webinar 3: the framework

(automated transcription)

With this we have started the feedback webinar on what I call the framework and that is the general context in which hyperfine interactions fit, so a kind of map you can use to navigate to the concept of hyperfine interactions. But before tackling this I want to go back to last week because I noticed after the webinar that I missed a few of your questions and yeah the questions are very important so therefore let's make some time in this webinar to answer a few of the questions of last week. And two of these questions, maybe this was the same person asking the question in two different ways, was about that nuclear wave function that was a few times mentioned. So where does that come from? And well here I want to draw a parallel to the electron wave function and the nuclear wave function. So what is the electron wave function? It's a probability distribution that tells you where it is most likely to find an electron. That can be anywhere in the atom but some places in the atom are more likely for the electron than other places. You can find that electron wave function as a solution of the Schrodinger equation which is a Hamiltonian equation where you have the kinetic energy of the electrons and the potential energy, the way how it interacts with sources of electric potential in its environment. And the first place of sources of electric potential are the nuclei that are present and the other electrons. It's exactly the same for the nucleus if you look at it from the point of view of nucleons, so neutrons and protons. You can wonder, and this is a question from nuclear physics, you can wonder if you have a collection of neutrons and protons, how will these interact? They interact via the Coulomb interaction but also and mainly via the strong force. So imagine that you could write down a Hamiltonian that describes the Coulomb interaction and the strong interaction between neutrons and protons. This would give a Schrodinger-like equation and you could try to solve that and you find the nuclear wave function. That gives you the probability where in the nucleus you find a proton or a neutron. You can have such one particle nuclear wave functions that give you the probability to find one of these particles, but just as for an atom you can also have the overall, the many-body nuclear wave function that describes the nucleus as a whole. And then it gives you the probability where you can find any of the neutrons and protons. So in nuclear physics, in principle, people can find that nuclear wave function that gives you all the properties of a nucleus just as the electron wave function or the atomic wave function can give you all the properties of a collection of electrons. In practice it is not so easy to get that nuclear wave function because in contrast to the electron problem we don't know the Hamiltonian because we don't know exactly how the strong force looks like. So if you cannot even write down the Hamiltonian, how can you hope to solve it? Nuclear physics can do that with some approximations, but anyway that's the concept of the nuclear wave function. So I hope this clarifies this concept a bit. So still about last week somebody asked this multipole radiation concept. Is that only for gamma radiation or does it also apply to other types of radiations, namely alpha radiation, beta radiation? It's something that is purely for gamma. Alpha and beta, these are particles, emitted particles. Gamma radiation that's emitted photons, so electromagnetic waves, and the concept of multipole radiation that's valid for electromagnetic waves. The next question is one that was asked this week, but that I can relate to a topic of last week. So I put it here. Somebody asked, and I find this a very interesting question, I first learned of the concept moment as force times distance. And I have to clarify here for the people who don't speak Dutch, this is the concept that is called in English torque. In Dutch this is something that sounds as force moment. So torque is indeed a force times a distance. And so the one who asked this question was wondering, is there a relation between moment as in torque and electric moments? And I can see some similarities because in electric moments you have a charge distribution and distances that are multiplied. But for force, how to connect that to force? Well I don't know the answer to this for sure, but I thought about it and I have a hypothesis. So the word moment comes from the Latin word for motion. So moment in physics very often refers to

something that affects motion. Motion is one of the first properties that physics has studied historically, so not surprising that a lot of our concepts refer to motion. So you have torque, force moment, that is something that affects the rotation of an object, so rotational motion. You have the moment of inertia, there in English as well as in Dutch the word moment is used. That is mass times distance squared and that is resistance against rotational motion. You have linear momentum, same origin, angular momentum, obviously related to motion. How can we relate a dipole moment to motion? A dipole is neutral, it has as many positive charges as negative charges. So you would expect if you put a neutral object in an electric field, then nothing happens. And people noticed in the early days of electromagnetism that if you put something that is neutral but that has what we call now a dipole moment in an electric field, I try to visualize it with my hands, a positive charge and a negative charge, you put them in an electric field, you calculate the forces on the positive and the negative charge, you will see that the forces are opposite and there is the tendency to bring the dipole parallel to the field and if there is no friction it will overshoot and you will get this kind of oscillating motion, there I use the word motion, this oscillating motion in an external field. So a neutral particle that has no dipole moment will not move in an electric field and a neutral particle that has a dipole moment will have this characteristic oscillating motion. And something with a quadrupole moment will oscillate in yet a different way and so on. So these multiple moments, they express how particles that have these moments will oscillate in some external field. That is my hypothesis how the word moment appears here. So there is no deep mathematical connection between these different types of moments, these different