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Last week we talked about-- we went quantum.

We had Dr. Quantum show us the way.

And this week, we're going to go quantum for electrons, right?

That's what we're going to do this week.

These are my two favorite quantum mechanicists of all time.

I believe that this sign is meant to teach us something about the double slit experiment.

And just as you're leaving the lot, knowing that there is some chance that your one car could actually split into two, go through both exits, and recombine.

Just like an electron does through two slits.

And in fact, we know that that's possible now.

And if we wanted to, you could write down-- from de Broglie-- you could write down like the wavelength of a car, right?

So like in a car-- I don't know, your lambda of the car would be equal to h over mv.

And if you plus some numbers in, this is going to be something like oh, you know, maybe 10 to the minus 37th meters.

It's small, but it's a wave.

Your car is a wave, you know?

The baseball is a wave.

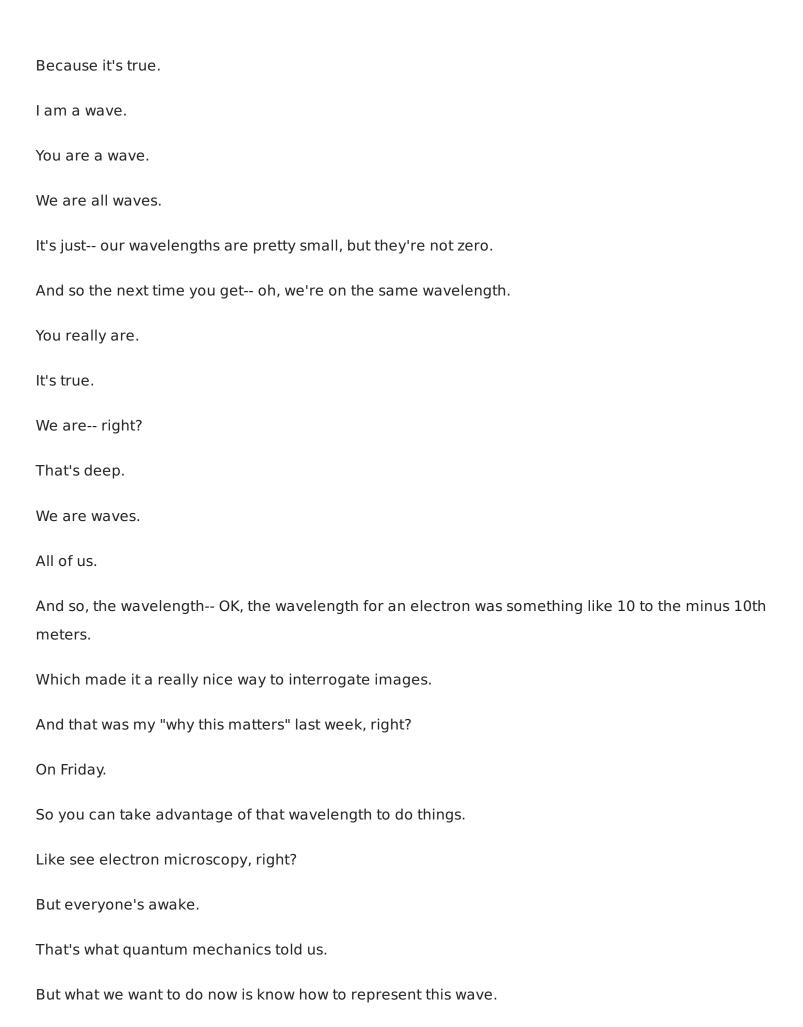
The electron-- we are all waves.

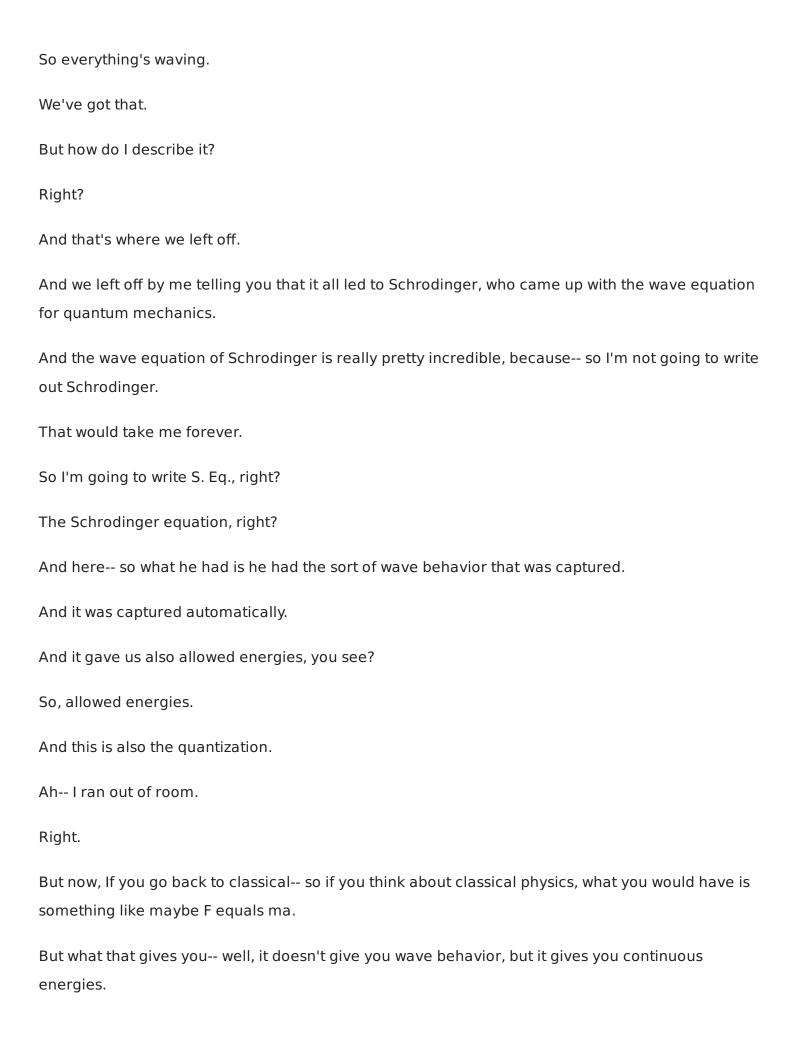
And I know, and that's what-- so the electron is a wave.

And I know-- hashtag, we are all waves.

