All right. I am going to start with Friday's lecture notes because there was a significant amount on them that I had not finished up yet. We had finally gotten to the point where we were talking about what does a wave function mean, what is the physical significance of it and how does it actually represent the presence of an electron? And what we saw was that the physically significant representation of the wave function, if you have some wave function Psi labeled by three quantum numbers, n, l and m. And, of course, it is a function of r, theta and phi. The physically significant quantity was this wave function squared. That wave function squared, that was interpreted as a probability density. The wave function squared has units. It has units of inverse volume. It is a density. It is a probability per unit volume. Now, as an aside, because someone asked me, I should tell you that the more comprehensive definition of the probability density is Psi, not squared, but Psi times Psi star, where Psi star is the complex conjugate. Because it turns out that some wave functions are imaginary functions. And so, if you took an imaginary function and squared it, then you would still get an imaginary function after it. And then it is hard to interpret an imaginary function as a probability density. And so the more comprehensive definition is Psi times Psi star, where Psi star is the complex conjugate of Psi. And, when you multiply Psi by Psi star, if Psi is a complex function, well, then you get a real function. This is the more comprehensive definition of the probability density, Psi times Psi star. We won't use that. I just wanted to let you know about it. So, probability density. Not only do we want to know something about the probability density. We also want to know something about the probability of finding the electron some distance away from the nucleus. And, to do that, what we were talking about was this quantity, this radial distribution, the radial probability distribution. And what that is, is the probability of finding an electron in a spherical shell of radius r and distance or thickness dr. For example, if this gray portion here represented the probability density of the 1s wave function in our dot density diagram. Remember, we squared the wave function, got the probability density and then represented it with a dot density diagram, where the density of the dots was proportional to the value of the wave function squared. And, in the case of the 1s wave function, we saw that the probability density was largest right at r equals 0, and that is exponentially decayed in all directions uniformly. That is what that gray part represents. But now, this blue, here, is my spherical shell. It has a radius r, and it has a thickness, here, dr. And the radial probability distribution is asking, what is the probability of finding the electron in this spherical shell? And that spherical shell has a thickness dr. Another way to ask that is the probability of finding the electron between r and r was dr. That is what we wanted to know, and that is what the radial probability distribution tells us. Now, how do you get a value out of that? How do you actually calculate the radial probability? Well, to do that, what we have to know is this volume, here, of the spherical shell. The volume of this spherical shell is just the surface area of that spherical shell, 4 pi r squared, and the volume is times this thickness, this thickness dr. It is a very thin shell. It is an infinitesimally thin shell of thickness dr. Well, if we know that volume, then what we can do is take our probability density, Psi squared, which has units of probability per unit volume. And we are multiplying it, here, by our unit volume. The unit volumes cancel, and we are left with a probability. So, that is our probability of finding that electron in a shell of radius r and a thickness dr. Let's look at the result of calculating the radial probability distribution for the 1s wave function. What did I do? I took Psi squared for the 1s wave function at some value of r, then I multiplied it by 4 pi r squared dr, and I did that for many different values of r and plotted the result here. That is what that radial probability is as a function of r. Well, the first thing you see is that the most probable value of r, or the value of r where the electron has the highest probability of being is at this value, a nought. The most probable value of r is this value, a nought. a nought is what we call the Bohr radius. And today, in a moment or so, I will tell you why it is called the Bohr radius. It has a numerical value of 0.529 angstroms. And so it is most likely that the electron is about a half an angstrom away from the nucleus, making, then, the diameter of the hydrogen atom, on the average, a little bit over one angstrom. That is how we think about the size of a hydrogen atom, is to take this most probable value of r and double it to get the diameter. The most probable value of r, or the most probable distance of the electron from the nucleus, is half an angstrom away. The most probable distance of the electron from the nucleus is not r equals 0 because the