things called moments, but they have a historical common root in the sense that they are describing different aspects of moving objects. How can I relate that to something you worked on in the first week? Well there is an extra interpretation possible of this dipole moment vector for configurations of charges, something I didn't point to last week. So I bring you back to the rectangle of four charges that we had last week and we calculated there or you calculated the dipole moment vector and we noticed that this is depending on the choice of the axis system. So if you had, and I switch on the pointer, if you had this rectangle with the origin of the axis system here, we find this vector as the dipole moment vector and if we took the origin of the axis system here in the center, we had the zero vector as the dipole moment vector. Well if you now divide these vectors by the monopole moment, so to have a kind of normalized monopole moment, obviously nothing will change here for the second case, we had already the zero vector, if you divide every component by the monopole moment 4q, nothing changes, but if you do that here, you get a over 2 times x and a times y, so a over 2 times x and a times y. So let me do that, this was the length a, a over 2 is here, and this length is 2a, so a is here half way, where do I end up? Exactly in the middle of this charge distribution. So these normalized dipole moment vectors, they point to exactly the same point in space. There is information in this, this is the position of the center of charge of this charge distribution, or if these would be masses, that would be the position of the center of mass, and that gives another view on why such a charge distribution has no dipole moment If you choose the origin at the center of charge, you can do that for every charge distribution, so you can always find an axis system in which there is no dipole moment vector, or in which the dipole moment vector is zero. So something triggered by that previous question I find is a useful insight. Okay, with this we are fully into the topic of the present week, and we start with this very important picture number 1, which you see repeated here, a summary of all the different ranges of energy splittings, with their own physical interpretation, and somebody asked a question here about that picture, wondering whether, well apparently this picture reminded this person to the difference between body centered and face centered crystal structures at different temperatures of steel, and if that is similar to that picture, is that related to this changing energy levels of nuclei. For those who do not have a material science background, let me show here part of the phase diagram of steel, in this case pure iron, it's a temperature pressure phase diagram, so we have to look just at the left hand side where you have the ambient pressure, and there you see at low temperature iron has the BCC crystal structure, if you increase the temperature it becomes FCC, if you increase it again it turns into BCC again, and if you then keep increasing the temperature it melts. So is that related to

these energy splittings in the very important picture number 1? No, not at all, because the energies that are involved in this thermal excitation that induces changes in the crystal structure, that's not at all at the scale where we have the hyperfine interactions, you will see that in the next slides in a different way. These phase transformations here are due to the electron system, the electron system organizes itself in a different way and that leads to different crystal structures being energetically more favorable at given temperatures, nothing to do with the nuclei. I asked you about that very important picture number 1 to reason a bit about this, namely to understand the scales, because that picture as we draw it is not to scale, and I asked you if you would imagine that the hyperfine splitting at the right hand side is 5 millimeters on the picture, how large would you have to draw the left hand side? This is just playing with some orders of magnitude, so if you start from 5 millimeters at the right hand side, you can realize that a nuclear transition at the left hand side that is of the order of kilo electron volts, that you would need to draw a separation between the levels of 5000 kilometers, which is roughly the radius of the earth, so really this picture is not to scale. If you would need a nuclear transition of mega electron volts, then you have 10 times the distance between the earth and the moon. If you want to have a visual picture how small hyperfine interactions are, then look at the moon, realize how long the distance is between you and the moon, then look at a fingernail, which with some approximation is maybe 5 millimeters in width, and then compare the width of your fingernail with the distance to the moon, and there you have the relative difference between hyperfine interactions and nuclear transitions. Hyperfine interactions are really, really, really small. So that relates to the confidence question, I can list the different energy scales in a system of electrons and nuclei, and I can relate them to the relevant physical processes. So at the left hand side, nucleus-nucleus, nucleon-nucleon interaction that gives rise to the nuclear transitions, then you have the, at the nucleus, electron interactions that can give rise to the energy levels in the atom, then the fine structure, which is related to spin-orbit coupling, relativistic effects, we will come to that, and then the hyperfine interaction, which is related to the shape of the nucleus. I gave you the suggestion to put that very important picture number 1 somewhere at a place where you can often see it, in order to let that message sink in, because it's really an important message for this course. And I also invited you to send me a picture where you have put it. I received this year only one picture, where there is not much detail visible, but according to the description, this is the door of the study room, and you see the very important picture number 1 every time you open and close the door of your room. So, you will meet it many times a day. In previous years I received similar pictures, so this may be a door as well, there are people who have put it as the background of their laptop, that also helps of course, or as an easy clickable file on your laptop, such that you can open it at any time, or in the kitchen above the hood, also