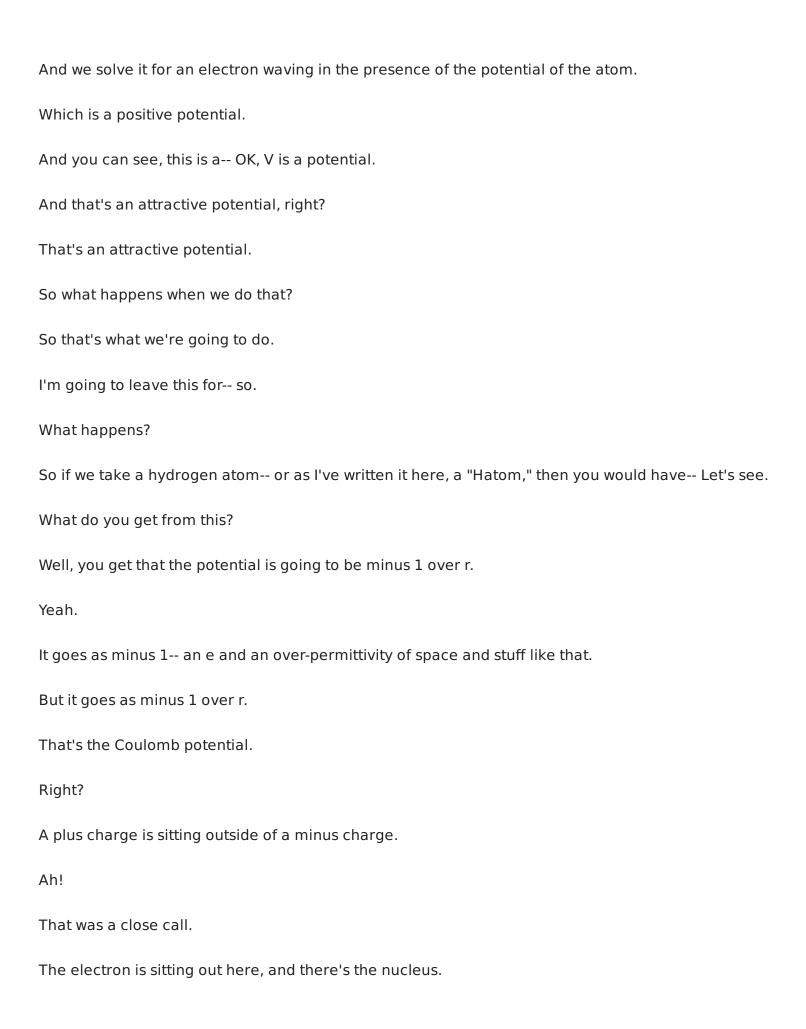
Because it's a thing.

It's really a thing.





Continuous energies. So the powerful point here is that from that equation-- and we don't need to know this equation. We're not going to derive it. Right? Today I'm going to tell you how it's solved, but you don't need to know how to solve it. But you need to know what the solutions mean. That's what we're talking about today. But that equation-- what it does is it sets up the energies as a function of the wave. Psi-- that function, psi-- is the wave function, OK? And so you get waves by default, because that's what you're solving for-- these waves. And then you have a minus second-- oh, there's an h bar. That's an h over 2 pi. Right? But it's like the same Planck's constant. OK. But the wave behavior gives you-- because there's only certain energies that solve that equation. So quantization falls out naturally. You don't have to put it in anymore. It is a direct result of solving this equation. If I take a wave-- think about this, right. If you take a wave and you put it in a box, then it can only have certain solutions. Once you define the box, if you throw a wave in it, well, that's where those things are on the right are. Maybe it's a standing wave. And so it's going to look-- no-- it's going to be like this. One solution. And some energy. Or maybe it's going to look-- I didn't leave myself any room-- like this. And it's going to have some other energy, right? 1, 2. That's it. If you throw a wave in a box-- like, here's the first one, second one. But there are only certain ones that are going to work. All right, and you can get that sense. Because otherwise it's not going to line up and then be able to wave and keep going. It's not going to be a standing wave. Right? So you get this sense right away of quantization. Only certain waves, and only certain energies, will solve this equation. Now, here's the key, is this-- we're going to throw an electron into this equation, right? But we're going to throw it into the right potential. And that is the potential that we know it sits in, in an atom. Which is simply a Coulomb potential. So this is how we get there, right? We take Schrodinger's equation of quantum mechanics.



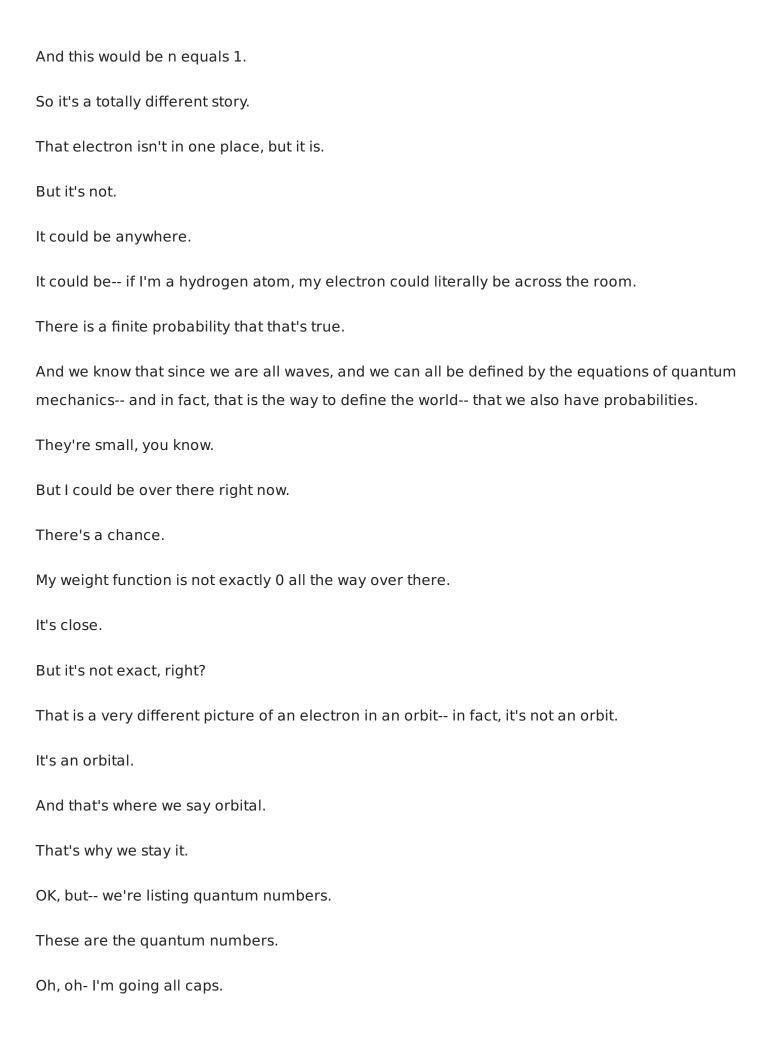
And the potential feels is a Coulomb potential.
OK, so that's point 1.
Point 2 is that we're going to apply the oh, I'm saving myself so much time.
I love it, when you're efficient like that S. Eq.
Schrodinger equation.
The Schrodinger equation.
But the way that we're going to do this is in spherical coordinates.
Spherical coords.
And all that means is that I'm going to write psi as a function of r, theta, and phi.
And the last thing that I'm going to do is I'm going to separate the variables.
And that's just a standard way to solve mathematical equations.
So I'm going to separate the variables.
So separate.
And so what that means is that psi can be written as one function let's call it r of the radius, times another function, p, of the theta, times another function f of phi.
So that's my separation of variables, OK?
Again, I'm not all about having you know how to solve this equation.
OK?
That you can learn in quantum mechanics.
But what I'm all about is what that quantum mechanics solution means for us here in chemistry.
And this is deep.
This is deep, because why?