radial probability here is zero at r equals 0. That seems a little strange because the other day we plotted the probability density for the 1s wave function. And, when we did that, here is Psi(1, 0, 0) squared versus r, what we saw was that the probability density was some maximum value at r equals 0 and that it exponentially decayed with increasing r. And that is the case. Probability density for the s wave functions is a maximum at r equals 0. But the radial probability here is actually zero at r equals 0. Why? Look at how we defined that radial probability, here. It is Psi squared times this volume element. Our volume element is this spherical shell. And, at r equals 0, the spherical shell goes to a volume of zero. So, our radial probability here is equal to zero at r equals 0. That is really important, that you understand that this radial probability here is always going to be zero at r equals 0 for all of the wave functions that we are going to look at. And we will talk about this a little bit more, the fact that the electron is about a half an angstrom away from the nucleus. But before I do that, I also just want to point out that in your textbook, and sometimes in the notes, that sometimes that radial probability is actually written as the following. It is written as the r squared, the distance variable, times the radial part of the wave function. That is the radial part squared. We talked about the radial and the angular part last time. And the radial part is labeled only by two quantum numbers, n and l. And so, for the 1s, that is n equals 1, l equals 0. Where does this come from? Well, let me just emphasize or explain where this comes from. This radial probability distribution here, we said for the s wave functions, was Psi squared. You could take Psi squared, the probability density, and multiply it by this unit volume or the volume of the shell, 4 pi r squared dr. Let's write that out again, but write it out now so that we write out Psi squared in terms of the radial part and the angular part. Remember, we said last time, for the hydrogen atom wave functions, that Psi is always a product of a factor only an r, which was the radial part, and a factor only in theta and phi.

that Psi is always a product of a factor only in r, which was the radial part, and a factor only in theta and phi, which are the angular parts. Now, what you also have to remember in looking at this is that the angular part for the 1s wave functions, 2s, 3s, all s wave functions, was equal to 1 over 4 pi to the 1/2. If you square that, you are going to get 1 over 4 pi. Therefore, the 4pi's here are going to cancel for the 1s wave functions. And what you are going to have left is this r squared times just the radial part dr. That is why the y-axis in your book is sometimes labeled this way for the radial probability distribution. But this is also important because if you were calculating the radial distribution function for something other than an s wave function. The way you would do it is to take just the radial part of that wave function times r squared, or just the radial part of that wave function and evaluate it at that value of r times r squared dr. You could not, for the other wave functions, take psi squared times 4 pi r squared dr. And that is because the angular part for the other wave functions that are not spherically symmetric is not the square root of 1 over 4 pi. This is a broader definition for what the radial probability distribution function is. It just works out, in the case for the s wave functions, these 4pi's cancel. And so you can write the radial probability for the s wave functions like that. So, those are just some definitions. I want to talk some more about this radial probability distribution function, here, for the 1s wave function. I want to talk about it and also explain why a nought is called the Bohr radius. The reason for that is the following. The nucleus was discovered in 1911, the electron was known before that, and SchrÉ†dinger did not write down his wave equation until 1926. And, in between that, 1911 to 1926, the scientific community was really working very hard to try to understand the structure of the atom. And we saw how the classical ideas, as predicted, would live a whopping 10^-10 seconds. And one of the people who were working on that problem was Niels Bohr. And, in 1919, Niels Bohr of course realized that classical physics fails this kind of planetary model for the atom where you put the nucleus in the center and the electron is going around that nucleus with some fixed orbit. We will call it r. Well, he knew that it was not going to work, that those classical ideas predicted that this would plummet into the nucleus in 10^-10 seconds. But, he said, obviously, that does not happen, so let me just forget classical physics at the moment. Then, what he did was to impose some quantization on this classical model for the hydrogen atom. And the reason he got this idea of quantization is because he already knew the hydrogen atom emission spectrum. He knew that in the hydrogen atom emission spectrum that light of only certain frequencies was emitted. That is, there was some idea