that is a place where you come often. And my favorite is this picture, this was a student with a young baby, and what is the place you visit most often as a parent with a young baby, that's the diaper changing room, or the diaper changing place, so that very important picture number 1 was put there, framed even, just above the diaper changing place. That was really a nice view. So wherever you put it, be sure to have it around, and for the next few weeks look at that picture every now and then, actively go through the different steps, and then hyperfine interactions, the concept of hyperfine interactions will be firmly planted in your mind, in order to never forget it. Well let's visit a few places of that very important picture number 1, and maybe I should first look at the chat to see if there is some question there, not yet. So let's look at a few places in this picture, and first of all we will look not yet at the hyperfine place, but the fine structure place, so the impact of relativity, and we do that because some of the reasonings that are relevant for fine structure can be copied later on to hyperfine structure. So by going through the fine structure reasoning that you may have seen in previous courses before, by going through the fine structure reasoning, we can remind ourselves about things that we will soon need in the next 1-2 weeks for hyperfine structures. And the question I asked you about the fine structure, mainly the spin-orbit coupling, which is the reason for the fine structure splitting, and what I asked you about is spin-orbit coupling, that is often said to be a relativistic effect. How can we understand that this is a relativistic effect? And a few answers you have given are listed here, and

these are answers that I would say are not really correct. These are answers that refer to the speed of the electrons, so how fast an electron is moving in the atom, and this leads to the spin-orbit coupling. It's not totally unrelated, but I would claim that speed is not the major reason for spin-orbit coupling. We have to search for relativity in a different way, or in a different place. And one reason why spin-orbit coupling can be said to be a relativistic effect is because it is a spontaneous consequence of the Dirac equation. What is the Dirac equation? I mentioned before the Schrodinger equation, which is the equation that gives you the wave function from which you know everything about your electron system. That Schrodinger equation, if we write it down in the original way, it does not know about spin, it does not know about relativistic effects, and it does not know about spin-orbit coupling, which is a relativistic effect. However, the Schrodinger equation can be mathematically upgraded in a rather easy way by adding spin to it. So this is not something that spontaneously follows from first principles, it's something you have to manually add. You can say I will use the Schrodinger equation not for one type of electrons, but for two types of electrons that have that property spin, spin up, spin down, and I will solve my Schrodinger equation under that assumption. It still doesn't have relativistic effects in this way, but one of these relativistic effects, spin-orbit coupling, can be added to the Schrodinger equation by perturbation theory. Again, a manual operation, it doesn't follow spontaneously, but you can choose to do it this way and such a Schrodinger equation with spin and spin-orbit coupling added, that gives a better description of your electron system. If however you would not have started from the Schrodinger equation, but from the Dirac equation, then all of these features are spontaneously present. The Dirac equation knows about spin intrinsically, it has spin-orbit coupling intrinsically, and all relativistic effects you can imagine are spontaneously contained in the Dirac equation. So therefore the splitting that is due to spin-orbit coupling, as you find it spontaneously from the Dirac equation, you can say this is a relativistic effect, spin-orbit coupling is a relativistic effect. The second argument by which you can say that spin-orbit coupling is a relativistic effect is that it is related to the Lorentz transformations. I read one sentence from this answer here, the transformation of the electric field in a magnetic field uses the Lorentz transformations. So I will not read the entire answer, let's go through a quick reasoning to see how this fits in. So quick reminder, what was the Lorentz transformation? It's something that solves a fundamental problem in electromagnetism. Imagine that you have an electric charge and a magnet next to each other in a moving train. For a passenger in the train, the charge is at rest, the magnet is at rest, so they don't interact with each other, a magnet does not interact with a static charge. But for an observer outside the train, who sees the train passing, that charge is moving, so that's a current, and then you have a magnet next to a current, so the magnet should feel something. How can you, these two things seem, it seems impossible that they are simultaneously true, either the magnet is interacting with the charge or is not interacting, but both people see it in a different way. So this can be reconciled by realizing that one observer is moving, the other is not, so you have two inertial systems from which you describe the same physics, and to transform one inertial system into another one, if they are at different speeds, you need the Lorentz transformation, and the Lorentz transformation changes what we call electricity and magnetism. Some features we call electric in one reference frame become magnetic in another reference frame and the other way around. And this relates to spin-orbit coupling, so for spin-orbit coupling we have an electron that is orbiting around a nucleus, we describe the motion of the electron by the orbital angular momentum, capital L, in a classical view, in a planetary approach to an atom, and this would be really the angular momentum vector that is perpendicular to the plane in which the planet orbits the sun, so we can mathematically represent this by a vector property. That electron also has spin, which is an intrinsic angular momentum, and that can be represented by a bar magnet, and what spin-orbit coupling tries to express is whether that bar magnet is oriented, well, how that bar magnet is oriented with respect to the orbital angular momentum vector. Is it parallel, anti-parallel, or something in between? And how does the Lorentz transformation enter? If you look from the point of view of the electron, then for an observer at the electron it appears to be the nucleus that is orbiting the electron, just as for us on earth it looks