Because this whole thing is quantized, right? So just like before, there's only certain allowed values for the wave function. There's only certain allowed values for these variables. Each one of them is quantized. Each one of them. OK? And that's what we need to learn about today, is what that means for chemistry. All right. So now we're going to go through the quantum numbers and see what they mean. And we're going to start with this first one, the radial function. So radial, and then two angular functions. OK. Now the radial-- so what do we get? Well, the radial function-- I'm using a word here, I got to tell you why. Orbital of hydrogen, right? So I've solved this now. I've solved this equation, and I'm plotting this orbital for first quantization-- n equals 1, n equals 2, n equals 3. We've got to talk about this, right? But I'm just plotting what that function looks like. Well, let's compare. Because if I'm Bohr, then what I have is this.

Remember this? I've got like this-- OK, there's 1, and it's going around, and it's very happy in an orbit. But see, we don't call these orbits anymore. And it's going to be clear as we talk about this picture, because these aren't distinct orbits, right? So now in quantum what you have-- I'm just going to take that n equals 1 solution. That's the first solution to the radial part, right? That's not a fixed distance. That's not a fixed distance, right? So now I'm just looking at the radial distribution of the probability. The probability of finding the electron. That's how we speak when we speak quantum. We don't say it's here, right? We say it could be here. I don't know. But there's a probability that it's there. So now it sort of has a probability cloud. Now it looks like it gets a little less-- why am I drawing spirals? It looks like it gets a little less probable as you go further out, right? So maybe the density of probability-- because look, right? It's got a peak there.

But even if I just plot that first orbital, even as I go all the way out to here, it is non-0, right?

So this is probability.



Didn't even know I was going to do that. So we have n, which is called the principle-- principle quantum number. And this is going to be related to the main energy, kind of e, 1, 1, right? E, 2, 2. So this is going to be related to the main energy level. Main energy level, right? And it's also related to the radial distance. Radial distance. And sometimes we call this the shell. So sometimes the principal quantum number, this is the shell, right? It's the first shell, or the second shell. So we can call this the shell. Come back to that later. And you can see right there. OK, we'll talk about n equals 2 and 3 in a second. But you know-- oh, let's talk about it now. You can see right there-- it I go from n equals 1 to n equals 2, then I'm further out.

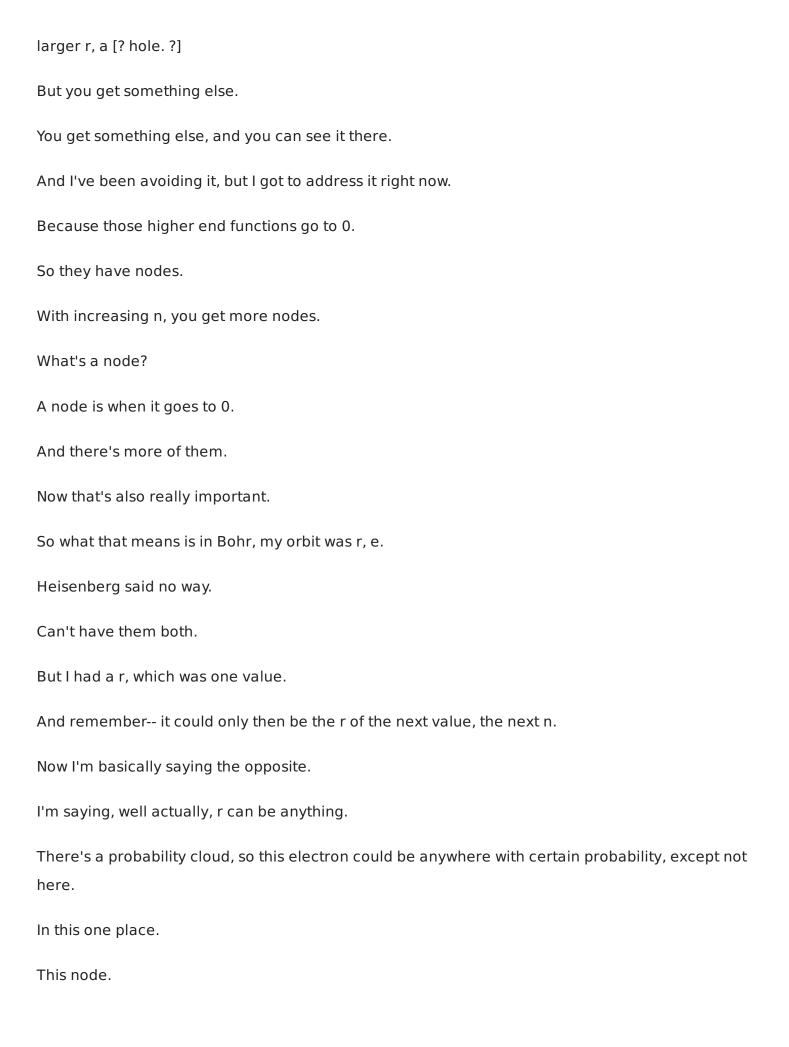
So with increasing n-- so another thing we can say about n is that with increasing n, you get higher

Yeah, I still got non-0.

Doesn't quite go to 0 like I just said there.

