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**PROFESSOR:**

So, a couple of announcements. Tomorrow we've got Quiz Two. Based on Homework Two. And then, Thursday, we'll have the periodic table quiz. I give you the numbers, you give me the letters. And Friday is the last day for the contest. I'll have office hours. I know when others have office hours. I'll be available 4:30 to 5:30 down the hall in my office. Where is Grant's, who's buried in Grant's Tomb? Grant. Where are my office hours held? In my office. Good. Last day. Last day. It was a rough weekend. I can't get a smile, can't get a laugh.

So, last day we looked at the validation of the Bohr model. And we had two pieces of experimental data. First were the hydrogen spectrum lines, measured in 1853 by Angstrom and fit to an equation by J.J. Balmer in 1885. And, secondly, we saw the Franck-Hertz experiment, in which we were able to get the sense that energy levels within a multi-electron atom, like, mercury, those energy levels are also quantized, which gave credence to the quantum condition. Which said that the movement of an electron, the movement of an electron, is quantized.

And then we started looking at the limitations of the Bohr model, problems with the Bohr model. And I said, in two words, fine structure. And we started looking at fine structure. We see that the 656 nanometer line in hydrogen, in point of fact, is a doublet. It's actually two lines very closely spaced. Bohr model is incapable of explaining this.

Zeeman looked at gas discharge tube, measured hydrogen spectrum in a magnetic field, and found line splitting proportional to the intensity of the field. Stark did similar experiments only in an electric field, and also found line splitting, the degree of which was proportional to the intensity of the field. And the Bohr model is incapable of explaining this.

Sommerfeld, in 1916, put a patch on the Bohr model and proposed that the electron moves not only in a circular orbit but also in elliptical orbits. And there's a plurality of these orbits. But overall, the distance from the nucleus to the electron orbits is more or less given by the principal quantum number  $n$ , and the degree of eccentricity is tiny. But, more or less, described by  $n$ . And then to further depict what's going on, he introduced the orbital quantum

number or, as your book calls it, the azimuthal quantum number. And the magnetic quantum number. And further said that the energy of the electron is given by the specifications according to all three quantum numbers.

And then, lastly, in order to get completeness, we jumped ahead in time to 1922 with the Stern-Gerlach experiment, which was the beam of silver. Atoms through a divergent magnetic field, the beam split in two symmetrically about the point at which the beam would land on the slide in the absence of a magnetic field. And that can lead to some deeper thinking by two graduate students in Leiden, Goudsmit and Uhlenbeck, who proposed the notion of electron spin. And from that came the fourth quantum number,  $s$ , and we're going to throw that into the mix even though Sommerfeld didn't give it to us back in 1916. But I just want to move forward with all of them.

And we recognize that  $s$  could take on two values, plus or minus  $1/2$ , or we could call it spin up or spin down. And, as you're going to learn in 802, the convention in electromagnetism is the right-hand rule. That is to say, the thumb indicates the vector and the curl of the fingers indicate the rotation. So we would argue that this is an electron spin from looking top-down anticlockwise and then vice versa.

So that's as far as we got. And so now what I'd like to do is to take a look at the periodic table and get a sense of electron filling. And whether that explains the trends in the periodic table. And for that I'm going to go to table 6-3 in your reading. And all we're going to do, basically, is say, well can we use this idea of  $n$ ,  $l$  and  $m$ , and explain the order of filling in a periodic table. So when  $n$  equals 1,  $l$  must be equal to 0. And the  $m$  must be equal to 0. So that means there's only one orbital. And, in that orbital, we can have two electrons. So we've got the possibility of two different electrons going into the  $1s$  orbital.

Then we go,  $n$  equals 2.  $l$  can take a value of 0. Which is the same as what we had before. Just one orbital in that subshell. Or we can have  $l$  equals 1, in which case  $m$  can take three different values; minus 1, 0, and plus 1. So there's three orbitals there. 3 plus 1 is 4. And that gives us the possibility of putting 8 electrons in. Because this is  $n$ ,  $l$ , and  $m$ . And then we've got the choice of  $s$  plus or minus  $1/2$ .

