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5.111 Principles of Chemical Science, Fall 2008
Transcript – Lecture 6

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PROFESSOR: All right. As everyone finishes getting settled in, why don't you take 10 more seconds on the clicker question here, and let's see how you did on that this, this is very similar to the clicker question that we had on Friday. OK, so let's get started here. It looks like we are doing a lot better. We now have 77% getting the correct answer, we only had about 30-something percent on Friday for a very similar question. So if you're not in this 77%, let's quickly go over why, in fact, this is the correct answer, $.9 \times 10^{-18}$ joules.

So I'm using the same kind of tricky language that we'd used before, not to trick you, but so that you're not tricked in the future. So if we're talking about the fourth excited state, and we talk instead about principle quantum numbers, what principle quantum number corresponds to the fourth excited state of a hydrogen atom.

STUDENT: Five.

PROFESSOR: Five. OK. So, hopefully that cleared up for some of you why you got the wrong answer. So we know that we're in the $n = 5$ state, so we can find what the binding energy is here. The ionization energy, of course, is just the negative of the binding energy. We know that binding energy is always negative, we know that ionization energy is always positive. So hopefully, putting all those things together, if you looked at this question again we'd get 100% on it, that our only option here is $.9$, and that it's not the negative, it's the positive version, because we're talking about how much energy we have to put into the system in order to eject an electron.

All right. And today we're going to mostly be talking about wave functions of electrons, but before we get to that, I wanted to review one last thing that's back on to Friday's topic, which was when we were solving the Schrodinger equation, or in fact, using the solution to the Schrodinger equation for the energy, the binding energy between an electron and a nucleus. And when we talked about that, what we found was that we could actually validate our predicted binding energies by looking at the emission spectra of the hydrogen atom, which is what we did as the demo, or we could think about the absorption spectra as well.

And what we predict as an energy difference between two levels, we know should correspond to the energy of light that's either emitted, if we're giving off a photon, or that's absorbed if we're going to take on a photon and jump from a lower to a higher energy level.

So we came up with two formulas, which are similar to the two that I'm showing here. The formula tells us the frequency of the light that's emitted or absorbed based on the energy difference between the two levels that we're going between, that the electron is transitioning between.

You'll notice that there's a little bit of a difference in these equations here from the ones from the other day, which is that you have this z squared value in there. So these are both called Rydberg formulas for figuring out the frequency of light emitted or absorbed, and before we were looking at the Rydberg formula specifically for the hydrogen atom, and now that we have this z squared term in the formula here, we're now talking about absolutely any one electron atom.

And it should make sense where we got this from, because we know that the binding energy, if we're talking about a hydrogen atom, what is the binding energy equal to? Negative Rydberg over what? Yes. So, it's negative Rydberg constant over n squared. But if we're talking more generally about any one electron atom, now we have a more general equation for the binding energy, which has this z squared term out in front of it, right, so it's negative z squared times the Rydberg constant all over n squared.

So, essentially when we're talking about these equations up here, all we're doing is talking about the regular Rydberg formulas, but instead we could go back and re-derive the equation for any one electron atom, which would just mean that we put that z squared term in the front.

So when you solve certain types of problems, such as problems later on in the second half of your p-set, if you need to talk about the frequency of light emitted or absorbed for a one electron atom, such as lithium plus 2, for example, then you would need to plug in z , and remember the z value for lithium would just be 3. The z value for hydrogen, of course, is 1, and that's why this term falls out of that equation when we're talking specifically about the hydrogen atom.

So, just to finish our review of what we talked about on Friday, when we're thinking about transitions between two different states, and we're talking about a situation where the final state, the n final, is greater than n initial, in this case, are we talking about absorption or are we talking about emission? Hearing a little bit of a mix here.

In fact, we're talking about absorption when n final is greater than n initial. We start at this lower energy state and go up -- that means we need to absorb a photon, we have to take in energy. Specifically, we have to take in this exact amount of energy in order to bump the electron up to the higher energy level. So that means that when instead we start high and go low, we're dealing with emission where we have excess energy that the electron's giving off, and that energy is going to be equal the energy of the photon that is released and, of course, through our equations we know how to get from energy to frequency or to wavelength of the photon that we're talking about.