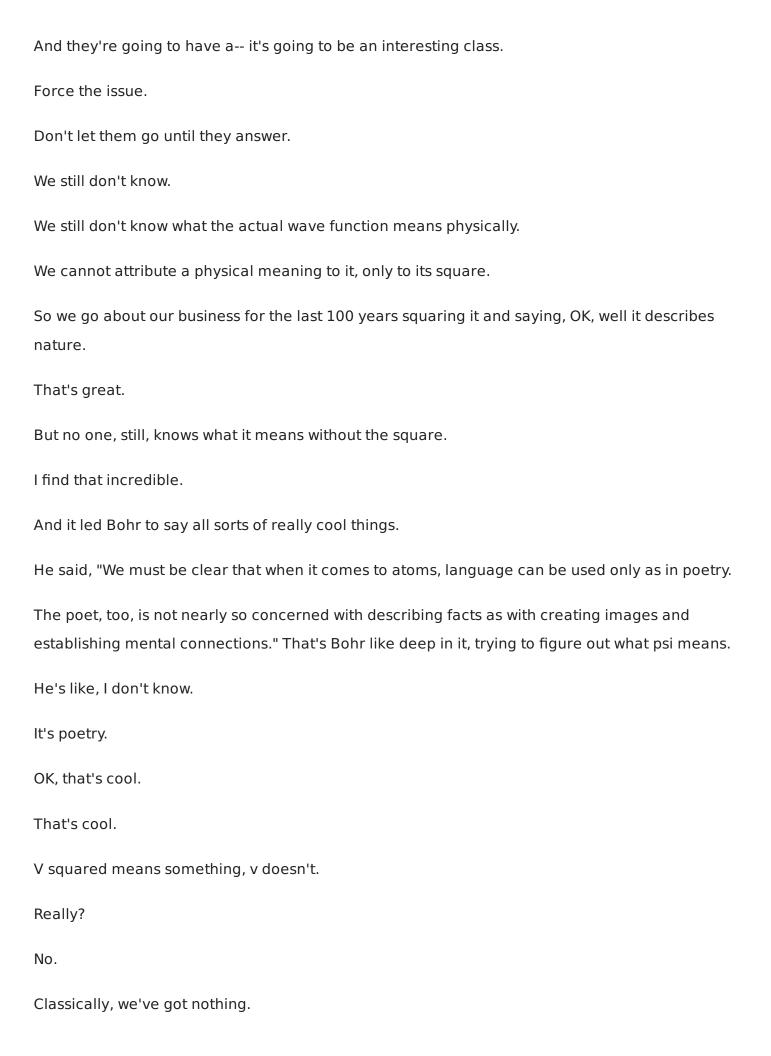
But it's further out, it's shifted out, right?

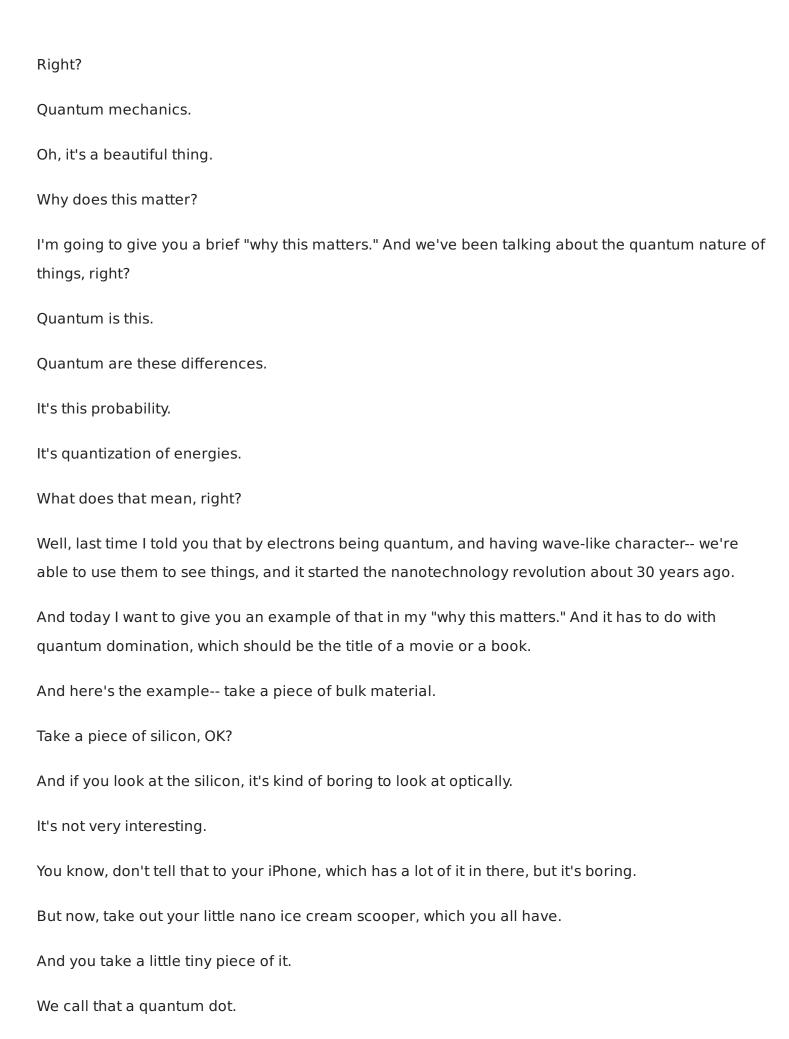
energies and larger distances.



It's 0.
It's literally 0.
The probability of finding the electron there is 0.
It cannot exist there.
But how bizarre is that?
The electron can exist with probability out here, and probability in here, but it can't exist in between
It's the same electron.
Try explaining how it goes back and forth.
It skips over a zero probability part, r.
Right?
But these nodes are very important.
And just to give you a sense of what this means, I found a very fancy animation, because I want to make sure you guys understand.
So here's the electron.
It's doing this, it's doing its waving thing.
But look at what happens with the nodes.
Uh uh.
The probability there is always 0.
You see that?
Can't go no.
Not gonna exist there.
Right?

That is super deep. Because there's no classical analog to these things. There's no classical analog. But this is what electrons do in an atom. Now, this is what the clouds look like-- a little better drawn than mine-- for n equals 1, n equals 2, and n equals 3. So again, you can see-- this is one electron. It's colored differently, just to contrast it, but this is one electron. Right? And These are plus and minus of this, right? So it'd be like a wavy wave, and you're just showing plus and minus with the yellow and blue. But that note in between is where it can never be. But it's one electron. It's not many, it's one. And this is its probability distribution. Now I want to make one really important point, which is that-- look at what I'm plotting here. Maybe something-- that's size squared, right? So it's only the square of the wave function that we can relate any physical meaning to. The physical meaning I just related to you is the probability of being somewhere. That's what size squared gives us-- the probability of being somewhere. But ask your teacher-- not me, your quantum teacher. Ask what psi means.





Why? We call it a quantum dot because it kind of looks like a dot-- its smallish. But we call it that because quantum mechanics takes over the properties. Here's an example-- shine light on this thing, or have it glow, and all of a sudden instead of being boring it can be any color you want. Why? Because if I shine light-- and here is a very sophisticated picture of a laser, which you can tell I had trouble making transparent. And so you shine a laser on this piece-- we know already, light excites charge in an atom. It does the same in solids. So here's my piece of silicon, and what that does is it sends an electron up in energy levels. But the electron is up in an energy level, and it left behind a hole. Which is something we'll talk about later when we talk about semiconductors. A hole is just a positive charge. And it turns out that that electron and that hole are attracted to each other, but not-- they can't get too close. But they want to kind of hang out at a certain distance. Where? How far? Yeah-- quantum mechanics.

N 2. 3. 4 tells us.

