JEFFREY GROSSMAN: Now, this is how we left on Tuesday. We got to this point where we had put a particle in a box. We put a quantum mechanical particle in a box. And it was an infinite square well. And what's this called?

AUDIENCE: Energy levels.

JEFFREY GROSSMAN: Energy levels, and what's really weird about them?

AUDIENCE: They're discrete.

JEFFREY GROSSMAN: Yeah, meaning if you have this one here and then you have another energy here, can it have energy in between? No. Can that quantum particle be in between? No, in energy.

And so the question was, can we connect that to things like what we see in the universe, like the spectral lines? So what I want to do-- there's a little bit more we need to do to do that connection. And so I want to spend some time today just going through that and going to the hydrogen atom, because this is not the hydrogen atom. It's not an infinite well.

And then from the hydrogen atom, we'll talk about how just from that, just by solving for the hydrogen atom, we literally have this incredibly deep understanding of the entire periodic table and all of chemistry. So it's a pretty powerful thing to do. So we're going to start with a little bit of review, and then this real-world example.

And then I've got to tell you a few things that are really important, like you have this thing called "spin." So we'll talk about that. We'll end with that, and talk about how from this solution, you get this-- pretty awesome, pretty amazing.

So some review-- so we went through this on Tuesday. So why did people even need quantum mechanics? Well, because things were failing, and crumbling, and catastrophing all around them. And so how long-- so classical atom, oh, no, there's a classical atom.

Photoelectric effect was one of them. Who can explain what happened here? These are some of the reasons why we needed a new theory after 400 years. What's going on with the photoelectric effect? Anyone remember? Yeah.

AUDIENCE: A description of the phenomenon or why it happened?

JEFFREY GROSSMAN: Yes.

AUDIENCE: OK, so basically, you take some light. You shine it at a metal, and a bunch of electrons come off. And if you increase the intensity of the light, the number of electrons coming off increases, but not the energy, which was sort of counterintuitive.

JEFFREY GROSSMAN: Why was that counterintuitive?

AUDIENCE: Because if light's not a particle, it's just like a wave, then you expect if you're shooting more light at it, that's more energy. So if an electron gets hit by a bunch of light, you'd think it would get a bunch of energy, and you'd also get a higher energy, but it doesn't. And the solution was that the photons are produced by electrons changing energy levels or something like that. And so they come in discrete packets of energy. And so when they hit an electron, they shoot it off at some particular energy.

JEFFREY GROSSMAN: And what's that?

AUDIENCE: It's frequency dependent.

JEFFREY GROSSMAN: It's just dependent on the frequency, exactly. That's exactly right. So does everybody see that?

So this was called the "photoelectric effect." And it was the reason Einstein was given the Nobel Prize. It's a very important explanation of this very confusing effect, which is that you increase the intensity, but the energy of those electrons-- see what's happening?

You're shining light on a piece of metal and electrons fly off. And you can measure how much energy those electrons have. And you increase the intensity of light, and they don't have any more energy, which was really bizarre if light is a wave.

What Einstein said is, no, actually, oh, but it does depend on the frequency of the light. So that makes sense if light can be considered as particles of zero mass-- that's weird-- that have an energy associated with their frequency. So that was really important. The energy of something you thought was a wave, light, actually can be considered as a particle associated with the frequency, have the energy of a particle associated with that frequency.

And then what was the classical atom? What's wrong with this one? How long do we live in a classical world? What's the most we could live in a classical world?

AUDIENCE: 10 to the minus 12 seconds.

JEFFREY GROSSMAN: 10 to the minus 12 seconds, it's game over. Why? What's happening?

AUDIENCE: [INAUDIBLE].

JEFFREY GROSSMAN: Why? What's happening? So it's accelerating, and we know that an accelerating charge-- radiation, and it loses energy. And if it loses energy, it should just spiral in, and that takes about 10 to the minus 12 seconds. So we know that's not true, either.

Actually, I wanted to put this out there. This is from Wikipedia, and it's a sort of explanation of that. And so if you want to understand more and read more about the classical atom, get a book on Lienard-Wiechert potentials. I'm sure just the name alone is inspiring you guys to want to dig deep.

And those are the ones. That's what you can do to get the time-varying EM field for a point charge in arbitrary motion. But look at that-- they're not corrected for quantum mechanical effects.

So that's what was such a problem. This was right around 1900. So they had it, but then they tried to apply it to an atom, and here's what happens.