All right. So that's all I'm going to say today in terms of solving the energy part of the Schrodinger equation, so what we're really going to focus on is the other part of the Schrodinger equation today, which is solving for ψ .

So we're going to for ψ , and before that, we're going to figure out that instead of just that one quantum number n , we're going to have a few other quantum numbers

that fall out of solving the Schrodinger equation for what ψ is. We're also going to talk more about what ψ actually means.

When we first introduced the Schrodinger equation, what I told you was think of ψ as being some representation of what an electron is. We'll get more specific here, more specific even than just saying you can think of it as an orbital. We'll really think about what ψ means. And in doing that, we'll also talk about the shapes of h atom wave functions, specifically the shapes of orbitals, and then something called radial probability distribution, which will make sense when we get to it.

But, as I said before that, we have some more quantum numbers to take care of, because it turns out that when you solve the Schrodinger equation for ψ , these other quantum numbers have to be defined. When we talked about binding energy, we just had one quantum number that came out of it. And that quantum number was n , which was our principle quantum number, and we know that n could be equal to any integer value, so, 1, 2, 3, all the way up to infinity. And this quantization that comes out of having n is what gives us the quantization of different energy levels. That's why we can't have a continuum of energy, we actually have those quantized points.

So, it turns out that n is not the only quantum number needed to describe a wave function, however. There's two more that you can see come out of it. And the first is l , and l is our angular momentum quantum number, and it's called that because it actually dictates the angular momentum that our electron has in our atom. And when we talk about l it is a quantum number, so because it's a quantum number, we know that it can only have discrete values, it can't just be any value we want, it's very specific values. And unlike n , l can start all the way down at 0, and it increases by integer value, so we go 1, 2, 3, and all the way up. But also unlike n , l cannot have just any value, we can't go into infinity. l is limited such that the highest value of l is $n - 1$. We can't get any higher than that.

So, it would be a good question to ask why are we limited -- clearly there's this relationship between l and n , and we can't get any higher than $n - 1$. We can actually think about why that is, and the reason is because l is our angular momentum. It describes the angular momentum of the electron. So another way to think about that is just the rotational kinetic energy of our electron. And we know that n describes the total energy, that total binding energy of the electron, so the total energy is going to be equal to potential energy plus kinetic energy. So if we say that l is just talking about our kinetic energy part, our rotational kinetic energy, and we know that electrons have potential energy, then it makes sense that l , in fact, can never go higher than n . And, in fact, it can't even reach n , because then we would have no potential energy at all in our electron, which is not correct.

So, that's the second quantum number. And the third one is called m , it's also m sub l . This is what we call the magnetic quantum number, and we won't deal with the fact of its being the magnetic quantum number here -- that kind of tells us the shape of the orbital or the way that the electron will behave in a magnetic field, but what's more relevant to thinking about the limits of this number is that it's also the z component of the angular momentum.

So since it's a component of the angular momentum, that means that it's never going to be able to go higher than l is, so it makes sense that, for example, it could start at 0 and then go all the way up to l . But since it is a component it can have a

direction, too, so can go up between negative l and positive l . So the allowed values for m sub l are going to be negative l , all the way up to 0, and then up to positive l .

So, if we think of just an example, we could say that $4 l$ equals 2, what would be our lowest value of m sub l ? Yup. So m sub l could equal negative 2, negative 1, 0, 1 or 2. So we could have five different values of m sub l .

So, those are our three quantum numbers. So if, in fact, we want to describe a wave function, we know that we need to describe it in terms of all three quantum numbers, and also as a function of our three positional factors, which are r , the radius, plus the two angles, θ and ϕ . So, we have now a complete description of a wave function that we can talk about.

So, we can think about what is it that we would call the ground state wave function. We knew from Friday, when we talked about energy, that ground state was that n equals 1 value, that was the lowest energy, that was the most stable place for the electron to be. But now we need to talk about l and m as well. So now when we talk about a ground state in terms of wave function, we need to talk about the wave function of 1, 0, 0, and again, as a function of r , θ and ϕ . So this is our complete description of the ground state wave function.