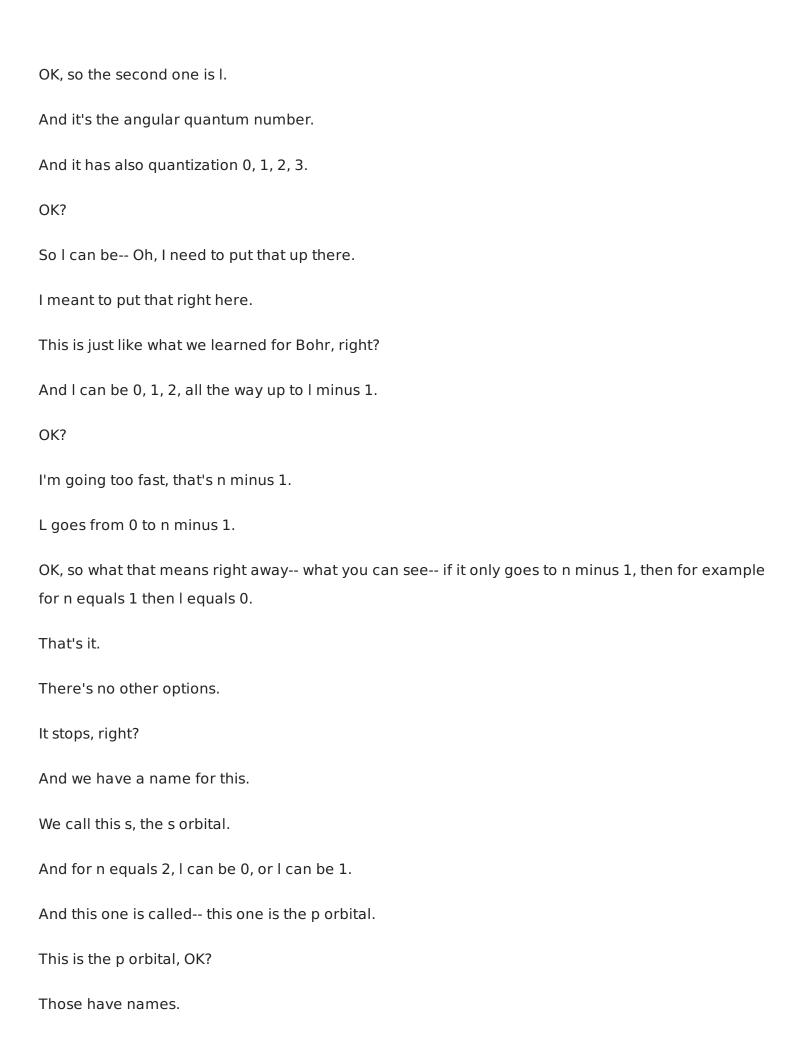
It tells us how far, right?

They want to hang out-- and now all of a sudden, I've nano-scooped them out, and I've made a quantum dot. But if I try to do the same thing there, that's how far they wanted to be. And they can't be. They literally ran out of real estate. They ran out of atoms. They cannot be out here, because there's no stuff out here. So they get squeezed. I am squeezing these quantum mechanical objects, this electron and this hole. And by squeezing them, I'm changing the way they interact with light. I'm changing the color, right? Oh. It's all stuff we've learned that explains something revolutionary. By the way, if you buy a QLED TV, is it as good as OLED? No. But is it better than LED? Yeah, a little bit. That's what they-- QLED-- quantum is quantum dots. They have coated the LED emitters with quantum dots to give you better color. Now what this means, why this matters, is nothing less than the periodic table itself. Because I think I showed you this-- we're living in these different ages, which I love. We have the periodic table that has-- the ability to work with it is what's brought us to the age of

materials design.

But see, now I've literally just told you that by changing the size-- nothing more than the size-- I can tune a property because of quantum mechanics. Because I'm changing its quantum mechanical interactions. It would be like saying, I can take a piece of this table-- I can break a piece of this table, and it's now going to be red. That's exactly what we're doing, but at a very tiny size. That is as if we are taking this periodic table and giving it a whole other dimension. Every element can do more things than we thought possible because we can tune these properties related to quantum mechanics. So that's a big deal. That's a very big deal. OK. Now back to our solution to the Schrodinger equation. For an electron in an atom. Because now we move on and we solve for the next one, which is-- OK, so we did r. Now we're going to do theta. And what happens with theta is, you get another quantization of that variable. And that's the second quantum number. So we're going to put it here. N-- I'll number them so we don't lose track. Who knows how many they'll be? OK.

Not three.



And so on and so on.
d, f This is old notation that we cannot get rid of.
This is called spectroscopic notation, because it comes from spectroscopists.
And remember, I told you never make a spectroscopist angry.
Don't do it.
Don't do it.
And so we use their notation still.
s was sharp.
Spherically symmetric.
p was principle, because it sort of dominated in some experiments. d was more diffuse.
f fundamental, because it looked kind of like the hydrogen atom sometimes.
These shouldn't be the names, but they are because they still stay with us.
Spectroscopic notation s, p, d, f.
What they really do is just correspond that looks like "porbital." Let's put a little more space there
P orbital.
Right?
Because what they really mean is nothing more than a quantum number for the second quantum number, which is the angular quantum number.
These are also sometimes called subshells, right?
Because they're underneath the shell.
And as you can see from this picture, it describes the angular shape.

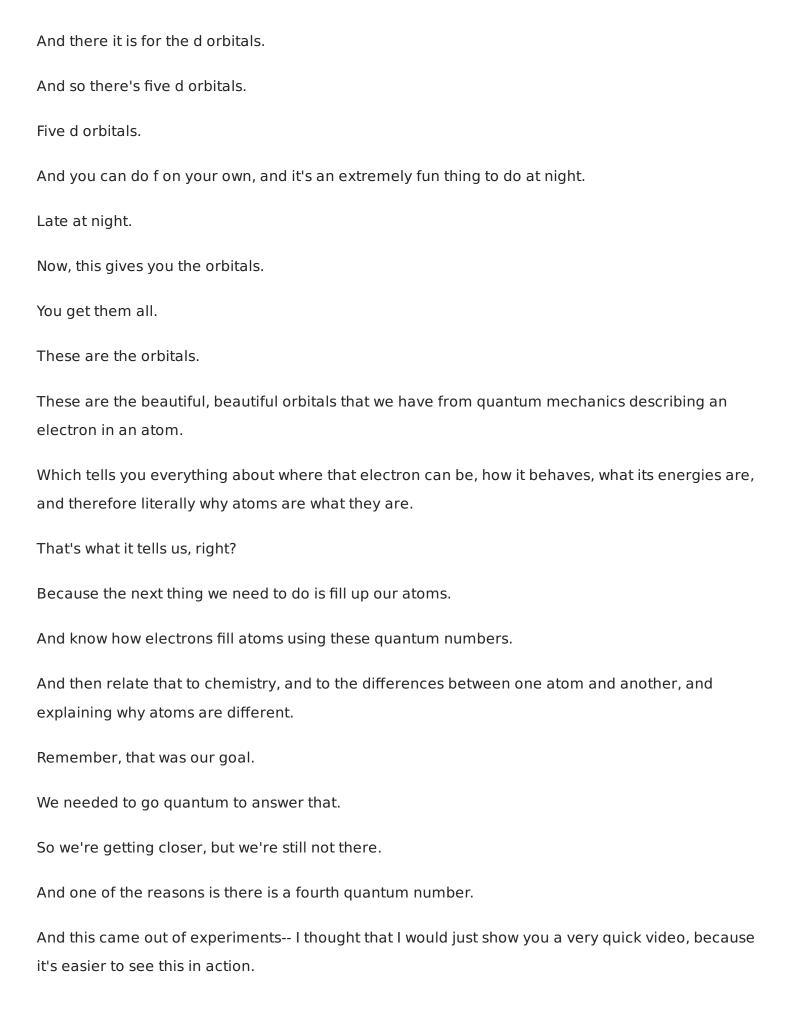
The angular shape of the orbital.

