PROFESSOR: Then let's talk about exciting physics, the Lamb shift. So we discussed the Lamb shift last Friday, and the Lamb shift is really due to the fact that, if you have a atom consisting of an electron, a Coulomb field, and the proton, this is not the complete description. The atom lives in a vacuum, and the vacuum is filled with electromagnetic waves.

So what we have to include, for an accurate description of atomic level structure, is the coupling of the atomic system, of the electron, to all of the modes the electromagnetic field, and this is radiation.

We will talk about the quantized electromagnetic field later, at this point I could introduce you to a simple model, fairly accurate model of the Lamb shift, by simply assuming, and that's what we did on Friday, that we have fluctuating electric fields, those fluctuating electric fields shake, accelerate, the electron and the electron performs some oscillatory motion and this oscillatory motion leads to an ever reaching of the Coulomb potential.

And similarly what we saw for the Darwin term, this ever reaching of the Coulomb potential takes away this singularity of the Coulomb potential and therefore lowers the binding energy of the electron. So today I want to just say a few more words about the result we derived, and then we have done what happens to an electron in a Coulomb field plus radiation. The next thing is, then, to discuss hyperfine structure.

So let me first make one comment, when we integrated over all modes of the electromagnetic spectrum, we needed an upper cutoff, and a lower cutoff due to logarithmic singularities. Eventually, an upper cutoff is relativistic rest mass of the electron we have to cut off things. I just want to say one more word about the lower cutoff. I suggested, as a cut off, the orbital frequency of the electron.

So the justification for that is the following, the electron, the free electron-- the free electron, when it's driven, has an amplitude which is 1 over the frequency squared. So if you drive it slower and slower, it's amplitude increases because it has more time to go in one direction.

So this divergence at low frequency, of course, happens only for the free system. When you have a bound system, like a mnemonic oscillate, and you drive it at lower and lower frequency, the response converges to a constant and not to 1 over high frequency squared singularity.

So therefore, when we reach the drive and the high frequencies on the order of-- oscillatory frequency of the bound system, the behavior changes. So when we mimic this with an effect cutoff because what you want to get rid of is a singularity, but in reality, of course, it should approach a constant at low frequency, and that is essentially the physics of the AC and then the DC Stark effect.

So that was a rational for the cutoff and let me just annotate it here. And let's say, for a free particle we had the situation that the amplitude was proportional to 1 over the high frequency. Whereas four bound particle is, you should approach a constant for low frequencies. And that's what we have introduced with a cutoff. OK.

So we have discussed the Lamb shift, but you've already discussed one contribution to the Lamb shift. So this was a contribution that the Coulomb potential is effectively smeared out, and the result of this is that there is a weaker binding energy. However, there is a second contribution to the Lamb shift.

I've sometimes seen sources where this is discussed as the main contribution to the Lamb shift, but this is not correct. This is only 3% off the total and contributes 27 megahertz. This is what is called the vacuum polarization.

So if you have a-- the proton positive charge and you have the electron, and they scatter off each other, and we use this kind of diagram to indicate that, now that there is an additional diagram which has this bubble which is this production of e minus and e plus pairs.

And you can say that if an electron and proton attract each other and you create, by virtual pair production-- because the vacuum is alive, things can happen in the vacuum-- it will virutally [INAUDIBLE] electron positron pair that now you create electron positron pairs, which shield the Coulomb field. And this is a second contribution in addition to the shaking motion of the electron.

So I want you to just think about it for 10 seconds before I tell you the answer. Does this vacuum polarization strengthen or weaken the binding energy? Anybody want to offer an opinion? Whatever you say, you can't be wrong because there are to aspects to the answers so.

Well then the actual answer is you would say, if you have charged-- if you create charges between the electron and the proton, you have a shielding effect and the shielding effect should weaken the Coulomb field. But the question is, what do we regard as the elementary charge, e, in our Schrodinger equation. And what we regard as the charge, what is measured in a Millikan Droplet experiment, is already the shielded charge.

So therefore, the fact that vacuum polarization exists means we always measure the shielded charge, but because vacuum polarization happens at a finite distance, the electron, in an s state, can sort of penetrate the shield and feel a somewhat stronger Coulomb potential. So therefore, accounting for the fact that we have these virtual electron positron pairs actually means that the binding energy is increased and the vacuum polarization has the opposite sign as the dominant effect we've mentioned earlier.

So the sum of e is, we observe the shielded charge and vacuum polarization implies that the s electron can penetrate the shield and sees a higher charge. So we normally observe the shielded charge, but the electron can see the higher charge. So therefore, that means, now, that we have, not an upshift in energy, but a downshift in energy for-- which for the two is one half state, is 27 megahertz, as I mentioned earlier.

Anyway, I'm not really deriving it, but I want to sort of uncover certain myths, so the vacuum polarization, number one, is not dominant and number two, has the opposite sign as everybody would naively assume. Questions? I hope not because I don't know anything more about that. All right. So we have dealt with Lamb shift. So is next now, in revealing the atomic structure, is we want to go beyond the Coulomb field created by a point charge.

