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**PROFESSOR:** All right, let's just take 10 more seconds. All right, so someone want to explain why this is the correct answer? And we have a syringe highlighter. You probably never had something like this before.

**AUDIENCE:** OK, so the fourth excited state is  $n$  equals 5. And then IE is opposite of the negative number shown. So it would be a positive reaction.

**PROFESSOR:** Right. So IE is always going to be positive. And you have to pay attention to what  $n$  equals when you're in the excited state.

So we've been talking about the hydrogen atom and binding energies. What comes out of the Schrodinger equation? We have the binding energies that come out. And we also have wave functions. So today we're going to be talking about wave functions, which are often referred to as orbitals in chemistry, for the hydrogen atom.

So when you solve the Schrodinger equation, you get out this information about wave functions. And what comes out of it is these quantum numbers. And we already saw quantum number  $n$  coming out. But there are three quantum numbers that are going to come out of the Schrodinger equation. And those three quantum numbers are necessary to describe the wave function or the orbital.

So we have  $n$ , the principle quantum number. We've already talked about that. And we've already seen that  $n$  is an integer. So I'll just put that down here. So  $n$  can equal 1, 2, 3, on to infinity. So this describes the energy level or the shell.

Then we have  $l$ , which we haven't talked about yet. So that's the angular momentum quantum number. So it tells you about the angular momentum. It also tells you about the subshell or the shape of the orbital. And so  $l$  is related to  $n$ . And it can be 0, 1, 2, 3, onward to  $n$  minus 1. So its biggest number is  $n$  minus 1.

Then we have  $m$ , the magnetic quantum number. And we often see this also listed as  $m$  sub  $l$

because  $m$  is related back to  $l$ . And this is equal to minus  $l$ , dot, dot, dot, to 0, dot, dot, dot to plus  $l$ . And  $m$  describes the behavior in a magnetic field. It also describes the orientation of the orbital with respect to an axes. And it tells you about the specific orbital in question. So we need all three of these to describe any orbital.

All right, so let's look at this in a slightly other way. So we're going to have lots of different sort of nomenclatures for the same thing. So to describe an orbital, we need those three quantum numbers. We need  $n$ ,  $l$ , and  $m$ . And this can also be expressed as our wave function sub  $nlm$ . And again, we talked about this last time. We're going to talk more about it. So our wave function is also described by  $r$ , the radius, and  $\theta$  and  $\phi$ , which are two angles. And we're going to talk a lot about those today.

So the wave function for the ground state is abbreviated wave function sub 1, 0, 0. Because it's the ground state. So  $n$  equals 1, and  $l$  and  $m$  are 0. So what you see down here, the 1, 0, 0, refers back to what is  $n$ , what is  $l$ , what is  $m$ .

And this also has another name. So in the terminology of chemists, we call the wave function 1, 0, 0 1s, or the 1s orbital.

So let's look again now at the same things we just talked about, but going through kind of chemistry lingo. So again,  $n$  describes the shell or the energy level. Again, it's integers, 1, 2, 3, et cetera.

$l$  in chemistry lingo, the subshell or the shape of the orbital. And instead of listing it this way, we have another way to list it if we're a chemist, and that is s, p, d, f, et cetera. So chemists like numbers, but we also throw in some letters every once in a while.

And then  $m$ , again, designates this orbital orientation or the specific orbital. So for s, there's only s. It doesn't have any other designation, as we'll talk more about later. But for p, we start having suborbitals. And there is a difference in terms of the orientation of this. So we have  $p_x$ ,  $p_y$ ,  $p_z$ . So that's what  $m$  tells us about. So if we have all three of these numbers, we get down to the specific orbital, we can say oh, that's  $p_z$ , for example. So we need all of these three numbers to define the orbital. And this is in then the chemistry lingo.

All right, also a little bit more chemistry lingo. So here we have  $l$  equals 0. So that is the s orbital. When  $l$  equals 1, that's the p orbital.  $l$  equals 2 is the d orbital. And  $l$  equals 3 is the f orbital. And frankly we don't really go much beyond that. And in this part of the course, we're

really only going to be talking mostly about s and p orbitals. We get to d orbitals around Thanksgiving time. So you can look forward to that. And pretty much we're not going to really talk about f orbitals very much at all. You'll need to know some things about them, but we're not going to go into them in any kind of detail.