that there was something about this hydrogen atom that is quantized. He said, well, let me just ignore classical physics for a moment. Let me give this a circular orbit. But let me quantize something about this hydrogen atom. And, in particular, what he went and did was quantized the angular momentum of that electron. He kind of just pasted the quantization onto a classical model for the atom, because he is trying to work toward explaining what the observations were. When he pasted that quantization onto this classic model, he was able to calculate a value of r. And that value of r is what we call the Bohr radius, a nought, and has the value 0.529 angstroms. That came out of it. And if you calculate for the radial probability distribution function for this model, which is called the Bohr atom, would be one where that radial probability is 1 right here at r equals a nought. In Bohr's model, the electron had a well-defined, precise orbit. The value of r at which it went around the nucleus was given by a nought. He knew exactly where the electron was in his model. This kind of model, which is this classical model, really, is what we call deterministic. It is deterministic because we know exactly where the particle, in this case the electron, is. I want you to contrast it with the quantum mechanical result from the SchrÉ†dinger equation. What you see, in the quantum mechanical result, is that we don't really know where the electron is, so to speak. The best we can tell you is a probability of finding the electron at some value r to r plus dr. That is the best we can do because quantum mechanics is non-deterministic. There is a limit to which we can know the position of a particle. That limit is given by something called the uncertainty principle. The uncertainty principle is not something we are going to discuss, but it tells us that there is a limit to which we can know both the position and the momentum of a particle. And that is the basis for why, here, we have a probability distribution and knowing sort of where the electron is. We don't exactly know where the electron is, here. This is the classical model on which Bohr just kind of pasted the quantization of the angular momentum of the electron onto it. In the case of the SchrÉ†dinger equation, the quantization drops out when you solve the differential equation. It comes out of the equation just naturally. We did not paste it onto it. We did not make an ad hoc kind of representation. That is the big difference here between quantum mechanics and classical mechanics. In quantum mechanics, it can only tell you about a probability. It cannot tell you exactly where the particle is going to be. Questions on that? Okay. Anyway, this value a nought, that is why it is called the Bohr radius. And then it turns out, quantum mechanically, that this value of r, the most probable value of r is, in fact, exactly a nought. In a sense, Bohr was pretty lucky. And this is kind of an accident that he got a nought out of this, and it has to do with the actual form of the Coulomb interaction. But, of course, this doesn't work for anything else, other than a hydrogen atom. Whereas, the SchrÉ†dinger equation, as we are going to see in a moment, is applicable to all the atoms that we know about. So that is the radial probability distribution function for the 1s atom, for the 1s state. We want to take a look at the radial probability distribution for 2s and for 3s. Let me plot those. And you can actually put these lights on here. That is okay. I am going to use this board for a moment. Here is the radial probability distribution function. I can write it as little r times R(2,0) squared of r, or RPD. This is for 2s versus r. And when I do that I get a function that looks like this. And, if I evaluate it here, what is this value of r at which the probability is a maximum? Well, this most probable value of r is 6 a nought. Look at that. The most probable value of r for 1s was a nought. In the case of the 2s state here, the electron, the most probable value is 6 a nought, six times as far from the nucleus. If you have a hydrogen atom in the first excited state, in a sense that hydrogen atom is bigger. It is bigger in the sense that the probability of you finding the electron at a larger distance away from the nucleus is larger. And that, in general, is the case. The radial probability distribution, here, also reflects the radial node that we talked about last time. That radial node is r equals a nought. Radial node is the value of r that makes your wave function go to zero. Notice, again, that this radial probability distribution function right here is zero at r equals 0. This is not a node. This is not a radial node. This is a consequence, right here, of our definition for the radial probability. Our volume element has gone to zero. r equals 0 is never a radial node in any wave function. What about 3s? Well, let's plot 3s. Here is 3s. This is the