And that means we want to address the fact that we don't have a point charge, but we have a nucleolus. And we are discussing, now, effects of the nucleus, which also go by the name hyperfine structure. So, just to summarize, so far we have treated, in pretty much complete detail, what happens for an atom which consists of a point charge and electrons.

But now we want to bring in that, what creates a Coulomb field, the nucleolus, has structure. And there are actually four different ways how the nucleolus has structure and contributions to observable effects on the atomic structure and atomic energy levels. The most important one is that the nucleus has a magnetic moment associated with the angular momentum of the nucleus I.

The second contribution is, in addition to magnetic moment, there may be a quadrupole moment. And since those effects can lead to a splitting-- this is actually, usually, called hyperfine structure, but then there are two more effects. One is the nucleus has finite mass, and the nucleus has a finite volume.

Both the mass and volume effect lead to energy shifts. But tiny energy shifts are hard to measure unless you have two different shifts, and therefore those effects go as isotope shifts because when you have an atom which comes in two different isotopes you find that, due to those two effects, the energy levels are not the same. So this goes by the name of isotope shifts.

By far the most important phenomenon is the first one. The fact that if a nucleus has angular momentum, we have hyperfine structure, and for the hydrogen atom that means that the ground state, the singlet S 1/2 state, actually splits into two states with total angular momentum quantum number F.

So the relevance of hyperfine splitting is, it's actually a huge relevance, one is, you don't have a single ground state of many atoms, you have several ground states.

So the lowest electronic state has several ground states, has several hyperfine states, due to angular momentum selection, where you can actually talk to them individually, you can prepare them individually, and many of you who do magnetic trapping know when need magnetic trapping you better prepare the atom in a single hyperfine state, otherwise you are in trouble. So you can prepare individual states.

In the old days this was done by optical pumping, and you can use several hyperfine states to great advantage for the manipulation of atoms. For instance, if you want to, you can put atoms into a hyperfine state where they don't absorb light, and then you can have resonant light for the other ones blast those away. So you can play, sort of, your tricks because you have two states between which you can juggle at the atoms.

Well, what else is relevance of hyperfine structure? OK if you have two levels, F equals 1, F equals 0, you can observe a transition. And the famous 21 centimeter line is used for astronomical observations. Hydrogen is the most abundant element in the universe, and how do you see hydrogen out there. Well it is due to hyperfine transition, the 21 centimeter line.

And finally, another aspect why hyperfine structure is relevant, where people use it, is for the determination of nuclear properties. How do you know what the properties of nuclei are? Well there are techniques in nuclear physics, but a lot, a lot about the knowledge of nuclei comes from atomic spectroscopy.

If you measure atomic energy levels with high accuracy, you figure out what the properties of the nucleus is, and one of the most outstanding examples we will discuss later on, and some of which is also on your homework assignment, is you can use atomic spectroscopy of hydrogen to contain the most accurate measurement, how big is the proton. And the big surprise is that there is, that there was, a surprise that people figured out that, until now, even in 2014, we do not fully understand how big the proton is but we'll talk about that later.

So for the level of this-- the level of this introduction, we can use it for determination of nuclear properties and actually, you cannot only determine properties of stable nuclei, you can also determine properties of unstable nuclei. At various accelerators, they have a facility when, by, you know, energy collisions they create unstable nuclei.

Maybe helium six, helium with four newtons, it exists. And you can take helium six, extract it, utilize it and then you've have a neutral helium atom which looks like your every days helium atom but it has two more neutrons in the nucleus.

And by performing atomic spectroscopy, you can figure out what is the deformation, what is the structure, of this-- I want to say alpha particle, but it's an alpha particle plus two neutrons. So people have really learned to do those atomic physics measurements within a few seconds after the element has been produced, and such determined nuclear properties even of unstable nuclei. OK. So that's my introduction.

So we are now discussing the most important effect due to the hyperfine structure. And this is the fact that the nucleolus has a magnetic moment, and this magnetic moment couples to the magnetic field even if you don't apply an external magnetic field, we talked about that on Wednesday, there is an internal magnetic field created by the electron with total angular momentum change. So this is, so to speak, the Zeeman Hamiltonian of the nucleus in the magnetic field created by the electron.

And I will show you quickly to, is a simple derivation, what the result of that is. But before I do that, I also want to mention out-- mention that there is-- I want to point out that there is an alternative. Right now, I said we say the nucleus experiences the magnetic field created by the electron. But we can also take the other approach, the nucleus creates a vector potential because of its magnetic moment, and the electron, which goes around the nucleus, is not only feeling the Coulomb potential but also feeling a vector potential.

And of course, both different perspectives, whether the electron moves in the magnetic field the nucleus, or the nucleus experiences the magnetic field of the electron, both treatments have to agree. I follow the more standard treatment, but the alternative treatment, where the electron moves in this electric and magnetic potential of the nucleus, is fully elaborated on the atomic physics wiki.