And we'll do one more. We'll go to  $n$  equals 3. So at  $l$  equals 0, we just have 1. When  $l$  equals 1, we have the same thing as we had with the  $2p$ . And then when  $l$  equals 2, we have what's known as the  $3d$ . Remember the spectroscopists there. They don't like numbers. So they use

s, p, d, f. But we're smart. We can go 0, 1, 2. It didn't hurt us.

And we go minus 2, minus 1, 0, 1, 2. So there's 5. So 5 plus 3 is 8, and 9. 9 times 2 is 18.

Now let's go to the periodic table and see if this reconciles. So, when we have 1s, there's hydrogen, helium. And then the next is  $n$  equals 2. So that should give us 4 times 2 is 8. So, 3, 4, 5, 6, 7, 8, 9, 10. So there's the 8 different electrons that get us all the way over to neon.

And now let's go to  $n$  equals 3. So, I have 1, 2, 3, 4, 5, 6, 7, 8. And then I'm over to 4. 4s. But look, this is saying I should have 18. 18 electrons in  $n$  equals 3. So what I'm pointing out here is that there's a disconnect, there's a disconnect between the populating of electrons just in ascending quantum number, and the way the elements are arranged in the periodic table. There's some other factor at work here. So we want to take a look at what that could possibly be. And, so what we need is to go to a modified energy level diagram. A modified energy level diagram, that can explain what the filling sequence is in the periodic table. And the modified energy level diagram is drawn on the basis of the Aufbau principle. The Aufbau principle. Aufbau, German, meaning construction. I think it actually means out-build. But, anyways, it generates the filling sequence.

So, there are three parts to the Aufbau principle. And the Aufbau principle is going to govern, it's going to govern or direct the electron filling sequence. Directs the electron filling sequence.

So, the first component of the Aufbau principle is the Pauli exclusion principle. Pauli exclusion principle. Wolfgang Pauli was an Austrian. He did his Ph.D under Sommerfeld in Munich, and then he post-docced with Born in Göttingen and on to Niels Bohr Copenhagen. These people worked together. They traveled from lab to lab, and it was a very vibrant conversation going on. Eventually, he became a professor physics in Hamburg.

And the Pauli exclusion principle, simply stated, is that in any electron system, each electron has a unique set of four quantum numbers. A unique set of four quantum numbers. Any atom set, four quantum numbers are unique for each electron. For each electron. So you can think of this as the set of  $n$ ,  $l$ ,  $m$  and  $s$  as sort of the social security number, if you like, for each of the electrons in the set. And he eventually gets the Nobel Prize for this, in 1929. Virtually everybody I'm going to talk about today, with the exception of Sommerfeld, gets the Nobel Prize. Sommerfeld is a very interesting character, though. While he himself never won the Nobel Prize, many, many of his students and proteges won Nobel Prizes, to which you must include that there was something very, very special about the quality of the mentoring that he

gave, that so many of his proteges went on to win the Nobel Prize.

So this is the first part of the Aufbau principle. The second part is that the electrons fill from lowest to highest energy. So electrons fill orbitals. You can think of the orbitals as placeholders. They're really energy concepts. But we populate orbitals from lowest to highest energy. From lowest to highest energy. Or if I wanted to be a wise guy, I would say, I'm going to define energy in such a way as I get that as the filling sequence. One's got to fit the other. And the energy is itself a function of the four quantum numbers. So energy, once I specify  $n$ ,  $l$ ,  $m$ , and  $s$ , you can give me the energy and away we go.

And the thing is that you need to realize that the energy levels are actually a function of electron occupancy. So you can look carefully, if you get down into the  $d$  orbitals and the  $f$  orbitals, as you add one more electron moving one element to the right on the periodic table, sometimes you see the population not adding by one, because the addition of an electron changes the relative energies of the various orbitals. So let's remember that, that energy is a function of electron occupancy. Energy is a function of electron occupancy.

And then the third part of the Aufbau principle is called Hund's rule. Hund's rule. Now, Hund is German for dog, but this isn't named after a dog. This is named after Friedrich Hund, a professor of physics at Frankfurt. He taught for many years. He died at the tender age of 101. And he spoke about degeneracy. Not societal degeneracy, but degeneracy in an atom. And this degeneracy is the condition where you have a plurality of orbitals at the same energy level. So, in orbitals of equivalent energy, in orbitals of equivalent energy, we strive for unpaired electrons. This is filling, now. This is how to direct the filling sequence. Strive for unpaired electrons. Let's say unpaired electron spins. Let's make it a little clearer. Unpaired electron spins.