So, a lot of you talked about different types of orbitals in high school, I'm sure, or in previous courses, and it might be less common that you actually talked about a wave function that was labeled like this. We're used to labelling orbitals as an s , or a p , or a d , for example, but it turns out that these correlate to those letters that we're more used to seeing. Does anyone know what the 1, 0, orbital is also called? Yeah. And specifically it's the 1 s , so not just the s , but the 1 s orbital.

So, using the terminology of chemists, which is a good thing to do, because in this course we are all chemists, we want to make sure that we're not using just the physical description of the numbers, but that we can correlate it to what we understand as orbitals, and instead of 1, 0, 0, we call this the 1 s orbital. The reason that we do this is because this is another way to completely describe it. The n designates the shell, so that's what this number is here, we're in the first shell. The l is what we call the sub shell. And instead of having a there, what we have here is an s .

So, if we look at what the other sub shells are called, essentially we're just converting the number to a letter. l equals 0 is s , what is l equals 1? Um-hmm, it's the p . What about 2? d , and 3? Yup, so 3 is f . So these names, they don't really make any sense if we're looking at them why they're called past s p and f , and it turns out that it comes from spectroscopy terms that are pre-quantum mechanics where, for example, this is called the sharp line, I think the principle, the diffuse, and the fundamental. It doesn't even make sense now, they're not used in spectroscopy anymore, but this is where the names originally came from and they did stick. So, we being chemists, we'll call that 1 s instead of 1, 0.

In addition to having another name to denote l , we also have another name for the m designation here. So, for example, when l is equal to 0, we're going to find that we have to call -- we have to specify what m is as well. All right. So, when we have, for example, l equal to 1, what kind of orbital is this? The p orbital. And for example, we could also in this case, have m is equal to 0. If m is equal to 0, in this case we would call it the p z orbital, so we would have the subscript z here.

Similarly, if m is equal to either plus 1 or minus 1, we would in turn call it the p_y orbital, or the p_x orbital. So you should know that any time m is equal to zero when we are talking about p orbitals, that it's the p_z . The p_y and the p_x are actually a bit more complicated, they're linear combinations of the m plus 1, and the m minus 1 orbital, where 1 is the positive linear combination, and 1 is the negative linear combination. You're not responsible for that, you're not responsible for correlating plus 1 to y , minus 1 to x . Just know that you have plus or minus 1, for our class, you can call it either x or y , either is fine, because it's a little bit more complicated than just the 1:1 translation between, for example, m equals and having a p_z orbital.

All right. So let's look at some of these wave functions and make sure that we know how to name all of them in terms of orbitals and not just in terms of their numbers. Once we can do that we can go on and say okay, what actually is a wave function, but first we need to know how to describe which ones were talking about. So we saw that our lowest, our ground state wave function is $1, 0, 0$. We can call that $\psi_{1,0}$, is how we write it as a wave function. We said that's the $1s$ orbital. We also know how to figure out the energy of this orbital, and we know how to figure out the energy using this formula here, which was the binding energy, which is negative r_h , and instead of n , we can plug it in because n equals 1, so over 1 squared, and the actual energy is here.

So, our next level up that we can go is going to be the n equals 2 energy level, but we also have an l and an m value, so our lowest l is going to be a there. So we'll call that $\psi_{2,0}$, wave function. What will we call that in terms of orbitals? Yup, so that's the $2s$ orbital. So something I actually wanted to point out that I forgot to here is you'll notice that there's no subscript to the s . We said we have a subscript to the p , for example, that describes what m is equal to. The reason that we have no subscript to the s , is because the only possibility for m when you have an s orbital is that m has to be equal to 0. So we just assume it, you don't actually have to write it because there is, in fact, only one possibility.

We can also figure out the energy of this orbital here, and the energy is equal to the Rydberg constant. The negative of the Rydberg constant now divided by 2 squared. So we can go on and do this for any orbital or any state function that we would like to. So, for example, if we talk about the $2, 1, 1$ state label, that's just $\psi_{2,1,1}$. What, in this case, would be our orbital? $2p$ what? OK, good, I heard mixed answers, which is correct. So you can either write $2p_x$ or $2p_y$, whichever one you want is fine. And again, you'll notice that our energy is absolutely the same for an electron in that $2p_x$ orbital and in the $2s$ orbital. So that's true for a hydrogen atom, it doesn't matter if you're in a p or an s orbital, their energies are the same.