It's accurate, but breaks down at the quantum level. Quantum mechanics sets important constraints on the ability of a particle to emit radiation, i.e., it doesn't in an atom. Sometimes, I think this is kind of interesting to look at.

Basically, we have this problem that an atom will sort of self-destruct, and the electrons just spiral down. The solution really, if you think about it, is it doesn't do that anymore. But now why?

Well, because of the fact that particles are waves and waves are particles. And it comes from the quantization. So I want to make sure that we're all on that page by the end of today, that we all kind of see that.

So that's the reason, is because particles can be both waves and particles. Waves can be waves and particles. Everything is one happy family. Can't we all just get along?

Here are some particles going through slits. Now what's happening here? Actually, you can think of this as a particle or it kind of looks like a water wave, doesn't it?

But see, that's the whole point. That's what particles are. So what's happening here?

Can somebody explain why it's showing this? What's going on? We've got on the left, how many slits?

AUDIENCE: One.

JEFFREY GROSSMAN: And on the right?

AUDIENCE: Two.

JEFFREY GROSSMAN: What's the difference?

AUDIENCE: Interference.

JEFFREY GROSSMAN: Yes. What's interference?

AUDIENCE: Two different waves, and you've got peaks and troughs.

JEFFREY GROSSMAN: Yeah, so that you get two waves coming out of-- but look, the same particle creates no interference here because it just bubbles through. But if you have two slits, it can create two little waves. And those interfere and they cause complex behavior. And that is what blew people away.

And oh, by the way, you can see that there's also some really cool interference going on in the backscattering from the edges, because you get a little scattering off the edges on both cases. But what we're looking at is what's happening over here. And so it's just really weird that you could throw particles through slits, and they were like water waves, not like particles. That was another really bizarre experiment.

And again, one of the big, important stepping stones was the fact that you could describe the energy of a particle by its frequency. And then de Broglie came and said, actually, not just light. No, everything-- all matter-- can be considered as both a particle and a wave. This is stuff we talked about Tuesday.

And so what that means is that I have a wavelength. What's my wavelength? 35, 10 to the minus 35. But I'm OK with that. I feel that quantum is right here. I feel it somewhere within.

But see, when things are really small like an electron, which is this part of the class-- we care about those electrons. And I motivated that on Tuesday, and we'll come back to that as we go through examples. So if I want to know about an electron, that's a really small thing.

And so its wavelength-- and we talked about this Tuesday-- the wavelength associated with the particle is about the same size as the distances the particle sort of goes out for a walk on, on a daily basis, otherwise known as its "chemical bond." If you're an electron, you kind of walk along this chemical bond. That's sort of what you do, if you're in a bonding situation.

And that distance of that walk is roughly the same as your wavelength, as your wave nature. Your wave nature-ness is important then. And so because of that, we can't describe it without quantum mechanics.

You have to have a way of describing it. And it has to be something that is based on a wave. So that's the breakthrough. And I'll go through that again just quickly.

But what we came out with is the fact that particles are waves. So they have wave functions. And this wave function is what we'll be solving for. This is what we want in this part of the class. We want that.

And so it'll have some form. And we showed a few forms, and I'll show you more today. But we showed a few for a particle in a box. That had a cosine, and then it had one node in the middle.

But what's amazing about this is that this has no meaning we know of. We do not understand what this means. So you have this intimate function that describes the particle, and we don't know how to interpret it.

The big breakthrough came in making the connection that the square of that function is meaningful. But that's pretty cool. So think about if I had a position.

Wait, you had this-- you did classical molecular dynamics, so you have the position of the particle. That's a function of time. Imagine saying that that has no meaning, or you don't know what it means, only the square of it.

So something as fundamental as the wave itself that is the solution to the equation to our f equals ma, which is Schrodinger, something as fundamental as that, we don't know what it means. But we do know what its square means. And what does the square mean?

AUDIENCE: Probability.

JEFFREY GROSSMAN: Probability. So tell me a little more about that.

AUDIENCE: [INAUDIBLE].

JEFFREY GROSSMAN: Yeah, so tell me-- this is a particle right here. You're starting to see it, I can tell. I can see that you're starting to see it. I can feel the excitement about this, too, in the room. It's tangible.

This is a particle. You see this now not as a wave, not as a particle. You see it as both.

Now, if this is a particle and that's why I'm going to show you a little video on it in a second. But if this is a particle, where is it?