So alternatively, electron moves in the potential of the nucleus, which is the Coulomb potential, we've discussed that, but then there is also vector potential created by the magnetic moment of the nucleus. So you simply assume this is a potential created with a nucleus, and then you just sort of Schrodinger's equation and this approach is carried out on the wiki.

However, since it's a little bit more standard, and there's an easy semi-classical derivation, let me now discuss this one. Because what I like about it is it addresses one intuitive quantity, namely the fact that there is an internal magnetic field. We're not just using the Schrodinger equation for the whole system, we are really estimating what is the magnetic field, which the electron creates, at the position of the nucleus.

So let's now do a semi-classical derivation of this internal magnetic field. And I have to-- I will immediately tell you, this derivation agrees quantitatively with the fully thermomechanical treatment. So, as often as these semi-classical derivations, we have to separate two parts. There are two ways how the electron creates a magnetic field at the nucleus.

One is due to it's orbital motion, the electron is a ring current and creates a magnetic field, but then the electron has magnetic moment for-- due to it's spin. The spin part is simply the potential of a magnetic dipole, you will need to vector-- you will need to vector where the magnetic dipole moment of the electron is proportional to it's spin with a g factor.

However, and you can find that in all textbooks on classical electrodynamics but, there is one important term which we have to add here, which is also part of classical E and M, and this is the delta function contribution. You've probably seen it, you find it in Jackson, if you haven't the model is that you can assume that a magnetic moment is created by ring current, and the ring current has-- creates a magnetic moment and you have the dipole potentially due to the magnetic moment.

However, if you have a ring current, there is-- you can also ask, what is the magnetic field inside the current loop and then eventually do the transition where you allow the current loop to go to 0. That's how you make a point model of a magnetic dipole, but what remains is, sorts of-- as a delta function, the location inside the loop.

I'm emphasizing it because it will be, eventually, the delta function contribution, which is important for s electrons, and therefore it is this contribution which is the dominant effect in many situations. OK. So this is the magnetic field created-- it's a classical expression, but it's buried in [? quantum ?] mechanics, the expression for the magnetic field created by the spin.

The second contribution is the orbital contribution, and for that semi-classical, we just use Biot-Savat. So Biot-Savat is usually the 3-Dimensional integral over the current density. The volume integral, or you can rewrite it as the current I, d, r cross r, over r cubed. And eventually, if you now put in the electron charge distribution, velocity course r, well, velocity cross r means we get, and that's what we want, the orbital angular momentum.

The 1 over r cubed term means we have to calculate an expectation value over the wave function which, is 1 over r cubed. And the prefactor leads us-- it's nothing else than two times the Bohr magenton. So, with those two terms, we can now obtain our final expression for the total magnetic field generated by the electron at the origin. And for that I use the g factor of two as it comes out of Dirac theory.

So now we have the total magnetic field. We had this contribution L over r cubed. If you inspect the dipole potential of the spin it has a contribution S over r cubed, then it is the second contribution to the dipole potential. And finally, most importantly for the following discussion, the delta function contribution which I discussed earlier.

If you have an s state, these first terms are 0 for L equals 0 because these are, sort of, terms which have dipole potential where positive and negative contributions cancel out when you do a spherical average, and the s electron performs a spherical average.

So it is 0 for L equals 0 due to the spherical average. Whereas the second part, it would be 0 for L non-equals to 0 because the probability for a non-s electron to be at the nucleus is 0. So pretty much this describes that. So this describes a hyperfine structure. Well, it describes the magnetic field created by the electron, and now we have to do the usual projection in the following way.

That the hyperfine structure is that Zeeman Hamiltonian of the internal magnetic field with a magnetic moment of the nucleus, and the magnetic moment of the nucleus is proportional to the angular momentum of the nucleus. Sort of this argument that even if it were not proportional, it would rapidly precess and eventually project it, and the only direction which survives is the direction of the angular momentum.

And similarly, you can-- the magnetic field, you have a contribution of S and L, but S and L rapidly precess around the result and angular momentum, J, and therefore, as a result, the internal magnetic field must be, can only be, parallel to the angular momentum chain. If you do a fully [? quantum ?] treatment, it comes out immediately.

But if you do it semi-classically, you calculate a magnetic field, you sort of have to fall in this argument that you always project on the axis of angular momentum and that means that the hyperfine interaction will be the Hamiltonian for it, or the operator, will be the dot product of I dot J. For fine structure, we had L dot S, for hyperfine structure, we had L dot J, this is always how we couple angular momentum with a dot product.

The hyperfine constant cause by the letter a, and since historically a is measured in frequency units, in Hertz, I have to put in h, Planck's quantum. No it's not h bar. For historical reasons, it's h.

AUDIENCE: Question.

PROFESSOR: Yes?

AUDIENCE: Are I and J dimensionless, or will they carry units in h bar?