Then we can also talk about the $2, 1$, state function, which would be $\psi_{2,1,0}$. What is this orbital? Yup. And there's only one correct answer here, which is to $2p_z$. Is the energy going to be the same or different as up here? It's going to be the same energy. Again, the reason for that is because the energy only depends on the n value here, it doesn't depend on l or on m .

So finally, if we talk about our last example of when n is going to be equal 2, we can have $2, 1$ for l and then minus 1 for m . We can re-write this as $\psi_{2,1,-1}$. And then our orbital is going to be just the opposite of whatever we said it was up here. So if you said $2p_x$ the first time, say $2p_y$ this time. And again, our energy is going to be the same where we again only depend on the n value.

All right. So hopefully we're pretty comfortable naming any type of wave function using the chemist terminology. Let's switch to a clicker question and just confirm that that is, in fact, true. So what's the corresponding orbital if we talk about this state, 5, 1, 0? And you can go ahead and give 10 seconds on that.

OK. All right, 77%. So, that's OK, you don't have to memorize things as I speak, you just need to go back and look at this and make sure you understand how to name it and that you'll be able to, for example, by next class, get a similar clicker question correct, and good job to the 77% that did get it. So I think we're safe to move on here.

And I just want to point out that now we have these three quantum numbers. The reason there are three quantum numbers is we're describing an orbital in three dimensions, so it makes sense that we would need to describe in terms of three different quantum numbers. And the complete description, as I said, is from n , l and m . And when you talk about n for an orbital, it's talking about the shell -- that shell is kind of what you picture when you think of a classical picture of an atom where you have 1 energy level, the next one is further out, the next one's further away. That's kind of your shell that we're discussing. l is the sub shell here, and then we have m , which is finally the complete description of the orbital. And what you can see is that for any n that has an l equals 0, you can see here how there's only one possibility for an orbital description, and that's why we don't need to include the m when we're talking about an s orbital.

The other thing that we know, which is what we were just discussing when we were going through the table is how this all relates to energy. And I want to really highlight here we're talking about for a hydrogen atom -- orbitals with the same n value have the same energy. Some of you might be saying in your heads, wait a second, I happen to know, I happen to remember from high school, that p orbitals have different energies than, for example, s orbitals. And that is not true for one electron atoms. We're going to get to more complicated atoms eventually where we're going to have more than one electron in it, but when we're talking about a single electron atom, we know that the binding energy is equal to the negative of the Rydberg constant over n squared, so it's only depends on n .

So, for example, if we're talking about the n equals 2 state, all of these four orbital descriptions are going to have the same energy. And we can generalize to figure out, based on any principle quantum number n , how many orbitals we have of the same energy, and what we can say is that for any shell n , there are n squared degenerate orbitals. And the word degenerate simply means same energy, so you have n squared orbitals that are of equal energy when they're degenerate.

So, let's look at where this comes from with an energy level diagram here. So what you can see is again, we've got this ground state. So if we go to the ground state, what you see is we're at that lowest energy level, and we only have one possibility for an orbital, because when n equals 1, that's all we can do. So that's the 1 s orbital -- we have n squared or 1 degenerate orbitals. When we talk about the n equals 2 state, we now have 2 squared or 4 degenerate same energy orbitals, and those are the 2 s orbital. And then we also have the l being equal to 1 orbital, so those are going to be the 2 p_x , the 2 p_z , and the 2 p_y orbital. All four of these orbitals have the same energy, they're degenerate.

And as we go up the next energy level, which is based on n equals 3 principle quantum number, well now we have again the s , so we have the $3s$ orbital, we're going to have three $3p$ orbitals, right, so we'll have $3p_x$, $3p_z$, and $3p_y$, and now we're actually also going to have five different possible l equals 2 orbitals. Does anyone remember the l equals 2? Yes, everyone remembers. Good. So we have five possible d orbitals. We'll call these here the $3d_{xy}$, as the subscript, the $3d_{yz}$, the $3d_{z^2}$, the $3d_{xz}$, and the $3d_{x^2 - y^2}$.