AUDIENCE: [INAUDIBLE] by chance [INAUDIBLE].

JEFFREY GROSSMAN: But I mean, I know that it can be a particle again. We it can go back and forth. That's what it did when you sent it through the two slits-- it became wave, then it became a particle. So can I say that it's spread out? Is it spread out? How do I interpret that?

AUDIENCE: The probability of finding a particle is 2 to the negative 3.

JEFFREY GROSSMAN: Good. That's sort of the way that I like to look at it. I mean, the particle is-- in a way, you can think about it is spread out until you measure it. It's sort of everywhere in here, because there's no here here. There's only a certain amount of chance to be here here.

So I have a kind of big chance, if I measure where it is, of finding it here. And then I have no chance of finding it here. And then it's sort of medium chance here, and a big chance there, if I measure it. So that's really what these functions mean.

And those functions are the ones that we solve for to find out where electrons are. And where those electrons are is what is absolutely critical to doing a whole lot of material science, as I mentioned on Tuesday, and as we'll talk about when we apply this to problems. And that's what you get. You get bizarre distributions of probabilities.

Here's an electron thrown into a wall that is infinite, and here is an electron thrown into a wall that's finite. So that's my quantum mechanical ball. Did I show this Tuesday? I don't think I did.

So if it's thrown into an infinite wall, it actually can't go through. The probability-- we worked this out. If you have an infinite boundary here-- we talked about that Tuesday-- you can't have any function. The only solution is 0.

So it can't penetrate at all. So it completely bounces back, although look at the weird things it does when it bounces back. That's the wave function of a ball thrown into a wall, or if you want, an electron thrown into a material.

But over here, you see it's not infinite, and all kinds of interesting things happen. It does bounce back in a similar way, but some of it goes through. What's that called?

AUDIENCE: Tunneling.

JEFFREY GROSSMAN: Tunneling, right. And you better believe that this is as effect we use in technology all the time-- tunneling of charges, very important. If I take my macroscopic ball and I throw it, or if I just run myself with a helmet on into the wall, how much of me is going to tunnel?

AUDIENCE: Not enough.

JEFFREY GROSSMAN: What is enough in that example? So why aren't I tunneling if I run into that wall?

AUDIENCE: [INAUDIBLE].

AUDIENCE: You're not running fast enough.

JEFFREY GROSSMAN: I'm not running-- so actually, that's true. I'm pretty slow. But the thing is that there's another reason. What is it about me that is really different here?

AUDIENCE: You're big.

JEFFREY GROSSMAN: I'm big, and so what does that mean? What's small?

AUDIENCE: Your wavelength.

JEFFREY GROSSMAN:

My wave function-- my wavelength, not my wave function. My wave function is everywhere, but it just doesn't really spread out that much. Because the wavelength of me is 10 to minus 35 meters, and remember, when quantum matters is when your wavelength is sort of on the same scale roughly as the stuff you're involved with.

And I'm involved with a thing that's a meter over there. So if I'm 35 orders of magnitude smaller in my wavelength, there's not going to be any quantum effects. You won't tunnel very often, not enough to make it worth trying.

Now, here's the goofy video, which is kind of fun. So I'll just play it, and then we'll move on.

[VIDEO PLAYING]

[MUSIC PLAYING]

I love the music.

- A true giant of quantum revolution was Werner Heisenberg. And from the vagueness of positions of electrons and de Beuys standing wave orbits, he drew a tremendous insight, which he stated like this-- "The more precisely the position is determined, the less precisely the momentum is known, and vice versa." And while it may seem like a bunch of gobbledygook, it was the insight necessary to understand how an object can be both a particle and a wave. This single statement led to the understanding that subatomic particles can disappear and reappear in another place.

JEFFREY GROSSMAN:

That's really weird.

- And they can do this without existing in the intervening space.

JEFFREY GROSSMAN:

That's really weird.

- When an electron is trapped inside an atom, the places it can disappear and reappear include specific locations around the nucleus. And that makes it look like a shell. Basic particles can also be in more than one place at a time, if the time is brief enough.

An electron can travel from here to there along all possible paths simultaneously. And even more astounding, these particles can appear out of the nothingness of space, exist for an extremely brief instant, and then disappear. Scientists call them "virtual particles."

They may be virtual, but they can have very real effects. All this jumping around makes particle descriptions so inexact. But then existence itself is inexact at these tiny scales.