PROFESSOR: Here they are dimensionless, thanks for the question, because each is in frequency units, it's in Hertz, and if you multiple with h you have an energy. So therefore, I and J measure the angular momentum in unit of h bar. So it's not in that sense, it's a normalized angular momentum operator. The quantum numbers of I and J are not 1/2, or 1h bar, it's just 1/2 or 1. Other questions? OK. I can now take this expression with, you know, L and S and S.r and evaluate further, but I feel I'm not providing any insight and you can read about it on the wiki.

So for a non-s state, how to simplify this expression and get the final textbook result, I defer to the wiki. I want to discuss the most important part, namely for s v electrons because hydrogen, all the alkaloids, have an s ground state.

So, in that case, all we have to consider is the delta function part and if we project the magnetic field onto the angular momentum axis, we get the probability of the s electron to be at the origin. And therefore, for s states, the hyperfine constant is-- oh, I forgot one thing. We have to parametrize the magnetic moment of the nucleus, and that is done by using a nuclear magnetron.

It's the same as a Bhor magneton, where you have replaced the electron mass by the proton mass, and you have the nuclear g factor. Just as a reminder, the g factor of the proton is 5.6, the g factor of the neutron is minus 3.8. So the g factor has nothing to do, not even close, to the factor of 2, which we obtained in the Dirac equation for the electron. That just shows that the nucleons, protons and neutrons, are more complicated. Well, they have quarks inside, they have a complicated internal structure.

OK. So therefore the hyperfine constant involves, now, the g factor of the nucleus, the product of the nuclear magnetron, with a Bohr magneton, and for hydrogen. This gives the famous result of 1420 megahertz. So this is hydrogen, and this h is now the Hamiltonian. So the hyperfine coupling Hamiltonian, which has I dot J, by using the expression for the total angular momentum I plus J and then we square it.

When you evaluate this square you get, on the right hand side, an expression for I dot J. So I dot J is nothing else than 1/2. F squared, minus I squared, minus J squared. And therefore, for hydrogen, where I, J and S are all 1/2, the proton has been 1/2, the electron has been 1/2, that's it.

You have only two values of the result and total angular momentum, 1/2 and 1/2 can add up to 1 or 0. And now the hyperfine splitting is into an F equals 1 and F equals 0 state. And one thing to remember is, if you inspect the above formula with the [? quantum ?] numbers you find immediately that, compared to the degenerate line, without hyperfine splitting, this-- so what comes out of the Dirac equation, the splitting is the fight-- is 1/4 and 3/4 of the hyperfine constant.

Since F equals 1 has a multiplicity of 3, 2 and F quantum numbers, plus minus 1 and 0, the rule is that the center of mass of this level does not change due to hyperfine splitting. So the center of mass of hyperfine states is not changing. So we introduce a level splitting, but no overall shift. Any questions about magnetic hyperfine structure? Yes?

AUDIENCE: Would you explain again the center of mass is not changing. Is this just for hydrogen? Or is this a general rule?

PROFESSOR: No, this is a general property, and you could actually show that when you evaluate the product of I dot J. So, the product of I dot J means that for arbitrary I and arbitrary J, if you calculate the hyperfine structure, the center of mass is the same. OK.

I've not done any experiment in my life where higher order moments became important, but I want to teach you about it because the discussion about whether those higher moments exist or not is really an interesting discussion about what is allowed by symmetry and what's not. So I'm bringing in a higher moments, not so much because you need it to understand the level structure of your favourite atom, but because it teaches us a really nice piece of physics.

So let me now discuss higher order moments and the leading one is the electric quadripole moment. So I want to raise, in general, the question, what further moments can a nucleus have. What we have discussed so far is the magnetic moment, mu. So beyond mu, what further electric or magnetic moments can a nucleus have?

Well, it's a question about symmetry and if you look at the parity of multiples, if you have an electric multiple-- well, you know if you have a dipole, plus minus, you invert it, the dipole becomes minus the dipole. So for L equals 1, it is minus 1, L is 1, but in general the it is minus L.

If you have a quadripole, you invert your coordinate system. It's L equals 2, plus plus, minus minus, you invert it nothing changes. So these I've shown you, for dipole and quadripole, that this formula is correct. So an electric multiple has this parity, and for, magnetic keys-- now, you know, magnetic we have axial vectors versus polar vectors, there's always an extra factor of minus 1.

So therefore if you go magnetic, magnetic multiples with L have a parity of minus L plus 1. So this really restricts what multiples are possible. Instead of giving you a general discussion, let me just look at the very important keys. Whether a magnet with a nucleus can have a electric dipole moment, and you will immediately see what it needs to-- and then I give you a general result.

So let's assume a nucleus has angular momentum I, and there is a magnetic moment, mu associated with it. So the general result is that odd electric and even magnetic multiple moments would violate not just one, but two symmetries, would violate parity and time reversal symmetry.