So, what do you need to know here? What you need to know is that when m equals 0, it's $3d_{z^2}$. That's it. Again, these other p -- or the d_{xy} , d_{yz} , those are going to be those more complicated linear combinations, you don't need to worry about them. Eventually you will, at least, need to know the labels and know a little bit more about them. And in the second half of this course, Professor Drennen's going to talk to us about transition metals in depth, and that's when we'll really delve into d orbitals. For right now, you can kind of put the d orbitals in the back of your head. You need to know how to think about them in the same way we think about s and p orbitals, but for example, you don't yet need to know what all of the names are except for this $3d_{z^2}$ here. So we'll wait on that until we start talking more specifically about atoms where the d orbital becomes very significant.

So, what we can see is this degeneracy. So what we know now is we can start thinking about the next step because we can fully describe the energy of orbitals, and we can fully describe a complete orbital in terms of its three quantum numbers, and its three positional variables, r , θ , and ϕ . So next we can think about okay, what is actually a wave function, and for example, what might the shape of different wave functions be.

So essentially, what we're asking for here is the physical interpretation of ψ , of the value of ψ for an electron. And it turns out that the answer to can we have this physical interpretation of thinking about what ψ means, the answer is really no, that we can't. There's no classical way to think about what a wave function is. There's no classical analogy that explains oh, this is what you can kind of picture when you picture a wave function. And that's somewhat inconvenient because we're working with wave functions, but it's a reality that comes out of quantum mechanics often, which is that we're describing a world that is so much different from the world that we observe on a day-to-day basis, that we're not always going to be able to make those one-to-one analogies.

But luckily we don't have to worry about how we're going to picture all this, now that I said that, because even though there's no physical interpretation for what a wave function is, there is a physical interpretation for what a wave function squared means. So when we talk about a wave function squared, we're taking the square of the wave function, any one that we specify between n , l and m , at any position that we specify based on r , θ , and ϕ . And if we go ahead and square that, then what we get is a probability density, and specifically it's the probability of finding an electron in a certain small defined volume away from the nucleus. So it's a probability density. The important point here is it's not just a probability, it's a density, so we know that it's a probability divided by volume.

And the person we have to thank for actually giving us this more concrete way to think about what a wave function squared is is Max Born here. And actually after the Schrodinger equation first was put forth, people had a lot of discussions about how is it that we can actually interpret what this wave function means, and a lot of ideas

were put forth, and none of them worked out to match up with observations until Max Born here came up with the idea that we just square the wave function, and that's the probability density of finding an electron in a certain defined volume.

And it's very helpful because it gives us a way to think about it. We can't actually go ahead and derive this equation of the wave function squared, because no one ever derived it, it's just an interpretation, but it's an interpretation that works essentially perfectly. Ever since this was first proposed, there has never been any observations that do not coincide with the idea, that did not match the fact that the probability density is equal to the wave function squared.

So, also about Max Born, just to give you a little bit of a trivial pursuit type knowledge, he not only gave us this relationship between wave function squared, he also gave us Olivia Newton-John. This is her grandfather, I don't know if you can see from the eyes, I feel like there's a little bit of a resemblance there. So, I don't know what she grew up hearing about when she went to her grandparents' house, but it might have been wave function squared. So, a little tidbit of knowledge for you that's somewhat trivial.

Then back to the non-trivial knowledge that is not trivial at all, in fact, is OK, how do we think about this probability density now that we have a little bit more of an idea.

We know that it's a density, it's not an actual probability. So, one way we could look at it is by looking at this density dot diagram, where the density of the dots correlates to the probability density. So, what you see is near the nucleus, the density is the strongest, the dots are closest together. As you get far away from the nucleus, the dots get farther and farther apart, meaning the probability density at those volumes far away from the nucleus is going to be quite low, eventually going to almost zero, although it turns out that it never goes to exactly zero, so if we're talking about any orbital or any atom, it never actually ends, it never goes to zero. But it turns out the probability is only significant within one angstrom. So you can either say that electrons are very, very tiny or that they're never ending, and both are pretty accurate ways to think about what an atom is.

So, that's probability density, but in terms of thinking about it in terms of actual solutions to the wave function, let's take a little bit of a step back here. I have yet to show you the solution to a wave function for the hydrogen atom, so let me do that here, and then we'll build back up to probability densities, and it turns out that if we're talking about any wave function, we can actually break it up into two components, which are called the radial wave function and angular wave function. So, essentially we're just breaking it up into two parts that can be separated, and the part that is only dealing with the radius, so it's only a function of the radius of the electron from the nucleus. And we abbreviate that by calling it r , which is specified by two quantum numbers, and an l as a function of little r , radius. And we have the angular wave function, which is specified by l and m , and it's a function of the two angles when we're describing the position of the electron, so θ and ϕ .