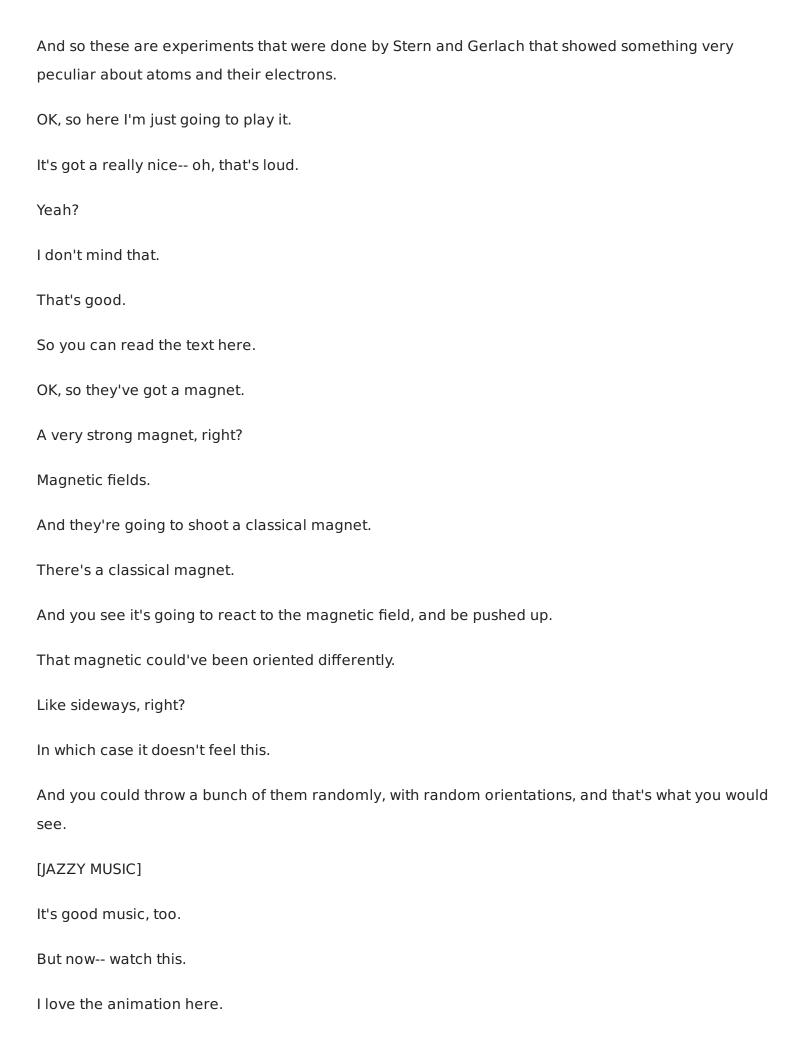
The shape, right? So it gives us a shape. Now-- if we think about it, and we think about that p orbital, that has a different shape than the [INAUDIBLE].. Then you think, well, this could be aligned in different directions, right? So if I think about that p orbital-- well, I could align it in three different ways. It could go along this axis, this axis, or that one, right? And so those are p orbitals in hydrogen that have three possible orientations, and that automatically gets us to another quantum number. In fact, it's the last one, and it makes sense just physically-- that's phi, right? So the last one-- or is it the last one-- is m. And we call it m sub I, which is the magnetic quantum number. And this one can have quantization equal to minus I, right? All the way up to plus I. So the number of orientations that the orbital can have-- if I'm a-- n equals 2, I equals 1, then m sub I equals minus 1, 0, 1. Three orientations. Right? It's got three orientations-- three possible magnetic quantum numbers. Why is it called the magnetic quantum number? Because those are the experiments.

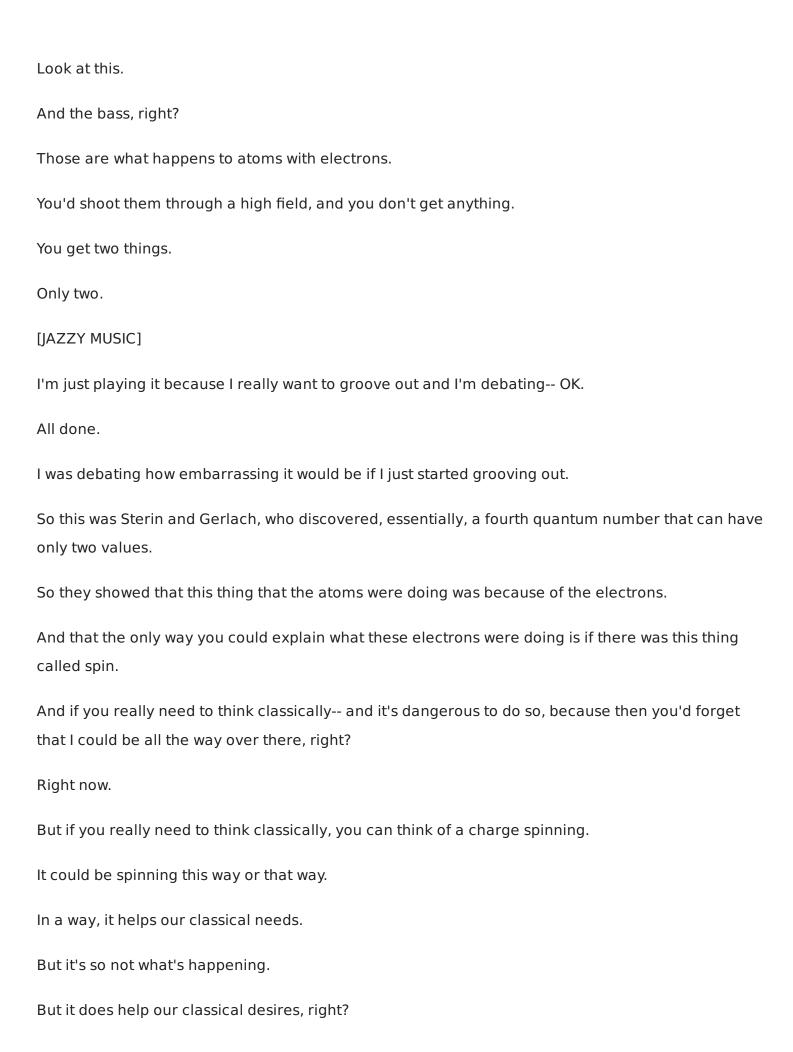
We're done using magnetization-- magnetic fields-- to discover these orientations, to sort through it.