radial probability distribution. I take Psi for 3s and square it, multiply by 4 pi r squared dr, and do so for all the values of r, and I am going to get something that looks like this. Now this most probable value of r here, where the 3s wave function is equal to 11.468 a nought. For the second excited state of a hydrogen atom, that electron, on the average, is 11.5 times farther out from the nucleus than it is in the case of the 1s state right here. Again, for that second excited state, that hydrogen atom is bigger in the sense that the probability of it being farther away from the nucleus is larger. That radial probability distribution of the 3s also reflects the two radial nodes in the 3s wave function. The radial nodes are at 1.9 a nought, here, and 7.1 a nought. Again, the value here at r equals 0 is not a radial node. Now, as you look at this, it is tempting to ask the following question. You might want to ask, if the electron can be at these values of r, and it can be at these values of r, and it can be at these values of r, how does the electron actually get from here to here to here if right at r equals 1.9 a nought and 7.1 a nought the probability is equal to zero? Well, you might say maybe this probability isn't exactly zero. It is something small. But I am telling you that it is zero, goose egg, zilch, zippo, nada, cipher, nix, nought. Anybody else have another name? Nil. It is nothing. It is zero. How do you answer that question? Well, it turns out, of course, that it isn't an appropriate question. And the reason it is not is because that question is asked in the framework of classical mechanics. When you ask, how does a particle get from one place to another, you are asking about a trajectory. You are asking about a path. Particles over here, over here, over here, how does it get from one place to another? And, in quantum mechanics, we don't have the concept of trajectories. Instead, what we have to think of is the electron as a wave. And we already know that a wave can have amplitude simultaneously at many different positions. And so it has simultaneous amplitude or probability here, here, and here, all at the same time. We cannot talk about trajectories anymore. And that, again, ties into the uncertainty principle, our inability to know exactly the position and the momentum of a particle at any given instance. The best we can tell you is a probability. We have to change the way we think about electrons. You cannot cast them in the framework of your everyday world. This is part of our world, but you have to go do a specific type of experiment to see this part of the world. That is why it seems so strange to you, because it is not part of your everyday experience. But this world works with different rules that you really do have to accept that it just works differently. Questions? Now, I am going to stop talking about the s wave functions and move on to talk about the p wave functions. With the s wave functions, we talked about the significance of the wave function, probability density, radial probability distribution. We talked about what a radial node was. Now it is time to move onto the p wave functions. And the p wave functions, of course, are not spherically symmetric. And to represent them, we are going to do our dot density diagram again. We are going to take the wave function and square it to get the probability density and then plot that probability density as a density of dots. We the dots are most dense, well, that means the highest probability density. Here is the result for the pz wave function. It is pz because you can see the highest probability, here, is along the z-axis. It is symmetric along the z-axis. Here is the probability density for the px wave function. You can see that the probability density is greatest along the x-axis. It is symmetric along the x-axis. And, if you look really carefully, you can see that there is no probability density in the y,z-plane for the px wave function. And, over here, if you look carefully, you can see that there is no probability density in the x,y-plane for the pz wave function. And here is a py wave function, the probability density of it. The probability density is concentrated along the y-axis. It is symmetric along the y-axis. And, if you look very carefully, there is no probability density, here, in the x,z-plane. Well, the fact that there is no probability density, here, in the x,y-plane, in the case of pz, indicates that we have an angular node. An angular node at theta equal 90 degrees. An angular node is the same thing as a radial node in the sense that it is the value of the angle that makes the wave function be equal to zero. Here is the wave function for pz. You can see that when theta is equal to zero, this wave function is going to be equal to zero. An angular node is the value of theta or phi that makes the wave function be zero. And the consequence, then, is that we have a nodal plane, because everywhere on the x,y-plane, theta is equal to 90 degrees. For the px wave function, the value of the angle that gives you that nodal plane is phi equals 90. That means everywhere in the y,z-plane is phi equal to 90. In the case of py, when phi is equal to zero, well, that is everywhere in the x,z-plane. Everywhere in the x,z-plane, phi is equal to zero. So, that is the angular nodes. In general, and this is something you do have to know, an orbital