So, let's look at what this actually is for what we're showing here is the $1s$ hydrogen atom. If you look in your book there's a whole table of different solutions to the Schrodinger equation for several different wave functions. So this is the $1s$, you can look it up if you're interested for the $2s$, or $3s$, or $5s$, or whatever you're curious about. But what I'm going to show you here is the $1s$ solution. So you can see there's this radial part here, and you have the angular part, you can combine the two

parts to get the total wave function. And what you can see is we have this new constant that we haven't seen before. So what do you see in there that is new?

Yeah. This is a sub-nought. That's a new constant for us in this course. This is what's called the Bohr radius, and we'll explain -- hopefully we'll get to it today where this Bohr radius name comes from, but for now what you need to know is just that it's a constant, just treat it like a constant, and it turns out to be equal to 5.29×10^{-9} picometers or about $1/2$ an angstrom.

The more important thing that I want you to notice when you're looking at this wave equation for a 1s atom, is the fact that if you look at the angular component of the wave function, you'll notice that it's a constant. It doesn't depend on theta, it doesn't depend on phi. No matter where you specify your electron is in terms of those two angles, it doesn't matter the angular part of your wave function is going to be the same.

So, what does that mean for us? Well, essentially what that tells us is that these s orbitals are spherically symmetrical. That should make sense, right, because they're only dependent on r. How far you are away from the nucleus in terms of a radius, they don't depend at all on those two angles, they're independent of theta and they're independent of phi.

So, what I'm showing in this picture here is just an electron cloud that you can see. Think of it as a probability density plot. And what here is just a graph of the 1s wave function going across some radius defined this way, and you can see that the probability -- well, this is the wave function, so we would have to square it and think about the probability. So this squared at the origin is going to be a very high probability, and it decays off as you get farther and farther away from the nucleus or from the center, and that's independent of the angle.

So, let's look at these probability plots of different s orbitals here, and up top here, we have the probability density plot and what you can see is what I just said, a very high probability density in the nucleus, decays as you go out. And what is plotted below is the actual wave function, so you can see it starts very high and then it decays down. More interesting is to look at the 2s wave function. So, if we look at the bottom here and the actual plot of the wave function, we see it starts high, very positive, and it goes down and it eventually hits zero, and goes through zero and then becomes negative and then never quite hits zero again, although it approaches zero.

So, at this place where it hits zero, that means that the square of the wave function is also going to be zero, right. So we can see if we look at the probability density plot, we can see there's a place where the probability density of finding an electron anywhere there is actually going to be zero.

So we can think of a third case where we have the 3s orbital, and in the 3s orbital we see something similar, we start high, we go through zero, where there will now be zero probability density, as we can see in the density plot graph. Then we go negative and we go through zero again, which correlates to the second area of zero, that shows up also in our probability density plot, and then we're positive again and approach zero as we go to infinity for r.

So, what this means is that when we're looking at an actual wave function, we're treating it as a wave, right, so waves can have both magnitude, but they can also have a direction, so they can be either positive or negative.

So, for example, if we were looking at the actual wave function, we would say that these parts here have a positive amplitude, and in here we have a negative amplitude. And when we're looking at the probability density graphs, it doesn't make a difference, it's okay, it has no meaning for our actual plot there, because we're squaring it, so it doesn't matter whether it's negative or positive, all that matters is the magnitude. But when we're thinking about actual wave behavior of electrons, it's just important to keep in the back of our head that some areas have positive amplitude and some have negative.

So we'll talk about this more we get into p orbitals and bonding is where it's going to become an issue. So I just want to kind of introduce that idea here. Because if we think about wave behavior of electrons and we're forming bonds, then what we have to do is have constructive interference of 2 different electrons, right, to form a bond, we want to add together those probabilities. So we want to have constructive interference to form a bond, whereas if we had destructive interference, we would not be forming a bond. So that's where you have to think about whether it's positive or negative. You don't have to think about it right now, but you might have heard in high school talking about p orbitals, the phase, sometimes you mark a p orbital as being a plus sign or negative sign. Did any of you do that in high school at all? A little bit, yeah. So, that's having to do with the actual wave function. So, that'll become more relevant later, bonding actually, a couple lectures down the road. But I just want to introduce it here while we do, in fact, have the wave function plots up here.