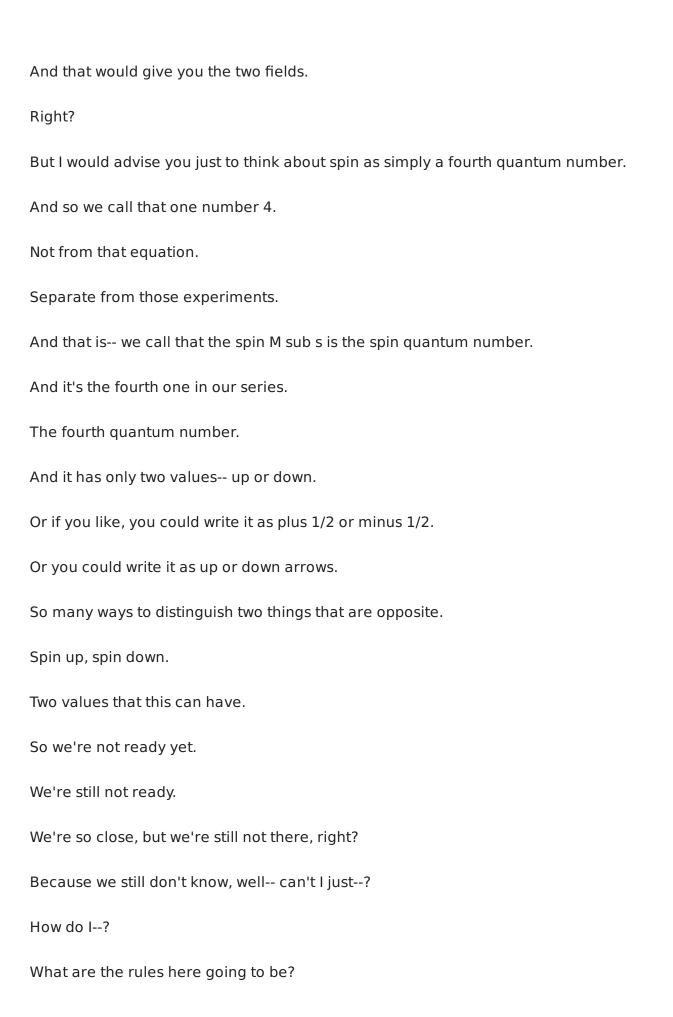
To see it.

OK.
So if I had I equals all right, so if I had, for example I equals 2.
Then m sub I would have five values.
Five possible values, right?
I should put a plus there, just to be sure we keep track of minus and plus.
These are quantum numbers.
That means they're integers, right?
But they can have these ranges and these rules, and again you may think, why did this come out like this?
Well, it comes out from solving this equation separation of variables with that potential.
That's it, right?
That's it.
You get these allowed values of these three variables, quantum numbers.
OK?
All right.
Now and there's the d.
These are called d So if n equals 2 OK.
So did I mess up here?
No, I didn't, because n would have to be 3 here, right?
For I to be 2.
Because I can't be equal to n, because I wrote it there as the list of allowed quantum numbers that I can have.

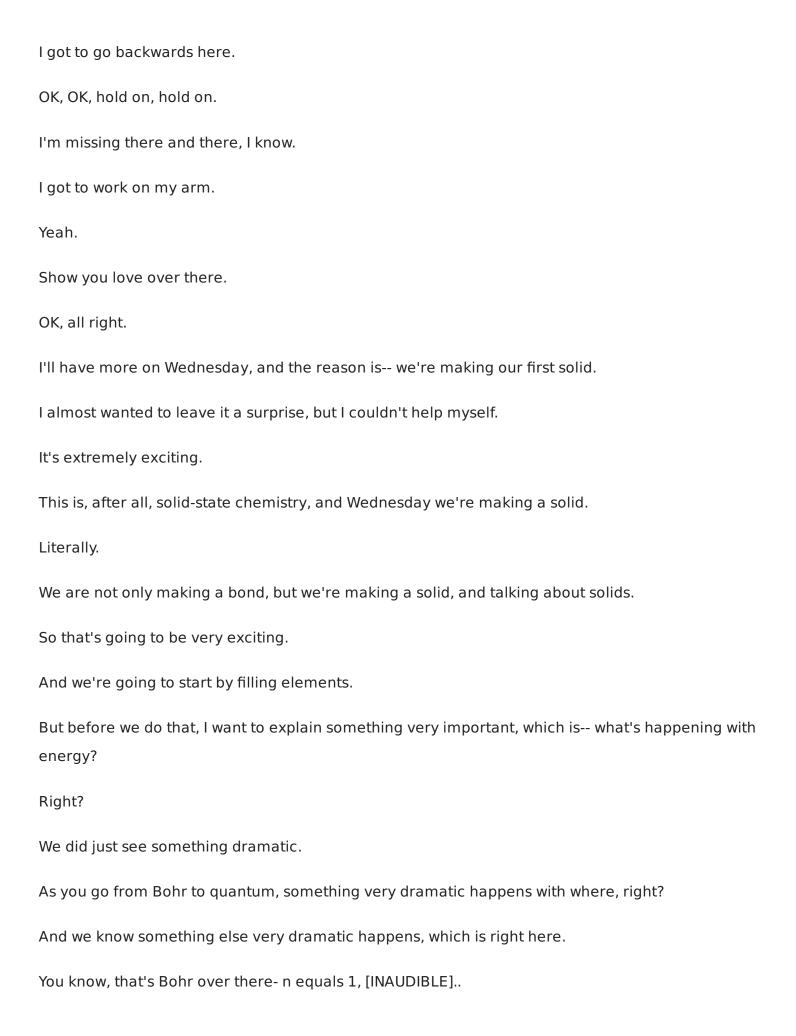








For populating atoms. And this is where Pauli said something very important, and made this incredibly important statement. Which is that-- no particles in the same system-- read that as, no electrons in the same atom-- can have the same quantum numbers. No electrons in the same atom can have the same quantum numbers. And that immediately tells you-- again, this has to do with the nature of quantum mechanics-- what that immediately tells you is that two electrons-- ho-ho, this is big! Two electrons-- I'm gonna write, two electrons, and watch this-- I'm going all caps-- only two electrons can occupy an orbital. An orbital. Or- bi- tal. That called the Pauli exclusion principle. OK. So we're going to use all of this information to fill stuff up, but I don't want to do that yet. On Wednesday, we're filling up the table, and we're making our first solid. I figure it's our three week anniversary. I know you've all been looking forward to it. I've been thinking about it a lot. And I think-- that makes me want to throw t-shirts. [STUDENTS CHEERING] I got to do this. All right, all right. I got to go-- I know.