All right, so if we keep going then, we can think about  $l$  equals 1 or our p orbitals. And then when  $l$  equals 1, then  $m$  can equal 0 plus 1 or minus 1. And when  $m$  equals 0, that's by definition the  $p_z$  orbital. So when you see  $m$  equals 0, that's going to be  $p_z$ . And when  $m$  is plus 1 or minus 1, those are the  $p_x$  or the  $p_y$  orbitals. And this is just something that you need to remember, that  $z$  is the one that's special. It's the one that has  $m$  equals 0.

All right, so we can take all of the nomenclatures now and use it to fill in this awesome table. So this will help you kind of keep track of all the different ways you can designate the same things. And we'll fill this in.

So first, state label. What do I mean by this? By this I mean this one 1, 0, 0 to generate this wave function where we have this 1, 0, 0 listed below the wave function here.

And so now this is just a little color coding. But it's blank in your handout. So  $n$  equals 1, so  $n$  is first.  $l$  is the second number. And  $m$  is the third here. So 1, 0, 0, and what kind of orbital is this? You can just yell it out.

**AUDIENCE:** 1s

**PROFESSOR:** Yep, so that's the 1s orbital. And so the 1,  $n$  equals 1, that's 1s. And now we have our binding energies again. And so we can write those in two different ways. So we saw for the hydrogen atom before what comes out of the Schrodinger equation, that the binding energy of the electron for the nucleus is minus the Rydberg constant  $R_H$ , divided by  $n$  squared. And here  $n$  is 1, so divided by 1 squared. So this is just the value for the Rydberg constant, the negative value. And binding energies, again, are always negative. So we have our first one down.

So now for the second, what number am I going to write here for the state label? You can just yell it out. Yep, 200 or 2, 0, 0. And then you would put it this way where the state label is by the wave function. What orbital is this-- 2s.

And then we also know the binding energies for this. So here we have minus  $R_H$  over  $n$  squared where  $n$  is 2, 2 squared. And we saw this number last time.

So we can keep going. Now we have 2, 1, 1. So we can write that down. We can write it both ways. What orbital is this?

**AUDIENCE:** [INAUDIBLE].

**PROFESSOR:** So it's a 2p. And because  $n$  is plus 1 and not 0, it's either  $x$  or  $y$ . Do we have a different or the same binding energy here? We have the same, right, because it's just over  $n$  squared. We're still talking about  $n$  equals 2, so 2 squared. So it's the same value here.

Now we have  $m$  equals 0. So we write 2, 1, 0. And now what is that orbital?

**AUDIENCE:** [INAUDIBLE].

**PROFESSOR:** 2p<sub>z</sub>, right, because that's  $m$  equals 0, by the definition I gave you. So we know that one for sure. And again, the energies are going to be the same.

And then the last one, so now we write 2, 1, minus 1. And now it's again a 2p orbital. And it's either  $y$  or  $x$ . And the energies are going to be the same.

So these are just a table that kind of interconverts different ways that you will see things written. And you'll know if you see it one way, what orbital to put down. And we can also think about the binding energies for those particular orbitals, or for electrons in those particular orbitals.

All right, so why don't you try a clicker question on this? 10 seconds. Ah, excellent. Right.

So you're getting the hang of this. It's great. Some things, it's always nice when there's some things that are pretty straightforward. So  $n$  equals 5,  $l$  equals 1, which means p orbital and  $m$  equals 0, means p<sub>z</sub>.

So let's think now about these orbitals again. And we looked at that table and saw that if we were talking about  $n$  equals 2, they all seem to have the same energy. So for a hydrogen atom-- and it will get more complicated when we start talking about things with more than one electron. But for a hydrogen atom, orbitals that have the same  $n$  value have the same energy.

So here we have  $n$  equals 1,  $l$  equals 0. This is our 1s. We have  $n$  equals 2, our 2s, and our 2p orbitals.  $n$  equals 3, we have our 3s, 3p, and 3d. And in this case, all these orbitals are what's known as degenerate with respect to each other. They have the same energy.

And so for any  $n$  with a hydrogen atom, or any one electron system, for  $n$  shells, there  $n^2$  orbitals degenerate-- or for any  $n$  there are  $n^2$  degenerate orbitals. So they're all going to be the same energy. And that changes when we go to more complicated systems. But for hydrogen, this holds.