So the argument goes as follows. Let us assume this is the magnetic moment, mu or the angular momentum I, it's a vector. And now we are asking, is it possible to have a vector of the dipole moment. And dipole moment, you should just think about it as a plus minus charge, separated.

We can now do the parity operation and the time reversal operation. If you do the time reversal operation, the current, which generates a magnetic moment if you want to think about it in this picture, goes the other way. So mu flips but nothing moves, of course, for an electric dipole moment, so reversing time is not changing anything.

So in other words, time reversal symmetry transforms parallel mu and d into anti-parallel mu and d. And similar, parity is not changing mu but it is changing d. So in both cases, would parity, or time reversal symmetry, if you had mu-d, a scalar product of mu and d which would be known 0, then both P or P would change the sign.

But that would mean that two kinds of particles would exist, one where the sign is positive, one where the sign is negative. But we have assumed that we have 1 nucleus and only 1 nucleus of this kind, so we cannot have one nucleus which has the properties of having, simultaneously, a magnetic and electric dipole moment.

So therefore, we conclude that mu times d has to be 0. And if you generalize this argument, we have ruled out that there is an electric dipole moment, an odd electric moment. The first, the lowest, possible electric moment is the quadripole moment, so the leading electric moment is not L equals 2, L equals 2, it's not L equals 1, the dipole, it's L equals 2 the quadripole.

And of course if you generalize the argument, L equals 4, L equals 6, would be possible but those effects would be very small. Questions so far? OK. So we've talked about parity and time reversal symmetry, which restricts what kind of magnetic and electric dipole moments particles may have.

And maybe in this context, I should just mention that John Doyle, Jerry Gabrielse, and Dave Demille at Harvard and Yale, they just published the most accurate result for the electric dipole moment of the electron. They found a bound, which was more than an order of magnitude lower than the best upper bound before and this has really made headlines. So to measure, accurately, that the electric dipole moment vanishes, in this case of the electron, but other people do it also for neutrons, is testing fundamental symmetries.

In particular, it tests whether nature is time reversal invariant. And the reason why, until now, everybody has found that the results are compatible with 0 is pretty much based on the argument I just gave you. OK so we have discussed those fundamental symmetries, but now I want to discuss something else related to it.

So let's assume you have a nucleus, and I want to discuss with you, is a minimum requirement for the nucleus for the angular momentum of the nucleus in order to have a magnetic dipole, or to have an electric quadripole. So let's formulate it as a quicker question. So here let's assume a is-- it's possible for any nucleus no matter what the angular momentum is. Here, we put in 1/2, or larger than 1, and for the electric quadripole we have the same choices.

So you should decide if I tell you, a nucleolus has a magnetic dipole. Does that imply that there is a minimum amount of angular momentum of the nucleus there? And then repeat the same question for the electric quadripole. So please tell me your opinion. So right now, what is a minimum requirement for I, for magnetic dipole, and if yes, what is it? Three, two, one. Stop. OK, so-- and let's immediately consider the electric quadripole moment.

So this was a majority opinion. I gave this answer for both of them together. So the question is, what is the minimum requirement for a nucleus to have an electric quadripole moment. OK, stop. Display. No requirement. OK. So the majority onset was a here.

So let me to discuss it, and I know some of you will have-- I always get into heated discussions with it. I actually just had a few minute discussion with one of my colleagues about it, who at least wanted to look at it from a different perspective than I did. So let me give you the short answer and we can go from there.

In order to the magnetic dipole you have to take an object, turn it around, and figure out that there's a different energy. So therefore, unless you have an object, which is has two orientations, you cannot figure out if it has a magnetic dipole or not. If you're in a state without angular momentum, I equals 0, there is no distinguishable states. You cannot orient a 0 angular momentum object in space.

So therefore you can never figure out that there's a magnetic moment, and now I'll make a bold statement, and this means there is no magnetic moment. So therefore, you need this because you need a minimum number of true orientations. OK. Now an electric quadripole means that the charge density is like ellipse. It has--

AUDIENCE: [INAUDIBLE]

PROFESSOR: Oh, 1/2, sorry. Thank you. So I should get larger than 1/2 because we need a minimum of two possible orientations. Now my question for you is, you think something is elliptical but how many different orientations do you need to figure out that it is elliptical and not round.

If I equal 0, you can only look at it, you can't rotate it, so will you never find any energies [? breathing. ?] It's just there and you cannot say where it's round or whether it has a quadripole or deformation. If I is equal to 1/2, you can take it and flip it around but can you tell from that that it's an ellipse. No because if you turn an ellipse around nothing changes. So it could be, as well, a sphere.

You can only figure out that it's an ellipse if you have an intermediate rotation, let's say, by 90 degrees. So in order to assess that something is elliptical, you have to at least resolve three positions, three angles, and three angles require that you have to three sublevels and this requires that I is larger, or equal, than one.