So I'm going to give you an example, work through an example. So, what have we got here? Here's carbon. And if you look at any element on the periodic table, you'll see this green. And this is the electronic configuration. This tells you what the sequence looks like for that particular element in the neutral form, et cetera, et cetera, subject to many, many considerations.

So let's look at carbon. So if we look at carbon, it tells us  $1s^2, 2s^2, 2p^2$ . So what's all this mean? Well, it's all written in code for us. So the first number here is the  $n$  number. So this means  $n$  equals 1.  $s$  is the spectroscopist's notation, so this means that  $l$  equals 0. And then the

2 here means 2 electron occupancy. So the 1s orbital is filled to the tune of two electrons. And the 2s orbital has two electrons, and the 2p orbital likewise has two electrons. So now we want to do is put these electronics into their orbitals. And we can use, there's a variety of notations. This is one I'll use today. This is a box notation. So this is 1s. This is 2s. And then this is 2p. If you recall, 2p there's going to be three of them. If you go back here, 2p has three orbitals in that sub-shell. And we said that this is the one time that m makes some sense with respect to Cartesian coordinates. m is -1, 0, +1 so we can call this 2p x, 2p y, and 2p z. And I don't know which is which. I don't know what the arbitrary standards of x, y, and z, I don't know where the origin of the universe is, so I can't tell you all this. But, arbitrarily, if I choose one as x, I know where the other two are according to right-hand rule. So let's start filling.

This says 2, so I'll put in one spin up, and one spin down. Now it says 2s 2. One spin up, one spin down. And now here's where the Hund rule comes in. I've got to put two electrons into these three boxes. Now, I could be a librarian and start left to right, and make them nice and neat. Or, I could just put them in wherever I want. What the Hund rule says is, strive for unpaired electron spin. So for the Hund rule, you'd put them in both same spin and in different orbitals. And then when you get to nitrogen, nitrogen will have a third one here. And when you get to oxygen you've got three plus the fourth one's going to be one of these three and I don't care. I mean, some people are really anal about it, and they want you to go from left to right. As long as you've got two of them unpaired and one of them paired for oxygen I'll be happy.

So now we can use this concept and look at the energy level diagram for multi-electron atoms. And this is taken from the book. So this is different from the energy level diagram for hydrogen, because you can see some compression here. And I want you to know first of all, all of these values are negative. It's true that energy increases vertically, but the zero is way up here. So these are all negative values. And I want to zoom in here. Because the energy difference between 1s and 2s is large. And we know in hydrogen it's 3/4 of the total energy difference. Because there's some compression in a multi-electron atom. But nevertheless, n equals 1 to n equals 2 is a huge energy difference. So let's zoom in on here.

And what do we see? Well, 2s, 2p, 3s, 3p and look. 4s lies below 3d. 4s lies below 3d. So that tells us, there's my 3s. 3s 1, 3s 2. There's 3p x1, 3p y1, 3p z1, 2, 2, 2. And now what's next? It says go to 4s. So potassium is 4s 1. Calcium's 4s 2. And scandium is 3d 1. So this energy level diagram is the map. It tells you how to put electronics in sequence.

So, this now gives us the rational basis for e equals n, l, m and s.

All right. Well this is nice. It's been graphical, and so on. Now I want to go to the same position. I want to get back to this, I want to get back to this point. But I want to go by different route. I want to go by different route, and for that we're going to go by wave mechanics. So, same destination. Same destination, via wave mechanics.

Now, you don't have partial differential equations as a prerequisite for 3.091, so I'm not going to go through the math. I'm going to give you the features of the wave mechanics. So that later on you're going to spiral around and study this again. You'll have seen it before. And again, there's going to be people involved, and they're all giants in modern physics.