So now I'm going to tell you why you should care a little about these energy levels again. And today you're going to hear in their own words from a graduate student in the physical chemistry division.

[VIDEO PLAYBACK]

- My name is Benjamin Ofori-Okai. I'm entering my third year of graduate school in the chemistry department here at MIT. And the work that I've been focusing on for the last couple of years involves nanoscale magnetic resonance imaging or nano MRI.

When you think of typical MRI, what comes to mind for most people is the image of a brain scan or a heart scan or some sort of organ scan inside the human body. The way that MRI works now, the way that you take a picture of anything in your body is you use water. And the reason that you use water is because it's made up of hydrogen atoms and oxygen atoms. And hydrogen atoms actually generate a magnetic signal. And so you can take a picture of that.

The idea behind nano MRI is that you want to take a picture. You want to do the same kind of imaging, but on a considerably smaller scale. We have this probe which is sensitive to local magnetic fields. And the way that the probe works is that you have these electrons. There's a ground state for these electrons and two excited states for these electrons, which are actually degenerate with each other. And degenerate means that they just have the exact same energy level.

As you move the probe around, anything that's in the environment that generates a magnetic field will change what the energy levels of these two excited states is. So when you're far away, there's no change and they're exactly the same. And as you get closer and closer, these levels start to split. And what we actually care about is what is the splitting between these two levels, because that's what tells us what the magnetic field is.

In traditional MRI, the probe that we use, the thing that measures the fields, itself is very, very big. It's person sized. The probe that we're using in this nano MRI is nanometer sized. So this gives us the ability to look at things that are on the nanometer scale. And to give you a sense

of size, that's like  $1/10,000$  the width of a human hair. So that includes viruses, cells, parts of proteins, not just the entire protein.

And on top of that, we'll be able to look within objects. So you're not just sensitive to what's on the surface. You can actually see how are things-- what's the constitution? What's the makeup of things within the object that you want to image?

So the long term goal, the one thing that I'd really love to see this technology be able to do is say, OK, we've got this virus. Let's just see how it works. Let's watch it in real time. Let's see if we can see how it attaches to cells and invades them and ultimately kills them.

[END PLAYBACK]

**PROFESSOR:**

OK, so I always think this is a great time of year to show this video because pretty much viruses, I think, start to be on people's minds. Everyone has sinuses and colds and other things going on. And so understanding, we're still very far away from having a real cure for the common cold. So I think it's very timely to be talking about, talking about this research.

I'll also use this to remind myself to tell you that if you qualify for extra time on the exam, you should get me your form for the exam. And it reminded me to say that because Ben, who is a former TA for this class, always proctors the extra time folks. So you'll get to meet him in real life if you qualify for extra time on exams.

So hydrogen is in fact important. I'm excited to get on to elements that have more than one electron. But hydrogen actually does turn out to be extremely important. A lot of imaging, as you heard from Ben, is based on hydrogen. So we're spending a lot of time on hydrogen, but hydrogen really, really is an important element.

So continuing on now, what is the significance of this wave function? Why do we care about this? And so really, we're interested in trying to understand not just how tightly the electron is bound to the nucleus, but kind of how the electrons exist around the nucleus. And so the wave function really gets at this. It gets at the probability density, the likelihood that you'll find an electron at a certain location, the probability per unit volume.

And again, this is a three dimensional problem. So our wave function depends on a radius  $r$ . But it also depends on two angles, the  $\theta$  and  $\phi$ . And so you can kind of think of those as latitude and longitude if you will. And so we want to know what the probability is that an electron will be at a certain  $r$ ,  $\theta$ , and  $\phi$  position in a particular small unit volume in that

area. How well can we understand where the electron is? And this gives rise to a lot of the properties of the elements. So probability density, density per unit volume.

So really, when we're talking about where electrons are, we're thinking about a shape of an orbital, a shape of a probability density of where that electron might be. So now we're going to think about shapes.

So we can define a wave function in terms of two properties, a radial wave function and an angular wave function. So again, the wave function has these three things. We are considered with a radius and these two angles. So we can rewrite this, breaking up these two different components-- the radial component that depends on the radius-- so that's easy to remember, radial, radius-- and the angular component that depends on the angles. So the nomenclature here is pretty good. All right, so we have these two components.