Sorry. Then one goes-- OK. I'm want to give you a formal argument using this spherical tensor, but I guess someone you are waiting for something simpler. So. I mean who wants to know the answer of the question, but what happens if it has a deformation. Does it just mean we can't measure it, but it has a deformation?

Let me explain that. So if I have a pencil and the pencil has zero angular momentum, I can't really figure out that it's an elongated object, because all I measure is a symmetric wave function. It's completely spherically symmetric.

The only way to figure out that it's a pencil is I have to localize it, that I can see that it's pointing somewhere. But to localize an object in space is actually an angular wave packet. It's not isotropic. It points somewhere. And an angular wave packet is a superposition of states of different angular momenta. So therefore, without assuming that there is a state with angular momentum, I cannot orient this pencil. OK.

I know you would all agree that even if this pencil is cooled to the ground state with zero angular momentum, it is a pencil. But what you're using here is now your knowledge that this object has higher angular momentum states. And those higher angular momentum states have nothing to do with the structure or the appearance of this object of being a pencil. So you sort of know that in addition to the i equals 0 state, there are i equals 1, 2, 3, 4, 5 states, and the pencil looks the same.

But if you have a nucleus, an i equals 0 state requires a certain configuration of quarks. And you cannot create an i equals 2, and i equals 4, higher states without messing around with the internal structure. So with a nucleus, all you have is an i equals 0 state. And to say that this i equals 0 state has a quadrupolar deformation doesn't make any sense.

If you would know that this nuclear state could be rotated without changing its internal structure, then you would say, yes, it has a quadrupole moment, I just can't see it. But usually, you cannot make this assumption. If all you have is an i equals 0 ground state, and the i equals 2 state is very, very different, because the quarks are spinning around each other in a different way, you have to see, i equals 0 is completely spherical. It doesn't couple to anything externally. And therefore, it has no moments whatsoever. So that's the story.

A lot of people get confused, because they think an object can have a deformation without rotating. But you need the rotation to resolve it. If you cannot create an angular wave packet, which is a superposition state of angular momenta, you can never figure out that there is a deformation.

And quantum mechanically, if you cannot figure out that there is a deformation, there is no deformation, because you can only use, in the language of quantum mechanics, where you have at least the possibility to measure it. Questions about that? OK.

I think that makes it now-- let me now kind of just give you a formal. A formal derivation. But I agree. I mean, the formal derivation, I'm just throwing a few equations at you, and say, that's it and everything follows from that. But I provided the insight for you.

Formally, you can define the quadrupole moment by the expectation operator. You take the nucleus with maximum MI. And now you calculate the expectation value of this operator. This is, of course, motivated by just electrostatics. If you take an expansion of the classical electrostatic energy into multi-poles, you find the quadrupole configuration to be related to a quadripole moment. Quadrupole moments couple to the derivative of electric fields.

And then in this purely classical description, you have this term, where beta is the angle between two symmetry axis, namely, between the symmetry axis of the electric field gradient and the quadrupole tensor-- just the classic quadrupole tensor as it comes out of *Jackson.* Yes.

You can see the quantum mechanical definition of the quadrupole moment, or more generally. So this is quadrupole moment. If you have a moment with l, the operator, which tells you whether you have a non-vanishing moment, a non-vanishing deformation, is actually a spherical tensor, Tlm.

And what you see above is a spherical tensor, T20-- l equals 2, m equals 0. And those spherical tensors are defined by the fact that they transform as spherical harmonics. And now you sort of realize what it means.

If you want a magnetic or electric moment with l, the operator for the moment transforms like angular momentum l. And now you realize that you have the triangle rule. If you want a matrix element where I and l overlap with I, you want to make sure that I, l, and I couple. And you have a triangle rule.

So therefore, if you want a magnetic moment, or electric moment, of l, and you evaluate this expectation value, well, at least the triangle rules can only be justified like this. Or in other words, you can only get a non-vanishing moment if l is smaller than 2I.

And this is what we discussed in the clicker question for the two cases of I equals 1 and l equals 2. So ultimately, it's a selection rule which is related to the triangle rule for the addition of angular momenta. But I like much better the argument, how many orientations do you need to find out that something is elliptical? It's formalized here. All right.

Let's just spend one more minute on the quadrupolar structure. So based on the expansion of the electrostatic energy, what determines the quadrupolar structure is this cosine angle, which is the angle between the axis of the nucleus and the axis of an electric field gradient. And that means it is the angle. It's a cosine of the angle between J, the outer environment, and I, the axis of the nucleus.

So therefore, when we would derive-- I'm not deriving it, but if we would derive an expression for quadrupolar structure, the quadrupolar structure would be proportional to a quantity C, which is nothing else than the dot product of I and J. And at least in my notes now, I and J have units of h bar. So I'm dividing it out here.

And as you know, I, dot, J can be expressed by quantum numbers F, F plus 1, minus I, I plus 1, minus J, J plus 1. So therefore, the quadrupolar energies-- E2, El equals 2-- involve the classical expression at cosine square.