has n minus 1 total nodes. And what I mean by total nodes is angular plus radial nodes. The number of angular nodes is given by this quantity, l. The quantum number l that labels your wave function always gives you the number of angular nodes. Therefore, if n minus 1 is the total and l is the number of angular, well then, the number of radial nodes is n minus 1 minus l. This is something that you do have to know. If I give you a wave function and ask you how many radial and angular nodes it has, you need to be able to calculate that, and vice versa. Sometimes I will tell you a function has three radial nodes and six or seven angular nodes or something, what is the wave function? So, we go both ways. Well, I also want to take a look at the radial probability distribution functions for the p wave functions. We looked at it for the s wave functions already. I actually want to contrast the radial probability distribution, say, for 2p, here it is, with that of 2s that we looked at a moment ago. Remember, how do you get the radial probability distribution function here for 2p? It is the radial part of the 2p wave function times r squared dr. It gives me the probability of finding the electron a distance between r and r plus dr. Again, what you see is that at r equals 0, that is zero. That is not a radial node. But what I really want to point out here is that the most probable value of r, for the 2p wave function, is actually smaller than it is for the 2s wave function. That is, it is more likely for the electron in a 2p state to be a little closer in to the nucleus than it is for the 2s state. In general, as you increase the angular momentum quantum number, the most probable value of r gets smaller for the same value of n. Similarly, here is the 3s radial probability distribution function that we looked at. Here is a radial probability distribution for 3p. Now, with the 3p, you can see the value of the radial node. You can see the radial probability distribution reflects a radial node, here. And here is the radial probability distribution function for 3d. We did not look at the probability density of 3d. You will do that with Professor Cummins when you talk about transition metals. But here, I just drew in the radial probability distribution for 3d. But the point again that I want to make is here is the most probable value of r for 3s, here it is for 3p, here it is for 3d, again, the most probable

value for 3d is smaller than it is for 3p, than it is for 3s. Again, as you increase the angular momentum quantum number, that most probable value gets smaller. However, ironically, if you actually look at the probability of the electron being very, very close to the nucleus, that probability is only significant for the s wave functions. Look at the 3s wave function. Here, you see that you really do have some probability very close to the nucleus. You don't see that in the 3p wave function. You certainly don't see that in the 3d wave function. Again, in the 2s wave function, you have some significant probability of the electron being really close to the nucleus in 2s, but you don't in 2p. That is important. And it seems in contradiction to the fact that on the average, the most probable value of r gets smaller as l gets larger. These two facts that look contradictory are important. They dictate the behavior of atoms. These two facts seem like kind of loose threads at the moment in the sense that you are probably wondering why I am telling you what I am telling you. But we are going to use that information in a few days, and you will see really the significance of this plot. And this plot will be an important one for you to refer back to. Yes? Probably. I am not exactly sure of the picture you drew in high school, but yes. If the electron in general is further out from the nucleus, that is a higher energy state. The electron is less strongly bound, as we are going to see in the multi-electron atoms here. Oh, no. For the hydrogen no. Let me explain that. For the hydrogen atom, the energies are only dictated by the n quantum number, so 3s, 3p, 3d all have the same energies. Where the energies become degenerate is with a multi-electron atom. And we are going to talk about that and how that reflects here, these wave functions in the next day. That is all I am going to say about the hydrogen atom. Now it is time to move on, to helium. And, of course, the SchrÈ†dinger equation predicts the binding energies of the electrons to the nucleus in a helium atom also very well. But, of course, it is a much more complicated SchrÈ†dinger equation. And I am not even going to write out the Hamiltonian in this case, but I want to show you the wave function here. See the wave function? The wave function is a function of six variables. It is a function of two r's, two distances from the nucleus, one for electron one, one for electron two, two theta's and two phi's. We have six variables for the wave function. And the consequence of this is that our solutions for the binding energies for the electrons in helium or any other atoms are not going to be nice analytical forms. We are no longer going to have e sub n equal minus the