So now I'm going to show you a table that is largely from your book. Don't let it scare you. You do not need to memorize any of these things. And I'm showing this to you because I want you to believe me about certain properties of these two functions. So here they are solved. You can look them up. Actually I think we just typed a new copy of this so it was easier to see. If you find any typos, please let me know.

But there's a couple of important points. So on this side, we have the radial wave function, and over here we have the angular wave function, for various values of  $n$  and  $l$ . So again, not an exhaustive list here. And a lot of these are written in terms of  $a_0$ , which is the Bohr radius, which is a constant, 52.9 picometers.

All right, so now let's just consider the ground state. So we'll start with that lowest energy state or most stable state, the 1s orbital for the hydrogen atom. So we have our wave function 1, 0, 0 here. And this is 1s up here. Again,  $n$  equals 1.  $l$  equals 0. So that's 1s. And  $z$  for hydrogen atom is 1. So I've gotten rid of all  $z$ 's to make it a little simpler.

So here we have the radial wave function times the angular wave function, which is listed up here. And the thing that I really want you to notice is that for all of the s orbitals, this is a constant. So this is always the angular component for all s orbitals. And in fact, there are no angular components in there. So all 1s, 2s, 3s, all have this same constant.

And that leads to a very important property of s orbitals, which is that they're spherically symmetrical. In other words, they're independent of those angles, of  $\theta$  and  $\phi$ . And so that

means that the probability of finding the electron away from the nucleus is just going to depend on  $r$ . There's only  $r$  in this equation. The angles are not part of the equation. So  $s$  is spherically symmetrical. The probability of finding the electron just depends on the radius.

So we can draw a picture, or multiple pictures, of what that could look like. And these are three common plots. So I'll tell you that on your handout, the plots are listed on one page, and then the plots are shown on the next page. And I'm going to kind of go back and forth between things. So the plots-- don't have to write this down. They're on the other page. But if you want to pay attention to which kind of plot goes with which plot.

So these are three different ways to, quote, visualize. And some people say, can you give me another visualization? We're really just trying to think about probabilities of finding electrons here. And so you can't sort of take a picture of an orbital. So these are just different ways to help people think about that possible distribution of electrons around the nucleus.

All right, so one thing that everyone's feeling pretty good about is that it should be spherically symmetric hole for an  $s$  orbital. And so we have a circle. And so the probability density, which is shown in this plot-- and the probability density parts are basically just dots where the more concentrated the dots are, the higher the probability density for that particular-- the probability for that particular volume exists. So in here there are sort of more dots and then less dots as you come out. And so that is a circle, which is what? It's symmetrical. So you can always recognize a  $1s$ . You have this symmetrical thing. So this is the wave function squared, is this probability density plot.

Another kind of plot that you can see looks at the radial wave function plotted against the distance  $r$  here, distance from the nucleus. And then a third kind of plot is another probability plot, like this one up here. But instead of the dots indicating the higher probability density, you have a radial probability distribution. And so at the nucleus, at  $0$ , well then the probability goes up. The electron is not going to crash into the nucleus, so it won't be right on top of the nucleus. But as you get out a little bit farther away, there's a high probability that it's there. And then that decreases again.

So the top one and the bottom one both talk about the probability of finding an electron in a particular unit. And I'll give you just a little more definition of this. And this is on the same page above those different plots.

So the radial probability distribution reports on the probability of finding an electron in the

spherical shell at some little distance  $dr$  from the origin. And one thing that comes out of this, which is pretty important, is the most probable value for that distance  $r$ , which is denoted  $r_{mp}$ , so most probable distance. And for a hydrogen atom, this is  $a_0$ , the Bohr radius. And you can see it expressed in different units over here. And from the plot, that will be the top part of the plot, the most probable distance. In this case, that's the Bohr radius for the hydrogen atom.

So we have now these three different kinds of plots that you'll see. And I want to point out that they're different plots. Sometimes people are thinking that there is sort of one plot and they're trying to read one of them as probability density, and that's not what it is. So we'll look at these again.

All right, so going back and we'll just look at them again now that we sort of talked about what all of them are, again, we have our sort of dot density, probability density plot, our wave function plot, and our radial probability distribution plot. And for  $1s$ , we have the dots closer to the nucleus here. Probability goes up and goes down. And here, you're thinking about this as the amplitude of finding an electron as you move away from the nucleus. So  $1s$  is pretty simple. And I think these plots are a lot more meaningful when we go on to look at other orbitals.