The first one is de Broglie. The first one is Louis-Victor de Broglie. Let's get his name on the board. Louis-Victor de Broglie, he was an aristocrat from Normandy, who had gone to the Sorbonne. He was studying humanities. Political science, literature, and around about the time of his senior year he decided to switch horses for graduate school and forget about a career in the diplomatic corps, do a Ph.D in physics. So, he did a Ph.D in physics. And in 1924 he published this Ph.D thesis, beautiful piece of elegant writings. Less than 30 pages long. And I'll give you sort of the summary, the one-liner that summarizes his Ph.D thesis.

Most of you are going to have to write a thesis. The word thesis comes from the Greek, and it means, sort of, my position. My statement. Before I have a thesis, I have something that is not a thesis. It's my trial balloon. That's a hypo-thesis, a hypothesis.

Now, the key to writing a good thesis is to ask a really good question. If you ask a pedestrian question, you're probably going to get some pedestrian answers and ho hum. If you ask a really interesting question, you give rise to the possibility of interesting answers. And what de Broglie did is, he asked a really interesting question. So here's his question: He says, if a photon, which has no mass, photon's just an energy packet. If a photon which has no mass can behave as a particle, and we've seen. We model ray optics as particle beams. And a photon, and Max Planck said equals  $h\nu$  got no mass, but we can think of it in our little anthropomorphic brains as, photon photon photon.

So if a photon, which has no mass, can behave as a particle, does it follow that an electron, which has mass, can behave as a wave? It's beautiful. Let's do it one more time. If a photon, which has no mass, can behave as a particle, does it follow that an electron which has mass, can behave as a wave? So he asked the question. And he answers it. In less than 30 pages.

So, let's get this on the board. Because this is beautiful. It's like, ask not what you can do for your country. If a photon, which has no mass, can behave as a particle, or can be modeled as a particle, behave really means, so that the theoreticians can model it as a particle, does it follow that an electron, which has mass, can behave as a wave? See, if you understand the question then the impact of the answer, and the answer is, if it does, this is what its wavelength is going to be. So de Broglie said, the wavelength of an electron, if it were to behave as a wave, would be given by the ratio of the Planck constant to the Newtonian momentum, which you know from 8.01 is simply  $h$  over the product of electron mass and its velocity. So that's de Broglie's thesis.

So let's take a look what we can do with this. Now, you remember in the Bohr model, recall Bohr. Well, Bohr taught us that  $mvr$ , that's the quantum, condition,  $mvr$  equals the ratio of  $h$  over  $2\pi$  times  $n$ , where  $n$  takes on the discrete values. 1, 2, 3, et cetera. That's the quantum condition.

Now let's take this idea of de Broglie. And first of all we have to put the electron in its orbit. So we'll put the electron in its orbit. And now I'm going to have it behave as a wave. So if it behaves as a wave, I'm going to draw it as a wave. Now, why did I draw it this way? There's two kinds of waves in this world. There's standing waves and there's traveling waves. Now, this orbit's stationary, it's in this orbit. So it better be a standing wave. I think there's a cartoon in the book. There you go, standing wave.

In order for this to be a standing wave, there's a geometric constraint on this. Listen carefully geometric constraint. I'm not saying anything about quantum mechanics. Geometric constraint, the geometric constraint for a standing wave is what? You know what this distance is, right? I mean, this is not to scale. This should be 10,000:1, in which case these ripples are barely visible. But here it looks kind of exaggerated. This is a hyper wave. This is emphasis added in proof. So that means that the circumference here,  $2\pi r$ , the circumference must be an integral number of wavelengths for a standing wave. But we know that from de Broglie, I can write  $n\lambda$  as  $n h$  over  $m v$ . I've just put in de Broglie's definition of the wavelength of an electron. And now I can cross-multiply and I get  $mvr$  equals  $h$  over  $2\pi$  times  $n$ . Which is Bohr's quantum condition. So we've got validation of the Bohr model, so that's a pretty compelling case that maybe the electron really does behave as a wave, and that explains why we have the quantum condition that we do.