like the sun is orbiting the earth, but then that nucleus is a moving charge and it generates a magnetic field, so there you can see, you can feel already that what we call a static nucleus may be a source of magnetism, and the Lorentz transformation describes more precisely how, from the point of view of the electron, that magnetism due to the orbit of the electron around the nucleus is felt. When is that effect, when is that magnetic field, or when is that interaction between the electron spin and that magnetic field due to the nucleus, when is that important? First of all, the electron should have a spin, that's true, and if the electron orbits fast around the nucleus, and therefore if the nucleus orbits fast around the electron, then that current will be larger, that magnetic field will be larger, so you expect that the faster the electron is orbiting, the stronger this effect will be, so therefore in heavy atoms where the orbital speed of the electrons become larger, for uranium the inner electrons are moving close to the speed of light around the nucleus, so for heavy electrons you expect that spin-orbit coupling will become more important. Did I say heavy electrons? No, I meant heavy atoms. So unlike what I said in the beginning, speed is not the reason, no, it's not the main reason, but indirectly due to the high speed you will see spin-orbit coupling more prominently present in heavy atoms. We saw an example, an observable example of spin-orbit coupling, and that was in the context of the orange light from the sodium lamp. I asked you to search some information about that, and here I copy-paste two of the answers you have given, so I will not read them, I just put them here on the screen, if you want to read them you can later look back at the video. This is a picture that represents what is happening, a sodium lamp emits orange light, which is a transition from an excited p-state to the ground s-state, but if you look closely you will see that these are two different types of orange light with a slightly different wave function, and that is because these are emitted by two of these levels that are split by spin-orbit coupling, with order of magnitude spin-orbit coupling, millielectron volts, so the frequencies will be quite close together, but they are observable. I said spin-orbit coupling, that expresses how the spin is oriented with respect to the orbital angular momentum, so let's illustrate that by wondering, in that lower of these two levels, how is the spin oriented, parallel, anti-parallel, or in-between with respect to the orbital angular momentum. In order to reason about that, we need term symbols, and I asked you about this in the confidence statements, I can explain how term symbols for the state of a free atom are constructed, there is some hesitation about that, so I will go through one example step by step, and then we will use that to answer the question, how is the orientation of spin with respect to orbital angular momentum for this particular state in the sodium atom. So sodium is at the left-hand side of the periodic table, it has one electron outside the noble gas configuration, so in the ground state that electron will be in an s-orbital. We need to construct these so-called term symbols, and these, well the general definition is given there, we need to know the spin angular momentum s for the entire atom, and we find that by summing over the ms quantum numbers for the individual electrons. We have only one electron here, it's a spin 1.5 electron, so the ms is 1.5 as well, we have to sum them, but there is only one electron, so s is 1.5, so twice 1.5 plus 1, that's 2. Wherever that electron is, in which orbital it is, it doesn't matter, the upper index of that term symbol will be 2, meaning we have 1.5, spin 1.5. The x, that is a character that expresses the orbital angular momentum of the entire atom, which means you have to make a sum over the ml quantum number. We have only one electron here, so if it is in an s-orbital, then the ml will be 0 necessarily, and that, so the total l is 0, and we note that by a capital S. If it is in a p-orbital, then it can be in an ml 1 0 or minus 1, so you have to apply Hund's rules to find out in which one, maximal l, so it will be in l equals 1, we note that by a p. If it would be in a d-orbital, that character would be 2, sorry, would be d. So we have, for this case, we have, if the electron is in the ground state, that x will be s, if it is in the excited state, where it is in a p-orbital, that x will be l. So l equals 0, that's the ground state, l equals 1, that's that excited state. So we had already s 1.5, sl is 1, and now we come to the j, the lower index, and j can have values ranging from the absolute value of l minus s, so 1 minus 1.5, that's 1.5, to l plus s, that's 3.5. So in steps of 1, so j can be 1.5 or 3.5. And j expresses the mutual orientation of spin and orbital angular momentum, that's the spin-orbit coupling. If in one extreme, l and s are pointing in opposite directions, so that's the minimal value of j, if they are

parallel, you have the maximal value of j, and everything in between. So for these three levels here, the turn symbols are 2s 1.5, 2p 1.5, 2p 3.5. So you see that in the lower level, that's Hundsterdroom, if you have seen this in previous courses, in the lower level the j is minimal, and that means that l and s in that level are anti-parallel. So for that level here, it's option C that applies, l and s are anti-parallel. So if you haven't seen this before, then this was quite fast, but I hope you see the overall reasoning, and we will use that same overall reasoning in two weeks when we will discuss the magnetic hyperfine structure. There will be quite some similarities between that and the reasoning for fine structure. If you have seen this before, then I hope this was just a quick reminder, a refresher of the spin-orbit coupling reasoning, and turn symbols, and everything. Some further pictures about the sodium lamp, so this is a spectrogram where you can see the two individual lines, and you can do these experiments where you take a pickled cucumber and you put some voltage about it, and in the salted vinegar that you have in the cucumber there are