The question is often asked, what is it that is wave when a particle is described as a wave? And after a lot of hem-hawing around the issue, the right answer is, existence is waving. The particles are jumping around, coming into and out of existence.

And those places where the wave crests are maximum, are the places where the particle materializes most of the time, while the places where the crests are minimum are the places the particle avoids. The wave is a map of the particles' existence. And as the wave changes, the particle changes as well.

[END PLAYBACK]

JEFFREY GROSSMAN: There you go. I love these kinds of videos, and not just for the soundtracks, because those are pretty cool. But I think that he got a little bit ahead of where I want to be, but does everybody see that weirdness? Is everybody getting a feel for it?

OK, he said something that's mind blowing. What did he say that I said was really deep. Anybody remember?

AUDIENCE: Existence is waving.

JEFFREY GROSSMAN: Existence is-- well, yeah. Oh, actually, there were so many things. You're going to have to see this again.

And again, this is one of those things-- you take this with Dr. Quantum, was it Dr. Quantum? You take this video with you, too-- to the bars, to the dorms, wherever you're going to do your next social thing. And you just see what the response is. You ask what their opinion is, and it's a great way to engage with people. Yeah.

AUDIENCE: Does the wave function exist all the time?

JEFFREY GROSSMAN: Sorry?

AUDIENCE: Does the wave function exist all the time, too?

JEFFREY GROSSMAN: That is a good question. And yes. I mean, it's changing all the time, but it exists all the time.

Here's the thing, though-- did anybody catch the other thing that's going on here? I'm going to talk about this at the end today. But--

AUDIENCE: [INAUDIBLE].

JEFFREY GROSSMAN: OK, yeah, I can't even go there, that's so crazy. What else? Yeah.

AUDIENCE: Virtual particles.

JEFFREY GROSSMAN: Vertical particles, vacuum fluctuations, but we're not going there either-- mind blowing. I mean, in quantum mechanics, stuff actually appears out of nowhere. Out of nothing you get something, and then it disappears. Those are called "vacuum fluctuations."

What else? But it's all related to this. Basically what he said is that particles can disappear and then reappear somewhere else. And actually, if you take field theory, which I really don't recommend for most people-- I still remember my final exam in field theory. It was 90 pages long. It was a 24-hour, take-home exam.

Anyway, I still remember asking my field theory teacher in graduate school, how can that be? How can a particle disappear? Because basically when you get down to it, that's pretty much how things move at the very smallest scales.

They disappear and then they reappear. That's what the math tells us, at least. How can that be?

I didn't get an answer. This gets deep. It's really cool and really mind blowing.

And we just don't really know. We don't connect it so much anymore in the classrooms to the mind-blowing awesomeness of it all. But I love it. Now, I'll get to that towards the end. I'll come back to that.

Now, what we need-- so we have these waves. We know that particles are waves and waves are particles. And we know that the particles we care about in this part of the class are going to have to be described by a wave.

How do we talk-- what's the F equals ma of that wave? It's dictated by-- it's the Schrodinger equation. That's it. That's our f equals ma. It's telling us how this wave is going to change in time and space.

And so we talked about that. And we basically just wrote this down and said this is the equation. We're not going to go into the details of where it comes from, but there's so many places where you can read more about that.

But this is our governing equation. And basically, what you have is a kind of kinetic energy of the wave. That's this del squared thing, kinetic energy operator, and a potential.

And that together, we call h, we call the Hamiltonian. That's got its own special name because just like T plus V in classical physics is the energy, we consider this thing, h squared over 2m del squared plus V to be the energy. That's h.

But it has to act on the wave function in order to get that energy. And that's basically what the Schrodinger equation is. Because we said, we're going to say that h doesn't depend on time usually, for the things we care about. And if it doesn't depend on time, then we can get rid of the t here, and we could separate the time dependence out, which is what we do.

And we're left with H psi equals E psi, which is the equation we need to solve. And I'll come back to it in a second. Here's the bit on Schrodinger I mentioned that I think is amazing. This is, again, from Wikipedia.

You see, he found the standing waves. See, there it is. He found the standing waves of this relativistic equation, but the relativistic corrections disagreed with Sommerfeld's formula. Discouraged, he put away his calculations and secluded himself in an isolated mountain cabin with a lover.

I find it amazing-- not that part, but I find it amazing that seriously, he had to be convinced. See, he came back from the cabin and he decided that his earlier calculations were novel enough to publish. It's a good thing, because it's pretty much one of the most important equations of the last century.