So therefore, you would expect there is a quadrupole constant. And then it is cosine square. But well, usually, quantum mechanic even, we have the square of a quantity, we have to write it as quantity times quantity plus 1. So this is the quadrupolar structure. And to remind you, we just discussed that for the hydrogen atom, the magnetic hyperfine structure had invoiced the same product of I, dot, J, but in a linear way.

So the reason why I'm not discussing quadrupolar structure in more detail is usually the hyperfine structure associated with quadrupole moments is much, much smaller than the hyperfine structure associated with magnetic moment, typically by a factor of 100.

The only exceptions are molecules, because molecules can have-- because of molecular binding mechanisms-- a much, much larger electric field gradient. So therefore, in molecules, quadrupolar structure is more important than in atoms. Questions about that?

With that, we have discussed the two effects of hyperfine structure due to magnetic moment of the nucleus. And we also discussed further deformations of the nucleus, in particular, the quadrupolar deformation. Let me now use the last 10 minutes to quickly discuss with you isotope effects.

And I know that many people here know about isotope effects, because if you lock your laser to a lithium cell or to a rubidium cell, you find lithium-6 and lithium-7 peaks. And in rubidium, rubidium-85 and rubidium-87. So there are two peaks which are spectrally very, very well resolved. And now I tell you what causes the splitting between the lines of rubidium-85 and rubidium-87.

Well, the first effect is really trivial. It's the mass effect. And I have to remind you that the Rydberg formula for a single electron energy level contains the reduced mass. In other words, the energy levels are the energy levels-- if you assume that the mass of the nucleus is infinite, that means you just take for the electron mass in the Rydberg constant the electron mass.

But in general, you have to take the reduced mass-- the big M is the nucleus. And small m is the electron. The simplest case is if you set the nuclear mass to infinity. Then you simply have the Rydberg constant with the electron mass.

So in the limit that the nuclear mass is much larger than the electron mass, this correction factor is 1 minus little m over big M. So therefore, the correction factor is on the order of 10 to the 4 or 10 to the 5. Visible frequencies are on the order of 10 to the 14. So 10 to the minus 4 or 10 to the minus 5 of it is between 1 and 10 gigahertz. So this is the scale for mass corrections due to the isotope effect.

What is the sine of the isotope effect? Does the fact that the nucleus has a finite mass-- does that mean that the binding energy of the electron is smaller or larger?

AUDIENCE: [INAUDIBLE] it would be larger.

PROFESSOR: The absolute value of the binding energy-- look at your signs. I would say it in the following. Let's start out with an infinite nucleus, and only the electron is moving. But now we make the nucleus lighter. And that means the nucleus also has to move, because it's a two-body problem.

And there is additional kinetic energy, additional kinetic energy of the nucleus. And kinetic energy is positive and weakens the binding energy of the total system. So therefore, the fact that the effective mass correction means the lighter the nucleus is, the more kinetic energy has to be added to the system for the nuclear motion, and the more the binding energy is weakened.

The most dramatic example is not the hydrogen atom. It is positronium, where your nucleus is not a nucleus, it's a positively charged electron to the positronium. And in this situation, you have an effective mass which is only 1/2 of the electron mass. And the 1s-2s transition, which is Lyman alpha for hydrogen, is now not even in the vacuum UV, it just happens at ordinary UV transitions.

And that means now the 1s-2s energy is smaller by a factor of 2. That really means the binding energy between an electron and a positron is only 50% of the binding energy of an electron in the hydrogen atom. OK. That's all I want to say about the mass effect.

Let's now talk about the volume effect. So if you would look at the charge distribution in a nucleus as a function of r, if we go from one isotope to a heavier isotope with more neutrons, the nuclear radius becomes larger and the charge becomes more spread out.

So if I plot now the electrostatic potential, the electrostatic potential is, of course, the Coulomb potential, 1 over r, until we enter the charge distribution. And then, as you know from electrostatics, it continues. This is 1 over r. And then it's flattened off. It continues quadratically for the heavier-- oops, I wanted to change color. For the heavier nucleus, it is like this, and for the lighter nucleus, it is like this.

So in other words, the finite size of the nucleus is cutting off the Coulomb potential where it is strongest. And this happens the earlier, the larger, or the heavier the nucleus is. So therefore, what you obtain is you obtain, in perturbation theory, a level shift. Since it only affects the electron when it's very close to the origin, this level shift is, as other effects we have discussed today, proportional to the probability of the electron to be at the center. This is only s electrons are effected.

What is the effect in terms of energy? Well, it's clear the Coulomb potential is weakened. Therefore, this effect, the volume effect weakens, decreases the binding energy of the electron. So we have two effects now-- we have the volume effect, which is the stronger the bigger and the heavier the nucleus is.

So it's largest for heavy nuclei. And the mass effect, or the effective mass effect, is of course largest for the lightest nuclei, with the extreme example of positronium. Any questions?

Well, we have five minutes left. But Cody.