these sodium ions, and you can let them emit this orange light. And that's the same orange light you have in the old type of highway illumination that is now gradually being replaced by LEDs, so the orange will soon disappear from our collective memory, which is a bit unfortunate because it is such a nice illustration of spin-orbit coupling, but that's how life and technology evolve. Okay, let me look at the chat, nothing there, so we continue. The gravitational analogue. Somebody asked why this was meant, I will come to that question at a place where it is more logical to discuss it. The answer to one of the tasks, so we started from the problem of two mass distributions, and we wrote down the gravitational interaction energy between these two static mass distributions, where we started from an axis system that was taken in the center of mass of mass distribution 1, and so in that axis system we write down the potential energy. It's very natural in that axis system to write it as the potential energy of mass distribution 2 in the gravitational potential field of mass distribution 1. But you could also write it the other way around, that you start from mass distribution 2, and I asked you, write down that expression, build that expression in two, three steps as we did it for the original expression, and verify that it is the same one. And yeah, many of you had no problems finding that this is the same one. It almost feels trivial, but for hyperfine interactions it is not trivial, and I will try to illustrate in the next slides with a very simple example why this is. So, go back to charge distributions and take a very classical picture of a hydrogen atom, a nucleus with a positive charge, and an orbiting electron with a negative charge. We wonder what is the potential energy, electric potential energy? Well, it's very natural to look at the electric potential due to the nucleus, which is proportional to the charge of the nucleus divided by the distance between the electron and the nucleus, so capital Q over r, and to multiply that with the charge of the electron, minus Q. That's just Coulomb's law. However, nothing forbids us to think from the point of view of the electron. So, just in the formula, replace the division, don't divide the nuclear charge by Q, but the electron charge by Q, so you can just visualize this as the electron generating an electric potential at the position of the nucleus, and then you evaluate the nuclear charge in that potential. That's totally equivalent. In atomic physics we will take the nucleus for granted and we will see what the effect of the nucleus is on the surrounding electrons, but in hyperfine interactions we will think in this second picture. We will take the fields generated by the electrons as the given and we will examine how the nucleus behaves in the fields generated by the electrons. So therefore, I asked you with the gravitational problem, just convince yourself that both approaches are identical, just the visualization, the imagination about what happens, that will be different. It will be more natural for hyperfine interactions to think in this second picture here. Somebody asked in this context about the order of integration, so in the way how we derived it, wouldn't it be more logical to have the symbols dr1 and dr2 interchanged in order to keep proper track of the order of integration? Yes, in strictly spoken I agree with that, but the order of integration for mathematically well-behaved functions, that doesn't matter. It's only if your functions are kind of weird that the order of integration is really important, so here we will be a bit sloppy about this. We assume that mathematicians have proven that in this case the order of integration doesn't matter and we just write the sequence as we want. There was something special about the dimensions of mass distribution 1, which will

represent the nucleus, and mass distribution 2. We had this coordinate r that was measuring distances r that was measuring distances for mass distribution 1 within mass distribution 1 and r prime which measures distances within mass distribution 2 within the electron cloud and we had this requirement that r should always be smaller than r prime. I will come to it why this was important again and I asked you to draw an example of a case where this condition is not fulfilled. So why was this important? We had this Laplace expansion of this potential energy and strictly spoken the mathematically correct Laplace expansion has these symbols r smaller than and r larger than which can be uniquely assigned to r and r prime only if that condition of r always smaller than r prime is satisfied and if you can do that then this Laplace expansion boils down to a summation of dot products between tensors of increasing rank where one tensor that is the multiple moment tensor has only properties of the nucleus and the other tensors the multiple field tensors have only properties of the electrons. But you can do that, you can have these pure multiple moments and pure multiple fields only if r is always smaller than r1. So we have to, we will need to take that into account and we will see in our development of hyperfine interactions that there are situations where we have to be careful that when this condition is not fulfilled. Before I continue somebody asked about this Laplace expression and about the y symbols there where do they come from? These are the so-called spherical harmonics and well this is from mathematical physics so depending on your background you may have met this or you may not have met this. It's not crucially important for this course so you can just take that for granted. And the person who asked this question may want to look at the Wikipedia page for the Laplace expansion where you will see that the Laplace expansion is basically the expansion over the is of one over a distance and in that expression you recognize here this r smaller than r larger than and this these y symbols that are spherical harmonics. There is a different link to spherical harmonics but you will rapidly go into more advanced mathematics if you start reading about this. They can be chosen to be real or in general a complex and whether or not you write these complex conjugates as I had on the previous slide but which are not on these slides well that can also be related to the sign of n the opposite sign of the index n is equivalent to a complex conjugation so well there are some variants of writing