So let's think about those other orbitals. And we'll finish the other plots. So this is just-- you can actually stay, in this case. So we're going a lot of back and forth today. So here is your table that we had before. And here's  $1s$ . Here's  $2s$ . Here's  $3s$ . These terms are in fact different, as you can see. But the angular term, as we mentioned before, is still the same. So that means  $2s$  and  $3s$  are still symmetrical. So we're still thinking about the probability of finding an electron in some volume as just going out as a distance of  $r$ .

So let's look now at the three plots, and compare those plots. And this is the one on your handouts we looked at. I showed you this. And now we have all of these three plots together here. And in the comparison of these three, I think it helps differentiate what you're seeing in these plots.

So important point, they're spherical.  $1s$ ,  $2s$ ,  $3s$ , they're all spherical. And here we see the dot density increase. And then the dot density goes to 0. And that's known as a node. So a node is a value of  $r$  or  $\theta$  or  $\phi$  for which the wave function and wave function squared, or the probability density, is 0. And in this particular case, the type of node that we're seeing is a radial node. And so that's a value of  $r$  for which the wave function, wave function squared

probability density is 0.

So it goes to 0. We have a node, a radial node. Then there's more probability. And then it increases, and then starts decreasing again. And so if you plot this with the radial wave function versus  $r$ , you see it go down. And it crosses the zero line here. And that's the node. And that's at  $2a_0$ . And then it goes back up.

And this plot often bothers people. They're saying, what, there's now negative probability? No, these are not the probability diagrams. This is thinking about the amplitude of finding an electron. So we don't have to worry. It can have a positive or a negative phase to it. And if you look at this plot, the radial probability distribution plot, then you'll see that actually the radius, the most probable radius is in this region over here. And you see that this is concentrated dots up here.

So if we think about these two, which are really probability distribution diagrams, we're thinking about the probability of finding an electron. You have a probability in here close to the nucleus. Then you get a node. And then you have another probability, high probability of finding the electron. In fact that's the most probable radius here for 2s. And then it decreases.

So this line shows you what a radial node looks like in all three plots. In this probability diagram, wave function squared plot, it looks like there's just an empty space, no dots at all. Down here, it's where it crosses the line. And in the bottom plot, it is where you go up and down and again touches the line before going back up. So you should be able to look at these plots and think about what they mean.

For 3s, we see the same thing. But now we have an intense spot in the middle near the nucleus. That is indicated down here. There is probability of finding the electron near the nucleus. Then there's a node. And that's in this plot where it crosses the line and in this plot where you have the empty space. Then you have more probability of finding the electron. You have another bump here. And then we have another node, indicated by touching the zero line here, touching here. That's at  $7.1a_0$ . And then we have more probability of finding the electron. And this is where the most probable radius is at  $11.5$ .

So again, you need to be able to look at these diagrams and recognize what constitutes a radial node. And a node is a place where there is no probability that you're going to find an electron.

So now let's think about how many nodes, or radial nodes you should have when you have different types of orbitals. And this is just a similar diagram to what I just showed. This is the wave function squared, probability diagram. And now instead of blue you have orange dots, but otherwise should be the same-- so for 1s, for 2s, and 3s.

So for the 1s orbital, we can calculate how many radial nodes that we should have by using this handy formula,  $n - 1 - l$ . So for 1s we have 1 minus 1. And  $l$  is 0. So we have zero radial nodes. And we can see that from that diagram there are zero radial nodes.

2s now-- 2,  $n$  is 2. Minus 1, minus 0-- so that's one radial node. And the radial node, again, in this kind of diagram is the empty space. And that radial node is at  $2a_0$ .

For 3s, we have  $n$  equals 3 minus 1 minus  $l$ , which is still 0. So we have two radial nodes. And so again, the empty space here at  $1.9a_0$  and then at  $7.1a_0$ . So why don't you give this a try now and tell me what kind of radial nodes you would expect for 4p.

OK, 10 seconds. These are pretty fast. Yep. So again, we have to do  $n$ , which is 4, minus 1. And then what is  $l$  in this case-- 1. So that gives you 2. All right, so 4 minus 1 minus 1 or 2 radial nodes.