But a real key in looking at these plots is where we, in fact, did go through zero and have this zero probability density. We call that a node, and a node, more specifically, is any value of either r , the radius, or the two angles for which the wave function, and that also means the wave function squared or the probability density, is going to be equal to zero.

So, we can see in our 1 s orbital, how many nodes do we have? There's no nodes, yeah. It looks like we hit zero, but we actually don't -- remember that we never go all the way to zero, so there's these little points if we were to look really carefully at an accurate probability density plot, it would never actually hit zero. And then, for example, how many nodes do we have in the 3 s orbital? two. That's correct. So we have two nodes in the 3 s orbital.

We can actually specify where those nodes are, which is written on your notes. For the 2 s orbital, at $2a_0$, so it's just 2 times that constant a_0 , which is the Bohr radius. And for the 3 s, we have one at $1.9a_0$, and one at $7.1a_0$.

We can also specify what kind of node we're talking about. We'll introduce in the next course angular nodes, but today we're just going to be talking about radial nodes, and a radial node is a value for r at which ψ , and therefore, also the probability ψ^2 is going to be equal to zero.

So, when we're talking about an s orbital, since there is no angular dependence, and it only depends on r , every single one of our nodes is actually going to specifically be

a radial node, right, because these are, for example, this 2 a nought is a value of r , a value of the radius, no matter which way you go around at which there's going to be a node at which there is zero probability density of finding an electron there.

So, it's very easy to calculate, however, the number of radial nodes, and this works not just for s orbitals, but also for p orbitals, or d orbitals, or whatever kind of work of orbitals you want to discuss. And that's just to take the principle quantum number and subtract it by 1, and then also subtract from that your l quantum number.

So what you can do for a 1 s is just take 1 minus 1 and then l is equal to 0, so you have zero radial nodes. And that matches up with what we saw. If we try this for the 2 s, we have 2 minus 1 minus 0. So what we should expect to see is one radial node, and that is what we see here in the probability density plot. And then if we think about 3 s, we want to start with 3, we subtract 1, again l is equal to 0, so minus and we have two radial nodes.

So, this should be pretty straight forward, let's see if we can get close to a 100% on this one, which is how many radial nodes does a 4 p orbital have? And let's give 10 seconds on that, make you think fast here.

OK, so most people were correct, or well, the majority, at least, were correct. And seeing that it's a 4 p has two nodes -- let's just write this out since not everyone did get it correct.

So, if we're talking about a 4 p orbital, and our equation is $n - 1 - l$, the principle quantum number is 4, l is 1 -- what is l for a p orbital?

STUDENT: 1.

PROFESSOR: 1. So, I tricked you a little, I guess I didn't put an s up there and that's what we had been talking about, so that was probably the issue. But what we find is that we have two radial nodes. All right. So we can switch back to our notes here.

So, doing those probability density dot graphs, we can get an idea of the shape of those orbitals, we know that they're spherically symmetrical. We're not going to talk about p orbitals today, we're going to talk about p orbitals exclusively on Friday, and as I said, d orbitals you'll get to with Professor Drennen.

But we can also think when we're talking about wave function squared, what we're really talking about is the probability density, right, the probability in some volume. But there's also a way to get rid of the volume part and actually talk about the probability of finding an electron at some certain area within the atom, and this is what we do using radial probability distribution graphs. And what that is the probability of finding an electron in some shell where we define the thickness as Δr , some distance, r , from the nucleus.

So, think about what we're saying here. We're saying the probability of finding an electron at some distance from the nucleus in some very thin shell that we describe by Δr . So if you think of a shell, you can actually just think of an egg shell, that's probably the easiest way to think of it, where the yolk, if you really maybe make it a lot smaller might be the nucleus. And let's also make our egg perfectly symmetric and perfectly round.

But still, when we're talking about the radial probability distribution, what we actually want to think about is what's the probability of finding the electron in that shell? Think of it as that egg shell part.