So de Broglie, that's his Ph.D in 1924. Einstein read the thesis, loved the thesis. But we don't

care what Einstein says, because he's a theoretician. So one theoretician praising another theoretician. That's not how science works. How does science work? Data. We need data. And the data come in 1927. 1927, at Bell Labs in New Jersey. At Bell Labs in New Jersey come the critical data. And they were taken by Davisson and Germer. Davisson and Germer. Davisson and Germer were studying crystals. They were studying crystals of various elements, and in particular metal crystals. Metal crystals, by X-ray analysis. And in order for you to appreciate what I'm going to show you of Davisson and Germer's work, I'm going to take you back to high school to those thrilling days with the wave tanks. Remember the wave tank? This is the top view, this is the side view of the wave tank. And you might have some kind of a mechanical device here that has a paddle. And it starts vibrating up and down, and it starts sending waves into the tank. So the waves come like this, from the edge it looks like this. Remember that? Sure you do. You're toying with me. Oh, I don't remember anything, we never did that. Sure you did.

OK, so you can send waves down. Now, what we can do is, we can put a dam here. I'm going to put a dam. And depending on, if this is the wavelength, this is the wavelength, it's the distance between two successive crests. And, if this spacing here, the gap between the wall and the edge of the dam,  $d$ , if  $d$  is greater than  $\lambda$ , the waves just propagate but for the place where they're blocked by the dam. So you get, you essentially cast a shadow. You've seen that.

And so I could model this system as a beam. This is a beam. This is a water beam. This is a water beam shadow. And this is equivalent to ray optics. Straight lines, if something gets in the way it's opaque. Blocks transmission. End of story. So you've seen all that.

But you also did this other experiment, I'm willing to bet. So let's do the other experiment. We're going to do the same thing. I'm going to send waves down here. Only, this time we're going to make the dam a little bit different. This time we're going to bring the dam in from the wall. And we're going to put a tiny opening. And I'm going to go some more into the tank. And then another tiny opening. It could be the same. It's probably best to keep it the same dimension.

Now, in this case, the spacing,  $d$ , is much less than  $\lambda$ .  $d$  is much less than  $\lambda$ . And what happens in this case? When  $d$  is much less than  $\lambda$ , you don't get the shadow. You don't get something like this instead, remember. You've got the rings. This is called diffraction. Diffraction. And there is no way to explain diffraction modeling water as a beam. You must



implore the wave-like behavior of water in order to explain diffraction. Explain only by invoking wave-like properties. So with wave-like properties, we get something that makes sense in terms of the data.

Now, let's do this same experiment, let's do this same experiment on a metal crystal. So if you go back to the gas discharge tube. Remember the gas discharge tube that we were looking at for lecture after lecture? If you take a look and go through the energetics of it. If you put one volt across the plates, you know the energy is going to be a product of charge times voltage. And that's equal to  $\frac{1}{2} mv^2$ . Which you know from 801 is  $p^2$  over  $2m$ . And  $p$  is equal to  $h$  over  $\lambda$ . Pretty soon you can come up with the wavelength. And that will give you the wavelength of the electron. This is a ballistic electron now.

See what I'm doing? See, once I said that this indicates that the electronic in stationary orbit can be modeled as a wave of a certain wavelength, so now the free electron. It's got  $m$ , it's got  $v$ , there's Planck constant. I can go ahead and compute its wavelength. I can compute the wavelength of a baseball. So, you go through it. And you get a value of about 12 Angstroms. 12 Angstroms. Now, if I want to see whether there's wave-like properties, I need to have a condition that gives me diffraction. So I'm going to have to find something that gives me a dam with an opening that's less than 12 Angstroms. If I'm going to use 1 volt.

So what can I do? Well, turns out you're going to learn this in greater detail later, but if this is a crystal of nickel. Crystal of nickel, the atoms are arranged in regular arrays. And this is what the face of nickel looks like, 4 atoms each at the corner. And one in the center of that face. This distance is 3.53 Angstroms. Perfect. Perfect.

So what Davisson and Germer did is, they irradiated this. They irradiated this first with X-rays on the order of  $\lambda$ , on the order of, say, 10 Angstroms. And what did they get? This is the output. This is the output. You get a diffraction pattern. It's a set of rings, concentric rings. So this is the X-ray diffraction. This is the X-ray diffractogram, if you like.

And then, what did they do next? They irradiate the same crystal with an electron beam.  $\lambda$  of the electron beam, 10 Angstroms. And what did they get? Are you ready? Drum roll.