this down. Here I would just take the idea of this expansion for granted and that this is something that will lead to the multiple field and multiple moment expansion. Well what did I ask here? Draw an example of two mass distributions where that condition of r always smaller than r prime is not fulfilled and you gave quite some interesting ideas. First I have some of them that are not correct and at the left hand side there is something about the origin so we have taken the assumption or the convention that we take the origin of our axis system always in mass distribution one. So this is not fulfilled in these examples but certainly not in the upper one. Maybe the lower one if the mass distribution would be weird it could still be okay but and the one at the right hand side cannot be correct because we work in one axis system so the position vectors r and r prime they start from the same origin and in this example here they started from different origins so that cannot be correct. A second series of suggestions so three examples you gave where this condition is not fulfilled and well you can you can trigger this by having mass distributions that overlap in a way as shown on these pictures. Mass distributions if this is in two dimensions strictly in two dimensions they cannot overlap because two masses cannot be at the same place but if you imagine this as flat mass distributions that are stacked in three dimensions then these solutions are proper solutions. There was a creative answer by somebody who even had this in a different way where you had a planet and inside the planet dark matter that as it doesn't interact with normal matter in the usual way can be at the same place as normal matter so also there you could construct something where the condition is not fulfilled. Another type of solutions is if you kind of reverse the roles and rather than having mass distribution 1 as the small nucleus that is inside the broader mass distribution 2 let the nucleus be large and encompassing mass distribution 2. So these are two realizations of this idea and there it's perfectly possible to have R smaller than R'. Of course you could then say well if I have such a situation let me just rename the system and 1 becomes 2 and 2 becomes 1 and then the condition is fulfilled again. So this is kind of it's valid but it's a bit artificial. Now there are two classes of

solutions that are genuinely correct and one of them is what I call the bulges. If you have a bulge on mass distribution 2 that enters the area where mass distribution 1 is present and each of these pictures show that in a different way but if you have that then it's definitely possible to have R smaller than R'. And the second set of solutions is when one or two of the mass distributions are rather long and flat then you can bring them together in such a way either next to each other or inside each other such that the condition is not fulfilled. And the yin-yang symbol is a kind of special case of this. Indeed with the yin-yang symbol you can perfectly have R smaller than R'. This year there were not really 3D solutions given but there are a few nice 3D solutions possible as well and I show you here some examples from last years. And also the example that I've always found the most, the nicest one which is this one here, a very simple case where you have a nice cylindrical rod and another hollow cylinder that is around that rod. This clearly is a situation where R can be smaller than R'. And therefore you cannot use the simple multipole expansion. You need the full Laplace expansion with the R smaller than and R larger than symbols. And it's interesting to realize that even in such a really easy and symmetrical situation where you would think well if I cannot apply a series expansion on this nice symmetrical mass distribution, well okay my sentence is a bit wrong, it looks like this would be a piece of cake but if you try it you see that you really need the full version of the Laplace expansion here. So you cannot tell just from the quick easy symmetry this looks easy so the multipole expansion will be perfectly valid. So now you really have to look at the condition R smaller than R'. Is that condition fulfilled or not? We continued to ask some questions about back monopole moments in the combination with mean square radii. So I gave you three charge distributions, two discrete ones and one continuous one where you had the same total charge Q and I asked you what is the where you had the same total charge Q and I asked you find the monopole moment and find the mean square radius. The monopole moment obviously we had done that one week ago is the total charge so for all of these charge distributions that's the same one. The mean square radius so I'm now time is running so I will go a bit quickly over this but if you had problems with the mathematical derivation of this you can later go back to the video and look at this slide. So this is the mean square radius for the first case a squared over four a squared over four and this one depends on the choice of the axis system again. So if we choose the axis system with origin in one of the charges we have a squared over two if we take it in the center of the two charges we have a squared over four and if these two charges would represent a nucleus well the convention for a nucleus will be that we always work from the center of charge of the nucleus so the right hand side that would be the choice of origin for the nucleus. So such a hypothetical nucleus would have a mean square radius of a squared over four. We can do this for the triangular nucleus as well apply the expressions and you find a mean square radius of a squared over three if you take the origin in the center of charge of the nucleus. This is the derivation for case a and case b and if you do this for the continuous charge distribution the cube I have a hint for the derivation in the first slide and you will find that it is again a squared over four. So why did we do this exercise that some of you found trivial? These three results together they give an important insight we have three different nuclei here hypothetical nuclei because of course nuclei are not as simple as here but three different nuclei that have the same monopole moment so it's always q but they have a different mean square radius. The left and the right hand side happen to have the same mean square radius the central one has a different mean square radius. So you can make nuclei that are in a first view just for the monopole moment for that charge that you always considered so far they are identical but they have other properties more subtle properties where they are different from each other and it's these properties that will play their role in hyperfine interactions. We will connect the mean square radius to what we will call the monopole shift that will be our first hyperfine interaction. We also met in this situation of in this context the principal axis system and I asked you where did you meet principal axis systems before in your education just to make the connection to things you already know and somebody said well I vaguely remember that we had to diagonalize matrices in my matrix algebra class and that's perfectly correct diagonalizing a matrix means search an axis system in which you represent that matrix that is chosen in such a way that the matrix is as simple as possible. We will do that a