AUDIENCE: What sort of scales are associated with the volume effect?

PROFESSOR: Pardon?

AUDIENCE: What sort of energy scales are associated with the volume effect? [INAUDIBLE] comparable?

PROFESSOR: What energy is-- no, it's actually-- wait. Let's estimate it. You're working with rubidium. What is your isotope shift in rubidium between 85 and 87?

AUDIENCE: I actually don't know.

PROFESSOR: Isn't it 170, 90-- no, I'm getting confused now with [INAUDIBLE]. So many people work with rubidium. What is the difference in transition frequency between rubidium-85 and -87?

AUDIENCE: [INAUDIBLE].

PROFESSOR: It's much more than gigahertz. You really have to tune your laser. I think if you look at the wave per cell, you will never accidentally see a rubidium-85 line. I just don't recall the number.

AUDIENCE: [INAUDIBLE].

AUDIENCE: [INAUDIBLE] together, you can see both of them.

PROFESSOR: OK. And for the mass effect, we said it's sort of-- then they would be comparable. The mass effect is easy to estimate, because the mass correction is one part in a few thousand. So that would mean on the order of 10 to the 10 gigahertz.

So the volume effect-- it really depends. It's tiny for light elements. Rubidium is already heavy. So right now I would say they are comparable. But since it's of interest, I will give you more accurate numbers on Wednesday. Any other questions? Yes?

AUDIENCE: Sorry. Could you explain the graph of the previous page, how the lines are joined off?

PROFESSOR: The potential?

AUDIENCE: Yes.

PROFESSOR: Yeah. So what happens is-- so if we're being cryptic, this is the charge distribution. And what I'm doing now is I'm solving Laplace equation. I'm solving Laplace equation and integrating from r equals infinity. And as long as I'm outside the charge radius, I get the 1 over r Coulomb potential. But the moment I heat the surface of the nucleus, I continue to indicate Laplace equation. But what is now inside is a smaller and smaller charge. I can also say I use a form of Gauss's law.

So I'm therefore not continuing on the 1 over r. And if you look at *Jackson,* or if you look at maybe a PSET you have solved, the 1 over r potential becomes now a parabola. And so what I wanted to sort of indicate here is once you heat the surface of the nucleus, you're not continuing on the 1 over r trajectory.

You have in a wave which is continuous and has a continuous deriviative-- you have to fit in a parabola. And for the heavier nucleus, this leads us to this potential. As for the lighter nucleus, the potential is deeper. And that explains why the binding energy for heavier nuclei is smaller than for lighter nuclei. Yes?

AUDIENCE: So for the other orbitals, is it exactly zero or [? near to ?] zero?

PROFESSOR: OK. For the other orbitals, what we have to do is-- and actually, you have a homework assignment to do it for hydrogen and the proton. You take the difference between the actual potential and the Coulomb potential. So you take the difference. And the difference is your perturbation operator for the finite size of the nucleus. And now you take this perturbation operator between your wave function and calculate the lowest order of the expectation value.

For the s electron, you can immediately factor out the probability for the electronic s equals 0. But s-- we discussed, if you have orbital angular momentum, let me just scribble it down here, the wave function is proportional to r to the l.

So therefore, you have actually an r to the l-- the wave function is exactly 0 only at r equals 0. And then it slowly grows. So therefore, given the finite size of the nucleus, you will get a tiny, an absolutely tiny effect if you integrate a wave function, r to the l, over your perturbation operator. So it's not mathematically zero. But for all practical purposes, it vanishes. Nancy.

AUDIENCE: For the different nuclei-- for example, in rubidium-- is mass and volume affecting anything? Or is [INAUDIBLE] structure also important in these isotopes? Because the nuclear structure would be different [INAUDIBLE].

PROFESSOR: Oh, yeah. When we talk isotope effects, I was talking about the isotope effects of mass and volume. But different isotopes will, in general, have different magnetic moments or different quadrupolar deformations. So what I discussed about hyperfine structure also applies to isotopes.

I only separated it, because usually when you don't have isotopes, you don't talk about, like, sodium. Who has ever talked about the mass shift or volume effect in sodium? Usually you don't, because sodium has 100% natural abundance in sodium-23.

So therefore, the hyperfine effects, they lead to observable splittings even if you have only one isotope. But in general, yes, different isotopes differ in all four effects-- the mass effect, the volume effect, the deformation effect, and the magnetic moment effect.

AUDIENCE: [INAUDIBLE] mass and volume effects are used more than [INAUDIBLE] splitting? Because I find there is a different rate for different isotopes. Like, in the starting of the lecture, you were talking about adding two positrons to the alpha particles. That would change [INAUDIBLE].

PROFESSOR: Oh, yeah, this would change. But you can separate those effects, because I mentioned that in hyperfine structure, the center of mass of the energy levels is the same. So if you see a splitting but take the center of mass, then the center of mass will only depend on volume and mass effects.

OK. Let's continue on Wednesday.