Now, there is no way that you can get a ring pattern from a beam of electrons acting as a particle beam. The only explanation for this is that the electrons were behaving as waves of this value to give us the same spacing as we got with X-rays. And you're comfortable if I say that X-rays are a type of light. So, therefore, it's got wave-like properties. And it's got particle-

like properties. Well, now I've just made the point that this is the electron diffractogram. So this is evidence of electron diffraction. And this shook the world. Because now it's real. There's no way you can get this otherwise. This is electron diffraction. This was 1927. 1929, de Broglie gets the Nobel Prize. 1937, Davisson gets the Nobel Prize.

So this means the wave-particle duality is complete. It applies not only to light, but it applies to matter. So, wave-particle duality, they call it. Wave-particle duality is complete. Matter can act as waves. Electromagnetic radiation can act as particles. So, sometimes people refer to de Broglie's accomplishment as matter waves. Matter waves. And what do you call the behavior of billiard balls banging around and so on? We call that mechanics. So now we're going to use what might seem as an oxymoron, contradiction, wave mechanics. Wave mechanics. That means matter behaving as a wave. But still behaving as a matter. So this is the dynamic. So that's pretty good for de Broglie.

So let's go to number two. I said there were going to be three people here. Number two is Werner Heisenberg. Werner Heisenberg. Heisenberg studied with Pauli. Sommerfeld. Did his Ph.D in Munich in 1923. Got his Ph.D with Sommerfeld at the age of 22. And then he decided to take a postdoc with Bohr. And he was working with Bohr for a couple of years, he was feeling a little bit burned-out. And decided to take three weeks off. Went up to a deserted island off the coast of Norway. Came back three weeks later with the mathematical formulation of quantum mechanics. I'm not kidding you, that's what he did in his time off, to kind of unwind.

And so one of the things that he used as a critical piece of this derivation is that the position and velocity of an electron cannot be fully specified. They cannot be fully specified below certain limits. There's a threshold below which we can't go. This is sort of like, if I asked you to time a 100-meter sprint, which typically takes less than 10 seconds. But I give you a clock, and the nearest unit on the clock is the minute. So you wouldn't be able to distinguish. So, he says - and the reason for this is, it's a consequence of quantization. Light itself is quantized. So, at some point you're asking for a continuous splitting and splitting and splitting into finer and finer time segments. And you can't get there. So we already knew this from Planck.

And so one of the ways that he expressed the inability to go below a certain threshold is the uncertainty principle. The uncertainty principle. And that's unfortunate that, see, it was originally published in German. And the idea really is the indeterminacy principle. But, English says uncertainty. So it's a limit to determination, but there it is. And so one expression of this is, the product of the velocity. Only, he wrote it in terms of momentum. So the mass isn't going

to change. So, think of this as the uncertainty and the velocity. And the uncertainty in the position. So this is the x-coordinate of particle. You can break its trajectory into three orthogonal components. So the uncertainty in the x direction of the momentum times the uncertainty in the position is greater than or equal to the Planck constant divided by 2 pi. The Planck constant divided by 2 pi.

And so what this means is that we're going to see a transition in models from individual atoms. If we want to describe what happens with individual atoms, we need what is known as a deterministic model. Sort of, Newtonian mechanics. You tell me the initial position and velocity. You tell me the forces, and I can predict where it's going and where it's going to be. So that's deterministic models. So, deterministic models describing individual atoms are going to give rise to probabilistic models. Probabilistic models.

And probabilistic models obviously can't be talking about individual atoms. Must be talking about ensembles of atoms. So I can't say where any individual atom will be, because I don't have the ability to do so. But I can tell you, if you give me a large number of them, I'll tell you roughly what the expected outcome could be in terms of energy. And ultimately predict the spectrum, and so on.

So instead of chicken and egg we have now chickenality and egg-ness. Everything is just sort of getting a little bit murky. Little bit murky. You can do a calculation on this. You can do a calculation on this, a very simple take. Take the Bohr model and take the ground state electron in hydrogen.  $n$  equals 1 in atomic hydrogen. And you know this is about half an Angstrom. So the distance across here is 1 Angstrom. So make 1 Angstrom your uncertainty, and you'll find that the uncertainty in the momentum is on the order of 15%.