Rydberg constant over n squared. If you actually solve for those energies, and you have to do it numerically, you are just going to get a list of numbers, a table of numbers, but not a nice analytical form. If you solve for the wave function, you are not going to get a nice analytical form, like we got for hydrogen. Instead, what you will get is a value for the amplitude of Psi as a function of r, theta and phi. But if you get actually much above three electrons, it turns out that even numerically, you cannot solve the SchrÈ†dinger equation, exactly. You have to use approximations. And we are going to look at the most basic approximation that is used that works, amazingly. It works well enough for us to have a framework in which to understand the reactions of these atoms. And what is that approximation? Well, that approximation is called the one-electron wave approximation or the one-electron orbital approximation. What does that mean? Well, that means this. I am going to take my wave function here for the helium atom, which strictly is a wave function that is a function of six variables, and I am going to separate it. I am going to let electron one have its own wave function and electron two have its own wave function. That is an approximation. In addition, what I am going to do is let the wave function for electron one have a hydrogen-like wave function. I am going to say that it has the 1s wave function, or the Psi(1, 0, 0) wave function of a hydrogen atom. And I am going to let electron two have the Psi(1, 0, 0) wave function of a hydrogen atom. Or, I am going to write it as 1s of 1, for electron one, times 1s of 2, for electron two. Or, another shorthand, I am going to write it as 1s. squared. And, if I continued on, here, it is for lithium. Lithium, the wave function strictly has nine coordinates, but I am going to let every one of those electrons, in the one electron wave approximation, have its own wave function. And I am going to let electron one have a wave function that looks like a hydrogen atom wavefunction. The 1s wave function. The same thing with electron two. And then I am going to let electron three have the 2s wave function of the hydrogen atom. And in simplified notation, that is just 1s squared 2s. And here is beryllium, 16 variables, but I am going to let every electron have its own wave function. And I am going to give electron one the 1s wave function, electron two, the 1s, electron three, the 2s, electron four, the 2s. I can also write that, as you have already done, 1s 2 2s 2. And I can keep going. And these electron configurations that you have been writing down in high school, that is what they are, electron configurations, well, they are nothing more than our shorthand notation for the electron wave functions within this one-electron wave approximation. That is what those were, that you were writing down. Those were a shorthand notation for the wave functions in SchrÈ†dinger's equation within this one-electron wave approximation. Now, one thing you do notice is that I did not, in the case of boron here, let all five electrons be in the 1s state, or let all five electrons be represented by a 1s hydrogen atom wave function. I didn't because of a quantity that you already know about, called spin. You already know that if you are going to put electrons in the 1s state here that one electron has to go in with spin up and the other spin down. And the 2s, spin up and spin down, etc. What is the phenomenon called spin? Well, spin is entirely a quantum mechanical phenomenon. There is no correct classical analogy to spin. Spin is intrinsic angular momentum. It is angular momentum that is just part of a particle, such as an electron. The spin quantum numbers actually come from solving the relativistic SchrÈ†dinger equation, which we did not even write down. When you solve the relativistic SchrÈ†dinger equation, out drops a fourth quantum number. That fourth quantum number we are going to call m sub s. And we find that m sub s has two allowed values. One of those values is one-half and the other is minus one-half. Here, we have a case where the quantum number is not an integer. It is one-half and it is minus one-half. Now, if it helps you to think about the electron spinning around its own axis, like I depict here, well, if that is the case, then the angular momentum quantum number is perpendicular, here ,to this plane in which it is rotating. And you might want to call that spin up. And, of course, if it is spinning in the other direction, well, then the angular momentum vector is pointed in the opposite direction. You might want to call this spin down. If it helps for you to think about this, okay, but remember that this is not correct. This is a classical analogy that we are trying to draw here. We are trying to say that this electron is rotating around its own axis. That is not true. This angular momentum is just an intrinsic part, the intrinsic nature of a particular

its own axis. That is not true. This angular momentum is just an intrinsic part, the intrinsic nature of a particular such as an electron. Next time, I will tell you about Uhlenbeck and Goudsmith. See you Wednesday.