So, we can do that by using this equation, which is for s orbitals where the radial probability distribution is going to be equal to $4\pi r^2$ times the wave function squared, $d r$. That should make sense to us, because when we talk about a wave function, we're talking about a probability divided by a volume, because we're talking about a probability density. So if we actually go ahead and multiply it by the volume of our shell, then we end up just with probability, which is kind of a nicer term to be thinking about here.

So, of course, if we're talking about a perfectly spherical shell at some distance, thickness, $d r$, we talk about it as $4\pi r^2 d r$, so we just multiply that by the probability density.

We can graph out what this is where we're graphing the radial probability density as a function of the radius. And what you see is that at zero, you start at zero. And so, the radial probability density at the nucleus is going to be zero, even though we know the probability density at the nucleus is very high, that's actually where is the highest. The reason in our radial probability distributions we start -- the reason, if you look at the zero point on the radius that we start at zero is because we're multiplying the probability density by some volume, and when we're not anywhere from the nucleus, that volume is defined as zero. So, it's a little bit artificial that we're seeing that zero point there.

So, actually I want you to go ahead in your notes and circle that zero point and write "not a node." This is not a node because a node is where we actually have no probability density. So this, where we start at zero is not a node, is the first thing to point out. And as we get further and further from the radius, the volume we're multiplying it by actually gets bigger and bigger, because you can see how the volume of that little thin shell is going to get larger and larger as you get further away.

So there's some distance where the probability of actually finding an electron there is going to be your maximum probability. And that's what we label as r_{mp} , or your most probable radius.

This is the point at which your probability is highest for finding an electron. This is equal to a sub nought for a hydrogen atom, and we remember that that's just our Bohr radius, which is . 5 2 9 angstroms. And basically, what that means is you can actually find an electron anywhere going away from the nucleus, but you're most likely to find that you have the highest probability at a distance of a sub nought, or the Bohr radius.

So, I said I'd tell you a little bit more about where this Bohr radius came from, and it came from a model of the atom that pre-dated quantum mechanics, and Neils Bohr is who came up with the idea of the Bohr radius, and here is hanging out with Einstein, so he had some pretty good company that he kept. And what you need to remember when we're thinking about this model of the atom is that in 1911 it had already been discovered that we have an electron, and we have a nucleus, and there needs to be some way that those two hang together, but it was not for another 15

years that we actually had the Schrodinger equation that allowed us to understand the interaction fully between the electron and the nucleus.

So all that Bohr, for example, had to go on at this point was a more classical picture of the atom, as you can see on the left side of the screen there, which is the idea that the electrons actually somehow just orbiting the nucleus. And even though he could figure out that this wasn't possible, he still used this as a starting point, and what he did know was that these energy levels that were within hydrogen atom were quantized. and he knew this the same way that we saw it in the last class, which is when we viewed the difference spectra coming out from the hydrogen, and we also did it for neon, but we saw in the hydrogen atom that it was very discrete energy levels that we could observe. He knew the same thing that had been observed by that point.

So, what he did was kind of impose a quantum mechanical model, not a full one, just the idea that those energy levels were quantized on to the classical picture of an atom that has a discrete orbit. And what he came out with when he did some calculations is that there's the radius that he could calculate was equal to this number a sub nought, which is what we call the Bohr radius, and it turns out that the Bohr radius happens to be the radius most probable for a hydrogen atom.

And the reason we won't talk any more about this Bohr model is because, of course, it's not correct. So we're not going to spend too much time on it here. But we can see, for example, one reason or one way in which is not correct. Because what it tells is that we can figure out exactly what the radius of an electron and a nucleus are in a hydrogen atom. That's a deterministic way of doing things, that's what you get from classical mechanics.

But the reality that we know from our quantum mechanical model, is that we can't know exactly what the radius is, all we can say is what the probability is of the radius being at certain different points. so, that's a more complete quantum mechanical picture of what is going on here. So if we superimpose our radial probability distribution onto the Bohr radius, we see it's much more complicated than just having a discrete radius. We can actually have any radius, but some radii just have much, much smaller probabilities of actually being significant or not.

So, I think we're a little bit out of time today, but we'll start next class with thinking about drawing radial probability distributions of more than just the 1 s orbital.