lot with the quadruple moment and that is exactly what diagonalization is about. One of the examples where you may have seen this in action is when you calculate moments of inertia of a rigid body you can do this in any axis system but there are axis systems in which your matrix with the moments of inertia becomes a diagonal matrix and then it's most easy and then it's most easy to discuss the rotation of that object in that axis system. Many people have given moments of inertia for rigid bodies as the context in which they met the principal axis system before but there are other ones you can have the stress tensor that is something you also describe most easily in the principal axis system or you have crystallography where some properties are simpler in a principal axis system. Somebody made a connection to optics geometrical optics where you had the principal axis of a lens and there I think that this is not a correct connection so the principal axis of a lens is a different concept than the principal axis system for a tensor. The principal axis for a lens that's just one direction whereas a principal axis system these are three directions so this is probably a false friend a confusion based on similarity of names rather than a real mathematical connection. We move on to the double ring system and here I want to discuss the question that someone raised. I do not quite understand the point that one tries to make here with this gravitational example. How can that help explaining these monopole dipoles and quadruples? Well I would say that the double ring system is a good illustration of this. So what do we have in the double ring system? It's a gravitational analog of an atom where we have in the center of the system a dumbbell so two masses connected by a massless rod and it can freely rotate in all directions and that dumbbell represents our nucleus whereas the electron cloud this one is represented by two rings two mass distributions in the shape of two rings and so this electron cloud mass distribution will gravitationally interact with the dumbbell that is the nucleus. If you would make electric charges out of all of this you would have an electric interaction so it would more look like an atom. But I chose gravitation because in gravitation we are totally sure that we don't have to use quantum physics. We have the nicely trusted formulae of classical mechanics so we can really concentrate on the features that are relevant for the multiple expansion only and that are not related to quantum physics. I try to demystify the hyperfine interactions a bit. They are appearing in nuclei and electrons so in atoms but they are not a quantum effect as such. The physics of hyperfine interactions is purely classical. It comes from the multipole expansion and so for this system of the double ring with the dumbbell you could make a multipole expansion and you can write what is the monopole contribution and that monopole contribution is the main contribution to the gravitational potential energy of that system and that monopole contribution does not depend on the orientation of the nucleus. It describes a feature of the nucleus namely the total mass that is not related to the orientation of that nucleus. The second term, the dipole term, turns out to be zero. The next term, the quadrupole term, that is a term that will depend on the orientation of the nucleus and the quadrupole energy is written here on the slide that you are watching already for a few minutes. You see that this quadrupole energy depends on the angle theta. The angle theta that describes the orientation of the nucleus of the dumbbell with respect to the z-axis. So this quadrupole energy depends on how the nucleus is oriented with respect to the electron cloud. So orientation of the nucleus can have an impact on the total gravitational energy of the system. That's the message of this example. You could write down a quadrupole moment tensor for that dumbbell and an electric field gradient tensor for the, well not an electric field, a gravitational field gradient tensor for the double ring system which is the quadrupole field tensor of that mass distribution and it's the interaction between this quadrupole moment tensor and quadrupole field tensor that gives the energy term that you see on the slide. An energy term that is orientation dependent. So I hope that if you understand this double ring system in this way that you will also understand the quadrupole interaction for nuclei and atoms better. It's an energy contribution to the electric potential energy of your system that depends on how the nucleus is oriented with respect to the electron cloud. Now after this long explanation what was the question, the task for this? We have here three different versions of that double ring system and predict which one has the lowest energy situation. Now most of you inspected that quantity alpha that comes there in front and did a little calculations about it and you find that alpha is that for an