All right, don't put your clickers away. Let's try something else. So now tell me which of these is correct both in terms of the indicated number of radial nodes and in terms of the plot for a 5s orbital.

All right, let's just do 10 more seconds. We're varying it up in terms of the plots. So maybe someone want to say what the right answer is here? Yeah?

**AUDIENCE:**

So by the formula we just did, that has four radial nodes. And if you look at the graph of one, there's three, and then there's another one at the origin. So that's four radial nodes. Right? Right?

**PROFESSOR:**

Actually, I just realized that-- let me count here. So this answer here, we should have four radial nodes. That is correct because we have  $n - 1 - l$ . Actually, I think this is going to this-- this should be going to this answer, because if we count 1, 2, 3, 4. Sorry, the new plot is highly confusing. I have to count.

So the one at the origin should actually not count.

**AUDIENCE:** It doesn't count?

**PROFESSOR:** This is not a node. So we have 1, 2, 3, 4, should be our four radial nodes. Because that's a nucleus, and there isn't one there. But that doesn't count as a node. So this should be here. I guess that's-- right. But thank you very much, and [INAUDIBLE], here. You were brave enough to answer. Yeah, there's a question?

**AUDIENCE:** Should there also be a certain number of peaks in the graph as well as nodes?

**PROFESSOR:** Yeah. So if you look at the peaks, these are really hard to draw. And I think that's partly what the problem is. But when we look later in the handout where they're drawn a little bit more carefully, it does increase. So there are different numbers. So we'll have nodes going down here. But then we'll have more distributions. But often the ones as you go along, it does indicate where the most probable radius is as the taller ones, and that it's usually drawn at the end. So we have some plots and I'll point this out later. We're going to look at more plots, don't worry.

So if anyone's good at drawing those, let me know, because they're really hard to draw. So a lot of them are copied from the book, but then they don't copy very well.

So let's consider other kinds of nodes. And we're going to come back to radial nodes. All right, so what about p orbitals? So here we have our table again. These are our p orbitals over here. And we have our  $n$  equals 2 cases here and our  $l$  equals 1. So these are x, y, and z-- so our 3p orbitals over here. And the important point is not to memorize what these values are. But now all of a sudden we have dependence on angles.

So we're going to have an angular component to these. And that means the probability density as you go out from the nucleus doesn't just depend on  $r$  anymore. It depends on  $\theta$  and  $\phi$ , which are sort of the equivalent to latitude and longitude, if you're thinking about geography.

All right, so let's see what that looks like. So that means then the p orbitals are not spherically symmetric, because it depends on angle. So you just don't go out and have the probability depend on the radius and it's symmetrical in all the different directions.

And here are what some of them look like. These figures are in your handouts. Here are some other figures. So the orbitals consists of two lobes. So you could view this as a lobe up here and a lobe down here. Or you have these lobes as these two different colors over here. And

the lobes are separated by a nodal plane. And the nodal plane is a plane on which the probability of finding the electrons is 0.

So in the top drawing, the nodal plane is drawn as a plane. And in the bottom drawings, you don't see a plane. You just see an empty space between the lobes. So empty space here, empty space here, empty space there. And so if it helps you to kind of think about an actual plane in between, that's good. Or you can just think that there's a break between these nodes.

And again, the nodal plane, there's no probability of finding an electron in the nodal planes. And the nodal planes are at the nucleus. Therefore, there is zero probability of finding a p electron at the nucleus. s can get pretty close to the nucleus. But with a p orbital, there's a nodal plane there. No electrons are going to be at the nucleus.

So now if you're going out from the nucleus, the probability of an electron, finding it, if you're going out in this direction, you're not going to do very well. If you're going in this direction, you should do a lot better. So here the angular components really matter. That defines the shape of the orbital. And where you're going, what direction you're going in, what angles you're going in matters in terms of whether you're going to find that electron or not.

So another way to think about this in sort of these nodal planes-- so here we'll just define what plane it is. So we have our  $p_z$  orbital. That's a nodal plane then in x and y. And so x and y are over here. Our  $p_x$  orbital is going to be in-- or the nodal plane is going to be in yz plane, so over here. And  $p_y$  will be in xz plane. So again, these nodal planes, there's no electron density there. And these arise from these angular nodes in the wave function.

So angular nodes then or these angular nodal planes are values of theta and phi for which the wave function, wave function squared are 0. So this is very different from the s case where we only had radial nodes. But now, when in the p orbitals where the angular component matters, they're angular nodes as well.