But what this is saying is, when you get down to atomic dimensions, you can't just shine light on it and reveal what's going on. Because you're going to disturb the very thing you're trying to measure. Some people say that, every time you try to work at the atomic level, it's as though you're trying to take a picture with the sun at your back and your shadow is in the picture. So you can't get there without disturbing the very thing. Another way to think about it is, the photons that are capable of this resolution are going to have such high energies they'll knock the very thing you're trying to measure.

All right. He gets Nobel Prize in 1932.

And then the third one is Erwin Schroedinger. Let's get him up here. Erwin Schroedinger. Also an Austrian, University of Zurich. He too was burned out. They get burned out, these guys. So at Christmastime, 1925, took a vacation. At Villa Herwig, in Aurora. And comes back two weeks later with the wave mechanics formulation, of quantum mechanics. See, sometimes going away on a vacation. So he took de Broglie's notion of the electron as a wave and wrote equations to model wave-like behavior. So, let's look at how to get there. And here's what he did.

So, you know, for example, that we could start with a violin string. And it has a geometric constraint. It must be fixed at both ends. And if I pluck that string, it can vibrate as long as it conforms to the geometric constraint of a standing wave. So here's one possibility. Wherein we would call this  $n$  equals 1. I have simply the entire string vibrating in the matter that's shown.

But here's a second possibility. I could have it vibrating as is shown here,  $n$  equals 2 with a node in the middle where that node doesn't move at all. The string is stationary at its midpoint. And what's the characteristic here? This is operating at a certain frequency. Let's say it's middle C. And this is the overtone. This is the first harmonic. And it's going to be an octave higher, because it's as though we have two strings, each fixed.

See, from a physics standpoint I could literally cut this string in half and fix it there, and this is now  $n$  equals 1 for the half-length. So it's going to have the same pitch as the half-length. Which means that this is an octave higher, and this is going to be two octaves higher, and so on. And all of these conform. So you get a plurality of solutions. You get a plurality of solutions. And the solutions look something like this. They'll eventually teach you the string as a simple harmonic oscillator. Simple harmonic oscillator. And it has equations that look like this. If you want to plot its position, this is  $x$  going from 0 to  $l$ . And this is the  $y$ -coordinate. So you can, for example, write something like this.

So, the function will look like this. Some pre-multiplier times cosine of  $kx$  plus another pre-multiplier  $b$  times the sine of  $kx$ . And the geometry will dictate that the value of  $k$  is  $n\pi$  over  $l$ . So,  $\pi$  over  $l$  is the geometry. And  $n$  takes multiple values. Just as you see here, there's not a unique solution. So listen carefully. Wave equation, plurality of solutions. But subject to some constraints. Subject to some constraints. So what Schroedinger did is, he wrote a wave equation to describe the motion of electron in its orbit. And guess what he gets? He gets a plurality of solutions. And when you look at the plurality of solutions, the plurality of solutions

ultimately map into what we know as the distinct values of  $n$ ,  $l$ ,  $m$  and  $s$ .

See, this is the one-dimensional. So this is giving us  $n$  numbers.  $n$  equals 1, this is now  $n$  equals 2. So I'm getting quantum numbers here. Now, if I did this in three dimensions, I'd have a plurality of quantum numbers. And Schroedinger gets us all the way to  $n$ ,  $l$ ,  $m$  and  $s$ . And so here's what it looks like. This is the equation, it's a wave equation, so there's a double derivative in space. There's a forcing function. And this is  $i$ , square root of minus 1 in a time base here. So it's a harmonic kind of equation.  $\Psi$  is the wave function, it's an abstract concept but we'll show you how to make sense of it. And these are the various solutions, the plurality of solutions. And we can now map those into what we know as  $1s$ ,  $2s$ ,  $2p_x$ ,  $2p_y$ ,  $2p_z$ , et cetera, et cetera. And you see this number  $a_0$ . That's our Bohr radius. Comes right out of the equations. 0.529 Angstroms.

So, this is quite good. But, as I said, the  $\Psi$  is the wave function. Or  $\psi$ , however you want to call this. This is called the wave function. Wave function. And we have plurality of solutions. We call these Eigenfunctions. Eigenfunctions. And the closest we can get to something physical is the product of  $\Psi$  and its complex conjugate. And that is related to the probability of finding the electron. Probability of finding the electron. Which, in essence, gives the boundaries of the orbitals.