Bohr is 1, 2, 3, right?

Now it's like-- oh no, wait, it's 1 and with 1s.

2-- I can put two electrons in there, thanks to Pauli.

I know I can put two, because I have all the quantum numbers in here the same except spin, which could be up or down, right?

N equals 1, I equals 0, m sub I equals 0, spin is up or down.

Two electrons.

But look, I'm now here at n equals 2, going from the Bohr model to quantum.

I've got this and I've got three p orbitals.

So now all of a sudden I've got eight electrons that can go into that quantum number.

That's very different than Bohr, right?

And that's called degeneracy, because you're taking something and you're saying, there are multiple variations that have the same n.

But there's something else that I want to explain right now that is can be understood very physically and intuitively.

And that is that the motivation-- one of the big motivations of this was that we needed more than one electron.

Our atoms are not all hydrogen and ionized atoms.

They are just neutral atoms going up above hydrogen.

So what happens when we go multi electron?

And there's two effects that I want to explain.

Here's what happens to this picture.

Those are the one electron levels, right?

There's Bohr over there.
This is what you really get in terms of energy.
Right?
This is energy along the vertical axis.
And there's two reasons, two very important reasons, why these are so different.
One is called shielding, and the other is called orbital penetration.
And I want to talk about both of them in the last seven minutes of class.
I'm going over here.
All right, so let's talk about let's do shielding first.
Shielding is something that you can kind of get a very good sense for it if you just look at what's happening in these atoms.
So in shielding let's take an example.
I'm going to give you an atom with 15 protons and 15 electrons.
What atom is it?
Anybody know?
Phosphorus.
OK, so I'm going to take an example of the phosphorus atom, OK?
And I've got 15 positive charges in the nucleus.
15.
Right?
Now, 15 protons.
Now I've got my levels, and it gets very difficult to draw levels as probability distributions.

So I'm going to draw them as rings, even though we know they're not, right?

These are my orbitals.

But I've got like an electron here, OK, an electron there.

All right.

So I've got two electrons in the n equals 1-- n equals 1 orbital.

So that's the 1s orbital, right there on the bottom.

But if I go out-- OK, so I'm going to go out now.

To n equals 2.

Well, now I've got 1, 2, 3, 4, and-- oh boy-- put one here.

5, 6, 7, 8.

Because here-- remember, I've got I equals 0 and I equals 1, and as we just said, because n sub s can be up or down, I've got eight electrons here.

So here, I've got n equals 1, here I've got n equals 2.

That's eight electrons.

And then out here-- oh, now it gets really interesting-- because for n equals 3, how many electrons do I have left?

1, 2, 3, 4, 5.

And you can already see what's happening.

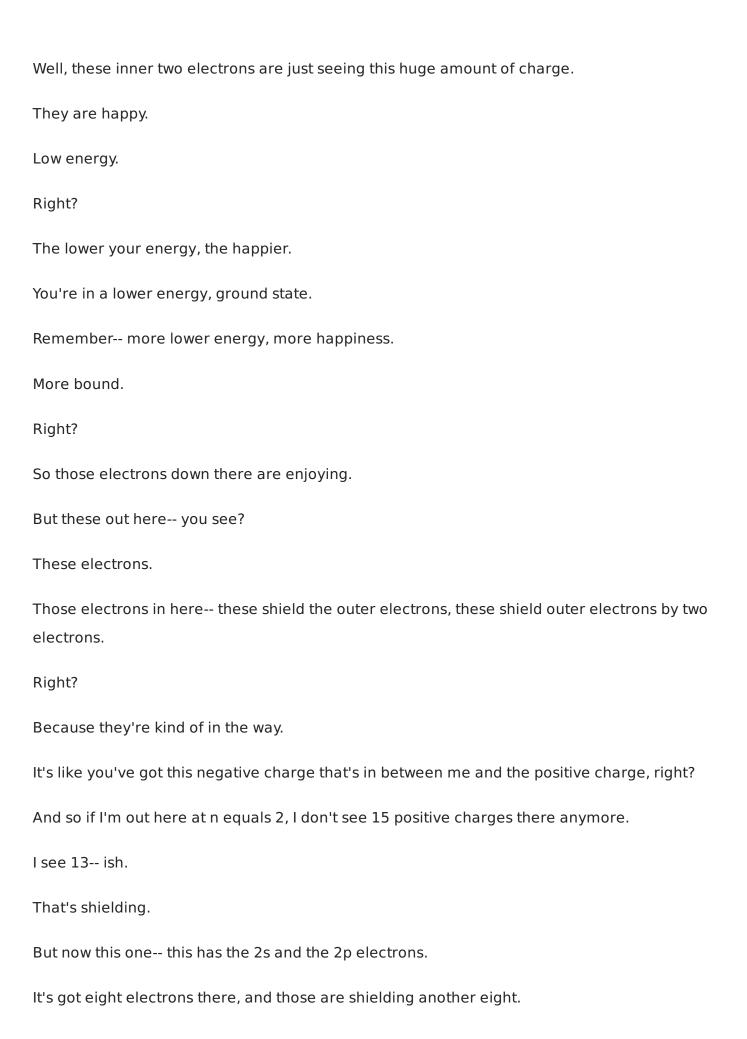
So remember, Rutherford told us this.

All this charge is in a tiny little point here.

You wouldn't even see it if we were drawing this to scale.

But what are these electrons seeing?

What are the electrons seeing?



Those are shielding another eight protons.
To things outside of them, right?
Shielding doesn't work going in.
If I'm this electron and I look out, all I see are repulsive I see repulsiveness.
In a good way I'm sure they're friends.
But two negative charges, right?
So I'm only looking in.
Looking in, shielded.
Looking in, shielded.
So these ones have sort of an effective z effective.
You know, that could be something like five.
This is not the z of the atom, but it's sort of like those very outer electrons don't see the whole proton cloud.
They get shielded.
And that's a very important part of what happens to orbitals when you put a lot of electrons in them.
And there's one more thing that happens, and it goes back to this plot that I showed you before, which is that the orbitals themselves are very different than just like a straight line from Bohr.
They have these shapes to them, right?
So the second thing that happens is that if I have that same s this is s, so this would now be the 1s.
And now I'm going to put remember that 2s looked like this.
And it had the node there.
Remember that?



It finds a lower happy place.

OK?

So we're going to use this, and on Wednesday, we're going to take these things and we're going to fill them up, and we're going to make our first solid.

Have a very good rest of your day.