And it's the equation we will be solving. That's why I think this history is interesting. OK, so there it is.

So we talked about how you can take the f out, because if H doesn't depend on time, then you can just set them equal to a constant. You can set each side having its own function dependent on its own variable, r and t in this case, and they equal a constant. And then you get the Schrodinger equation we care about, which is the one we'll be solving, which is H psi equals E psi.

And then we did this, and we said, well, how do you solve it? What if you have a very simple particle in a box. And the box's walls go up to infinity.

Then you can solve it. And it's because you have basically the particle is either between 0 and L, in which case here, then v is 0, and so you get this equation, or it's out here in this region, in which case V is infinity, which means psi has to be 0. That's the only solution.

And then this is the interesting part. And when you look at this, you see that the general solution is sines and cosines. So we did that, but then there was the very important thing that happened. What is it?

And you get a solution for E. Once you say the general solution, you get a solution for E. So this is just a standing wave, and you get a solution for E, which depends on k squared. But what's really important that we did next?

AUDIENCE: [INAUDIBLE].

JEFFREY GROSSMAN: And that does-- yes, and what did that do?

AUDIENCE: It quantizes.

JEFFREY GROSSMAN: Quantizes. Once you have the boundary conditions, it limits what this can be. We didn't limit it until we applied the boundary conditions. Then we applied the boundary conditions and boom, this thing is quantized, and out from that drops such a relief for the world, which can exist for more than 10 to the minus 12 seconds.

Because that quantization is, in fact, the answer. It's that those electrons can only be at certain energies. They cannot radiate energy off of the atom and spiral to the middle because they can't be at another energy except the one it's in, and then the next one.

And it's real. I think I may have shown this on Tuesday-- that you can actually visualize the spatial extent of the orbitals. And I put some more-- this is actually cutting-edge research.

Visualizing the shape of electrons is not easy, but it can be done. There's been some really phenomenal breakthrough experiments. This was in *Scientific American* a decade ago.

Now I want to move from particle in a box to real stuff. And the first real stuff that's relevant is hydrogen. And it's only one element, and I mentioned last time that it's not necessarily useful enough to do, say, materials engineering.

And so you'd like to have a little bit more of the periodic table. That's true, but you'll see that with hydrogen alone, we get our answers to so many questions about the whole periodic table. And it is a real useful material. How much of the universe is made of hydrogen, does anybody know?

AUDIENCE: 70?

JEFFREY GROSSMAN: That's a really good guess. It's about 75%. That's a lot of hydrogen. Now, how much of that is in usable form on Earth for the hydrogen economy?

How much hydrogen is usable for hydrogen-powered cars on this planet right now, in an immediate form? Zero. That's part one of the hydrogen economy problem. You've got to make the hydrogen.

There isn't any more. It's too light. This planet's gravity couldn't hold it. So anything that was free, left or bonded to something else.

You've got to make the hydrogen. What's part two of the hydrogen economy problem? Storing it. So you've got two big problems with the hydrogen economy. I'm not saying it's not worth looking at.

We will not be driving around this way, but I'll talk a little bit more about hydrogen. I just love motivating the topic we're about to go into. And since I want to talk about the hydrogen atom, I will talk a little more about hydrogen storage materials.

And we will calculate some properties of them using quantum mechanics. But I love this. The history of hydrogen is a very interesting one, but I love going back to Jules Verne.

In 1874, Jules Verne said, "I believe that one day hydrogen and oxygen, which together form water, will be used either alone or together as an inexhaustible source of heat and light." I love that. Anyway, we're not there, not even close. I think a hydrogen economy is a possibility.

And I think there's some great research going on. And it should stay as research for at least another 30, 40 years. I'll come back to-- it's going to need about that much research to really make an impact in the energy scene. I'll come back to that later.

So that's a little motivation for hydrogen. Now here it is. Hydrogen has a proton, an electron, and it's got some distance that that electron sits away from the proton. What do I need to know?

Well, I need to know the potential. So what's the potential here between these two charges? One's negative, one's positive. They feel an attraction.

How does it go with r? Yeah. It goes as 1 over r. So now that-- I got my V. It's the potential that charges feel. And that's got to go now into the Schrodinger equation, which I then need to solve. And that'll tell me what the possible wave functions are.

And so here's what it looks like, see? We had H psi equals E psi. That's our master equation.