So we can think about how to calculate the angular nodes. So total nodes is going to be equal to  $n - 1$ . The angular nodes is  $l$ . And as we saw before, the radial nodes are  $n - 1 - l$ .

So let's have more practice in calculating these. And then we'll look at some more diagrams. So for 2s, total nodes-- and you can just yell this out. Total nodes will be what?

**AUDIENCE:** 1

**PROFESSOR:** 1-- 2 minus 1 or 1. Angular nodes are?

**AUDIENCE:** 0

**PROFESSOR:** 0. For 1s, there is none. And if you forget,  $l$  equals 0 there. Radial nodes is going to be?

**AUDIENCE:** 1

**PROFESSOR:** Right, 2 minus 1 minus 0, or 1. All right, let's try 3-- or sorry, 2p is next. Total nodes? 1 again, so 2 minus 1 or 1. Angular nodes? 1--  $l$  equals 1 here. And radial node? Right, 2 minus 1 minus 1, or 0. So since there's only one total node, if you figured out there was one angular node, you could even realize that there had to be zero there. It's a way to check maybe your equations.

All right, so let's try for 3d now. How are we doing? All right, let's just do 10 more seconds.

And let's just work that out over here. So total nodes for 3d, we have 3 minus 1 or 2. Angular nodes,  $l$  equals 2 for d. So radial nodes, we have 3 minus 1 minus 2, or 0.

All right, so bring these handouts on Wednesday because we need to go back and look at more radial probability diagrams. And talk more about nodes.

All right, let's just do 10 more seconds. OK, good job everyone.

Let's look through this a little bit. And you can sort of-- everyone can help. Yell out some responses. So this was 2s. And that was the correct answer. Which type of orbital is this-- 2p. And if you couldn't read this information here, you should have been able to read the information about the nodes. What equation is that for nodes? Yeah,  $n$  minus 1 minus  $l$ , for what kind of nodes?

**AUDIENCE:** Radial.

**PROFESSOR:** Radial nodes, right. So if you know what it means if  $l$  equals 0 versus  $l$  equals 1, and you knew this was  $l$ , then you could tell if it was an s orbital or a p orbital. And then whether it was 2 or 3p is from the  $n$ . So even if you couldn't read this, if you knew that expression, then you were OK.

What kind of orbital was in plot C? This was a 3s.  $l$  equals 0. And then this is a what, 3p and?  $l$

equals 2. Louder. D, right? So do 3px, 3py, and 3pz have different plots? No, they wouldn't have different plots.

So we'll continue to look at this. And we're going to be starting with the handout from last time. And so let's continue with Monday and continue with these radial probability distributions.

So this is again from Monday, page 6. We're talking about orbital size. And we've already looked at this a little bit today. So we should be able to go through this now in a little bit more detail. You've already thought about it.

So here we have the 2s orbital. And we're going to have one node using our equation that you just told me,  $n - 1 - l$ . And when we go from 2s to 2p, here we have no radial nodes. And we can look at  $r$  and  $p$ , which is the radius of the maximal probability of finding an electron. And you can note that when you go from the 2s to the 2p, the radius actually decreases. So the most probable radius for 2p is less than that of 2s.

Now let's consider the 3,  $n$  equals 3. So we have the 3s situation over here. And so  $l$  equals 0. We have two nodes here. And now if you look at the radius, the axis over here, you'll see that the most probable for 2s is close to  $5a_0$ , where  $a_0$  is the Bohr radius. And over here you're talking between 10 and 15. So we see an increase in size going this way.

And then when we go from 3s to 3p-- so here we have  $3 - 1 - l$ , which is 1. So we have one node, down to 3d,  $3 - 1 - 2$ , zero nodes. And you see that there is a decrease here in the most probable radius. So, OK, interesting.

All right, so 3d has the smallest, next 3p, next 3s. So there's two different trends we're seeing. One, as we increase  $l$  within the same  $n$  number, and one going from a smaller value of  $n$  to a larger value, and then again within the 3, within the  $n$  value as we change  $l$ .

So again, to say the same thing in a different way, as  $n$  increases from 2 to 3, the radius, most probable radius or the size increases. So from here to here we have an increase in size. I just want to make sure people have time to kind of get all of this down, but it should be good. I have a little picture that just shows they're very different in size.