So now I'm going to put, we're going to get a Cartesian shape. I told you,  $1s$ ,  $2s$ . What do they look like? Here's what they look like. So these are the square of the wave function plotted. So this is in a radial distribution function. It's only in one direction, out from the radius. Now, if you whip this around in 3-D, you'll generate the surface. But already you can see, here's  $1s$ , and it peaks at about  $1/2$  an Angstrom. And here's  $2s$ , and it peaks at 4 times the Bohr radius. And  $\Psi^2$   $3s$  about 9 times. This is from your book. So it's a maximum. But there's some uncertainty. See, it's not a simple line fixed at 0.529 Angstroms. This is another way of plotting. So these are spherical. What we were calling circular now becomes namely spherical. And there's this node here. This is the  $p$  orbitals. They're dumbbell-shaped. With two lobes. And if you have a single electron, it doesn't reside in one lobe. It can jump from one side to the other. You might say, well, how does it get from one lobe to the other when halfway between, there's a nodal plane. It has zero probability.

Well, it's behaving as a wave. Behaves as a particle, you can't get through a wall that says zero permission. That's how, you can transfer energy from here to here and have that node's perfectly stationary. Anybody skip rope? You know how this works.

Now, this is where I quarrel with the book. This is another drawing. But I'm uncomfortable with the fact that they chose different colors. Because I think to the first time learner, you might be tempted to think, well, one electron lives here and the other electron lives here. No, the electron, if there's only one, it can go from one to the other. If there are two, they can go from one to the other. And, see, they do this all the way through. So please don't start rationalizing in your mind that one electron goes in the yellow and the other electron goes in the grey. There's the d. Aren't they pretty? If you find the f orbitals, that's wild.

So I think this is probably a good place to stop. We've got a few minutes here. If you want to read more about uncertainty, this is a very nice book by David Peat that goes into the meanings, including this indeterminacy, and so on. Good book here on hydrogen.

Please, I don't want noise. We've got, still, a few more minutes. Still got a few more minutes.

This book here talks about hydrogen. Goes right back to Democritus. One chapter is a beautiful thing on the use of hydrogen as a potential fuel. All the Bohr and whatnot.

This is a play that won the Tony Award in the year 2000. Written by Michael Frayn. And it's about the fact that Niels Bohr was the mentor to Werner Heisenberg. And now it's 1941, the Nazis have invaded Denmark. And Bohr is essentially waiting to get out of Denmark before the war overtakes the rest of Europe. Meanwhile, Heisenberg is now the head of the Nazi equivalent of the Manhattan Project. And he goes to Copenhagen to visit his old mentor. That's a fact. They have dinner. That's a fact. They go for a walk. That's a fact. They never speak to each other after that night. That's a fact. So the question is, what went on that night. And that's what Michael Frayn uses as the dramatic point of departure. So, did Heisenberg go to Bohr to get Bohr's opinion about nuclear weaponry? Did he try to find out whether the Allies were working on a bomb? Did he go to say, look, we should on both sides not develop nuclear weaponry? What went on in that conversation? And so you see Bohr at the center. There's Heisenberg who's the one electron. And there's Margaret, who is Bohr's wife, who was the observer. And so there's the play between the uncertainty in quantum mechanics and the uncertainty in human relations. It's a really nice play.

Here's a rendition of it. This is Stephen Rea playing Bohr, Francesca Annis playing Margaret Bohr, and playing Werner Heisenberg is, do you recognize him, it's Daniel Craig.

This is a book that came out not too long ago about Heisenberg. A lot of controversy about

him. Some people accused him of being a collaborator. Other people say that he was absolutely brilliant in the right amount of foot-dragging. He did not want to give Hitler nuclear weapons. If he'd been a total disaster he would have been replaced by somebody who might have been more zealous. And if he went too fast, he might have figured out how to make nuclear weapons. So, very interesting book about him.

And here's a nice photo. This is Bohr. This is Werner Heisenberg. And this is Wolfgang Pauli. Undoubtedly talking about what goes on when you pluck that string. So we'll see you on Wednesday.