Then we said, that's the kinetic plus potential. And then we said, that's the momentum term, remember, we talked about Tuesday, which is just a second derivative. It's a second partial derivative.

It's a del squared, and plus this potential term, which I now put in here explicitly for the hydrogen atom, E squared over 4 pi epsilon 0 r. And that's the question I need to solve. And it turns out that you can solve this exactly.

You can solve this exactly, just like you could the particle in the box with the infinite boundaries. And that's really cool. So you've got an electron. You've got one particle, just one electron.

These are its spatial coordinates. And you can solve for it in this potential, in this 1 over r potential exactly. And the easy way to do that is to switch it to spherical coordinates.

So I won't go through the math in detail. There's literally like 100 sites and 50 Wolfram Alpha apps you can look at that go through this, and really, really wonderful material on this. But basically, the key point is that when you write it in spherical coordinates, you switch from XYZ Cartesian to spherical coordinates, you can actually separate this into essentially three quantized problems-- theta, r, and phi.

And so you can write psi now as a function of the r and a function of the theta and a function of the phi. And what ends up happening-- and then so you put that in. And there's a little bit of math. It's actually not that much. I'm not going to go through it.

But you put that in, and basically, just like that particle in the box, just like that, each one of these variables gets quantized. It gets its own sort of E-type term, and it gets a quantization. So these are the equations that it leads to when you do the separation of variables.

And I think I have-- yes, and the quantization is-- I think maybe on the next page I have the actual energies. But the solution-- remember, just like the quantization of a particle in a box, the same here. It only can happen, you can only have a solution, if in this case, we're going to have a quantum number called n is 1, 2, 3, or something else going up.

Or in this case, we'll have a quantum number called l. That's also, by the way, the main quantum number, the orbital quantum number, and then we have this little m sub l, which is the magnetic one. How many of you have not seen these?

So you've all seen these? How many of you have seen this? OK, so I'm glad to see all the hands go up.

And so that's what you have. And it's a very special case. And how many of you remember that s stands for "sharp?" See, I forget that.

Seriously, did you all remember this sharp principle and diffuse? And I love f, which is "fundamental." So I want to know what's not fundamental about silicon, which has no f electrons? Anyway, I thought that was an interesting label.

So this is how we designate, from these quantum numbers, which come from just solving the Schrodinger equation for one electron in a 1 over r potential-- that's how we get all of these designations that you're used to-- s orbitals, p orbitals. And you see, you get different wave functions. You get these functions, these same wiggly functions that I've been showing you.

You get four different values of these quantum numbers. And those functions can be plotted in space. This is just given those spherical coordinates and the functions of those, you can plot them.

And you see that they make really funny shapes. Why is this so important? I said it on Tuesday. Why is the funniness of those shapes important?

AUDIENCE: [INAUDIBLE].

JEFFREY GROSSMAN: Yeah, because what am I looking at? Actually, let's go to the next one. That's kind of fun.

What am I looking at here? This is the 1s orbital of hydrogen, 2s orbital, 3s, 4s. Look at how they're all spheres. They're all spherically symmetric.

And then you go 2p orbital and you see that it has a different shape. So its function, these are wave functions. Remember, the wave function is-- what's the wave function?

Who knows? Does any of you know? If anybody has some ideas, this is like an open problem, an open discussion.

But what is interesting about these? So these are the wave functions. From that, what can I get?

AUDIENCE: [INAUDIBLE].

JEFFREY GROSSMAN: Yeah, if I do what?

AUDIENCE: Square it.

JEFFREY GROSSMAN: Square it. So these landscapes squared tell me what? Where the electron is. And that is incredibly important.

That's it-- where is that electron? Well, if you are fundamental as opposed to diffuse, you have some really bizarre places you can be and not be. You can't be anywhere where this isn't.

That's the point. It's a probability distribution. It dictates-- basically, all the behavior of materials comes from these, these distributions. They dictate what materials do and become.

Now in the hydrogen atom-- so what happens? So you get these shapes of the size, and then you also get those E's. And remember, we solved for the E's and then we put the boundary conditions on, and then it was quantized.

And the quantization in hydrogen can be calculated exactly. So the quantization of the energy levels in hydrogen is exactly minus 13.6 over n squared, where n is the principle quantum number. How many of you have seen this? Sort of half.

So 13.6 eV over n squared is the quantization. That means the energy of an electron in this first orbital, that one up there, if I put an electron in that orbital, its energy is bound to the atom by 13.6 eV. So what does that mean? Yeah.