So we'll go back to this again. And then as I also said, as  $l$  increases for a given  $n$ -- so from  $l$  equals 0 to  $l$  equals 1 here, then we have a decrease in the size. So you can see the most probable radius moves over. And then here is another within  $n$ . And  $n$  equals 3. We see,

again, this decrease. So those are the two trends that you observe when you look at these radial probability distributions.

So for exam one next week, you should be able to draw distributions like this. You should be able to tell me how many radial nodes you have for different types of orbitals. And you should know these trends in size. So I think in the exam instructions it says up to a 5 case. You don't have to go on forever to be able to draw them, but you should be able to look at these and tell what kind of orbital it is and where the nodes are, be able to draw where the nodes are-- one node here, one, two, one node here. This kind of thing will be on the exam next week.

So there's something that's a little counterintuitive when it comes to this size issue. And that has to do with how this correlates to the amount of shielding, and as we see later, to the energy levels.

So only electrons in the s state here really have any kind of substantial probability that they'll be close to the nucleus. So we have this little blip over here that is close to the nucleus, that at are very small radii, very small values of  $r$ . Even though the most probable is out here, if we compare 3s to 3p and look at where the electrons are that are closest to the nucleus, they're quite a bit farther away than in the 3s. Or there's more probability that there's going to be some closer here. And then the closest probability over here for these electrons is quite a bit farther away. So we see these circles kind of move out.

So even though the overall radius, the sort of size of the whole thing is decreasing, the probability that there are going to be electrons really close is actually going in the opposite direction. And so what this means is that s electrons are the least shielded because there's higher probability that they'll be some close to the nucleus. There's more penetration close to the nucleus. So s electrons are the least shielded.

And we're going to come back to this when we move on to today's handout. This is really important in terms of thinking about the energy levels. And I'm going to have these diagrams on the handout for today. So we'll see them again.

All right, so before we move to that handout, we've got to finish our quantum numbers and talk about electron spin. So the fourth quantum number describes the spin on the electron. And we already saw the magnetic quantum number  $m$ . We saw  $m_{\text{sub } l}$ . And now we have  $m_{\text{sub } s}$ . And the s stands for spin. So there's some nomenclature that actually makes sense.

So there are two possible spin values for an electron. And  $s$  can equal plus  $1/2$ , spin up, or minus  $1/2$ , spin down. And here are some little pictures of that.

So this  $m_s$  term, this spin magnetic quantum number, completes the description of the electron. But it's not dependent on the orbital. To describe an orbital completely, you only need three quantum numbers. But to describe the electron, you need four.

And that is shown, again, here on this picture, or on this slide. You need three quantum numbers. You need  $n$ ,  $l$ , and  $m_l$  to describe the quantum number, describe the orbital completely. But you need a fourth one, this  $m_s$  to describe the electron. So if you see wave function  $n$ ,  $l$ ,  $m_l$ , you say that's telling me what the orbital is. And if we add the  $m_s$ , then you look at that and say oh, that's going to tell me all the way to the electron what is going on.

So this final quantum number led to what we know as Pauli's exclusion principle, which is that no two electrons can have the same four quantum numbers. They can't have the same-- no two electrons can have the same spin, in other words.

So if we are drawing a configuration for neon with 10 electrons, we are going to have with one electron being up spin, the next one is going to be down. Because if we had two of these both going up, they would have the same four quantum numbers. And that's not allowed by Pauli's exclusion principle.

So when you have two here, one spin up, one spin down in an orbital, then we say that those electrons are paired. And an important thing that kind of comes out of all of this is that one orbital can't hold more than two electrons. If it did, there'd be another electron that would have the same four quantum numbers. Because you need three quantum numbers to describe the electron, or the orbital. We need three to describe, say, that it's  $n$  equals 1, and then its  $s$  state. So we need those other ones to describe the orbital and then the fourth one to describe the spin. So if we add another electron, you'd have two that were spin up, say. And that just wouldn't work. So you cannot have more than two electrons in the same orbital.

And this makes a lot of sense when you think about why you would be putting electrons in orbitals that are higher energy. Why not just keep putting him in the low energy orbital? And it's because you can't do that. You can't put more than two electrons in. And so therefore once you've filled a lower energy orbital, you've got to move up to the next lowest energy orbital.