alpha being positive that then the energy of the system is lowest when the dumbbell is parallel with the z-axis so when the angle theta is zero and if alpha is negative the angle theta should be 90 degrees to make that energy expression as negative as possible and that's correct but here I want to draw your attention to a more visual way of coming to the same conclusion. If alpha is zero what does that geometrically mean? It means that you have rather small rings compared to the distance between the ring and in the limiting case your rings become so small that they are points so you have two point masses and in the center the dumbbell. How can the dumbbell lower the energy? By being as close as possible to the point masses and that means being parallel with the z-direction. In the other extreme you have two rings that are very large and almost touching each other so in the limit you have one ring. The two rings merge to one ring in the limit and how can the dumbbell be as close as possible to the masses in that ring? By being in the same plane as the ring. So the lowest energy situation is the horizontal one so without doing the mathematics just by visually imagining the limiting cases you can see the two different types of lowest energy orientation. I'm going a bit fast because time is running but we will well almost finish in time. The last part is the multipole expansion for the quantum case so because so far with the gravitational example everything was done deliberately in classical physics. What changes if we use quantum physics and that will be related to perturbation theory. So I asked you what would happen if you would try to use perturbation theory to describe a general nucleus and I deliberately draw here some very complicated shape. So a nucleus with that shape if you would try to use perturbation theory without having used the multipole expansion and by the way I use the word perturbation theory as if you know this. So I assume that if you have had an introductory course to quantum physics you may have met perturbation theory before. If that is not the case then please look at the refresher section where you have a quick summary of that idea. So back to this problem what would happen if you use perturbation theory without using the multipole expansion. So you take the unperturbed system the point nucleus and then everything that comes on top of the simple system to bring us to the complicated system. So that would be the complicated shape without the point aspect of it which is visualized there as a shape with a hole. Now you would need to evaluate the energy contributions of that additional term but that still looks complicated. So yes you can use perturbation theory to have a zero order contribution and a perturbation but if your perturbation is complicated this will not help you. Therefore it's much better if you first do a multipole expansion. So you describe your complicated shape by a point, then by a sphere, then by a deformed sphere in ellipsoid. So all the different terms in the multipole expansion with and without overlap and then you use these simple terms as perturbations because these shapes are easier so you can evaluate their impact on the energy. Did we win by doing that? Well therefore we have to think about when is it meaningful to use the multipole expansion and to truncate it and when is it meaningful to do perturbation theory and to stop after a few orders and can we do that simultaneously? Can we use the multipole expansion in combination with perturbation theory without running into too many extra terms that need to be calculated? Asking the question is perhaps more difficult than answering it. So let's look at the first one. When is it valid to truncate the multipole expansion early on? I flash a few of your answers that are correct ones and I give you my summarizing answer. When is the multipole expansion valid? When can we truncate it after only a few terms? If the dimensions of the nucleus are much smaller than the dimensions of the electron cloud. If you look at these expressions it's the nuclear distances divided by the electron distances to some power. The power that always increases and you will see because the nucleus is so small compared to the electrons that ratio is a very small number. If you raise that to some power that number will become even smaller. So these higher order terms of the multipole expansion they will really rapidly become very very small. So stopping the multipole expansion after say the quadrupole term that will be already a very good approximation for a system with a nucleus and an electron cloud. When is it valid to stop at first order perturbation theory? Well if you look at the mathematical expression for first order perturbation theory or for first and second order perturbation theory you have here on the slide you see that these terms depend on expectation values. Expectation values of what will be the multipole operators evaluated for some

state of the electron cloud. And because these multipole operators are already small, see previous argument, these expectation values will be small as well and therefore these terms in the perturbation theory expansion will also be small and the ones that have a higher power will be even smaller. So stopping after the first order perturbation will already be a good approximation. So we are very lucky here the multipole expansion converges quickly for a system that has the properties of a nucleus and an electron cloud and perturbation theory gives an already after the first term a good approximation. So we can use them together. That is the conclusion that is reached here. And therefore I can summarize this message as follows. If you have a classical system like two interacting mass distributions with complicated shapes you can make this tractable by making a multipole expansion and truncating this at the term where you want. If you do this with a quantum system then you still use the multipole expansion but on top of that you have to use perturbation theory and we are in the fortunate situation where for both of these numerical approximations it is justified to stop after the first few terms. So we will not run into many, many, many contributions that all have to be evaluated separately. No, first order perturbation theory on the lowest orders in the multipole expansion will be sufficient and every of our hyperfine interaction contributions will be one of these terms. Good, a little bit longer than I was planning so we try to finish in one hour 15 minutes. It's one hour 20 minutes but well so be it. Let me look for a last time at the chat as there is a few seconds of delay between the stream and my words. I will wait for one minute more to see whether questions arrive. I don't see any, perfect. So don't hesitate to keep submitting your questions via the question forum, also questions about the topics of the previous weeks and with this you're ready to tackle module 3. So see you next week, same place, same time. Bye bye.