. And the latter gives you a first way to see where this can be experimentally detected. Imagine that you have two isotopes of the same element, so an additional neutron in one of the isotopes, that will modify the average radius of the nucleus. So in one of the isotopes, the radius of the nucleus will be larger than in the other isotope. So that will influence this first order electric monopole shift. The energy levels, the atomic energy levels of two different isotopes of the same element will not be exactly identical. An example of this effect is shown in this diagram here for the lithium atom, where you see the energy levels for lithium 6 compared to lithium 7, and compared to a hypothetical lithium atom with a nucleus that has an infinite mass. We need to distinguish two effects here, because remember the infinite mass of the nucleus was one of the approximations you made in the very beginning, and I said that we wouldn't drop that approximation explicitly, because if we would need to do so, then there was a straightforward classical correction that we could apply to take the finite mass of the nucleus into account. Well this classical correction is present in this picture, part of the reason why the energy levels of lithium 6, 7 and infinity are different is due to that finite mass correction. But another part of the reason of the difference is the difference in radius between lithium 6 and lithium 7. So part of the reason why all these energy levels in these three isotopes are different is due to the first order electric monopole shift. The first order electric monopole shift is experimentally quite easy to determine, and some of the nuclear methods that we will meet in the second half of this course will explicitly measure this. It will turn out to be a very useful property to identify positions in crystals. In a few very exotic cases that we will never meet in practice, one can even see the presence of this second order monopole shift, that is always many many times smaller than the first order monopole shift. How can you see that it is smaller? Well the first order monopole shift depends on the square of the nuclear radius, which is the square of a very small number, while the second order monopole shift depends on the fourth power of the same very small number, so it will be many orders of magnitude smaller in general. But there are a few exotic cases, like the case of muonic atoms, where you can detect the presence of this term. So what is a muonic atom? It's an artificially constructed atom, where one of the electrons of the atom is replaced by a muon, a muon that has more or less the same properties of the electron, except for the fact that its mass is 200 times heavier than the electron. That will bring the muon much closer to the nucleus than the electron is, and therefore the probability to find the muon inside the nucleus will be also much larger than it is for the electron. So that will give rise to a much much larger value for the first order monopole contribution, for the first order monopole shift, and as a result also the second order monopole shift will be larger and will be detectable. Now muonic atoms have been produced in the 60s, nowadays I don't think there are facilities anymore available where this can be produced again, but the effect is there and has been observed.