AUDIENCE: If you give it 13.6 eV or greater, it'll become free.

JEFFREY GROSSMAN: Yeah. That's the ionization energy of that electron. But hydrogen has all of these other orbitals accessible to it. Maybe I could put an electron up to another level, like the 2s level.

And if I do that, it's all the way up to 3.4. So now it's only bound by 3.4 eV in the atom. And what does that make it? Is it sort of less stable, more stable?

AUDIENCE: Less stable.

JEFFREY GROSSMAN: Less stable. So it'd be much more easy to pull it off. Now, do you think that that has something to do with bonding?

You better believe it. Where electrons sit in energy relative to other electrons in other atoms, or in their own atom, has everything to do with how things bond together. And that bonding is the one that you've been just fitting to like a Lennard-Jones potential.

You've just been fitting it. All that bonding is what you just-- in classical physics, in classical modeling, you have to have some potential form. And all of the intricacies of the bonding get swept up into that. But you can see why that's so much more complicated than that, just by looking at these.

OK, but now, that series that we just got from a simple particle in 1 over r potential explains all of these levels that are observed. So does everybody remember this? And poor number six who didn't get named?

What are these? When you see these, what does it make you think? Spectral-- now explain what's happening in the Lymann series. What's happening?

AUDIENCE: You're moving from one orbital down to the ground one and it's emitting photons at those wavelengths.

JEFFREY GROSSMAN: And why are they different? Why do I have all these different ones in one series?

AUDIENCE: The amount of energy it gives off as it goes from n equals 7 to n equals 1 is different from n equals 2 to n equals 1.

JEFFREY GROSSMAN: Yeah, exactly. And if you go up to 2 and you stop at 2, then you have other energies. Because it all comes down to, then, what the differences are. To get an electron to go from here to here, you need the difference in these energies.

And to go from here to here, you need that difference. No more and no less will do. Now, when the electron comes back down, what happens? Anybody know what happens?

AUDIENCE: It emits light.

JEFFREY GROSSMAN: It emits light. It gives that energy back out as light. And that's what you see when you look out at these spectral lines. So it emits light at exactly this energy.

Can it emit light at something else, at a different amount of energy, or a different frequency? Because we know for light, the energy is equal to the frequency times a constant. Can it emit light at this frequency, something in between? Why not?

AUDIENCE: Quantized.

JEFFREY GROSSMAN: Yeah, it just can't because it's a wave problem that has as its solution quantization. And now, I come to the question of, well then how does-- so that's what's happening. That's the picture of these electrons coming back down, and emitting different colors of light.

It explains what people saw and couldn't understand for so long. This simple solution, mathematical solution, does it all. It really crystallized what was going on, and it really confirmed that this is the right way to picture things-- the wave equation and the Schrodinger equation.

Now, what's happening when an electron goes from here to here? How does it do that? It cannot go in between, but we know it does do this all the time.

We just look out in space and we see it happening all the time, but we can do it here. We can build materials that do this for a living. Where are those electrons going when they go from the 2p to the 1s? Where are they going? Who can tell me? Yeah.

AUDIENCE: They're all sort of described by a wave function, right? So it has some non-zero probability to be in one place and a non-zero probability to be in another place. And if you hit it with a photon or something, or have some perturbation to your hydrogen atom, then it's going to have a non-zero probability to be in one electron energy level than another. And so it just sort of ends up falling into one of them.

JEFFREY GROSSMAN: That actually works. That is a great interpretation of what's happening. And that actually works, and it even works all the way down to the nucleus.

By the way, decay to the nucleus is possible because those s orbitals-- I was just showing you a slice of them, an isosurface. But they have a non-zero magnitude all the way down to the nucleus. It just won't happen very often, because the probability is so low that it's why we have a universe.

If that overlap was more, if the wave function going into the middle-- if this is the nucleus and this is the electron, and the wave function of the s orbital looks like this, and it's almost 0, that's why we are alive today. But if this looks more like this, no, we wouldn't make it. There's just too much probability for the electron to decay into the nucleus, and give off that amount of energy, and the atom collapses. So we should be very thankful to quantum mechanics.

Now, there are situations, though, when you actually have nodes in between. And that's a tougher one. The node means the wave function goes exactly to 0. Now what's happening?

And here, we go back to this world of particles, this field theory world, basically, of how particles move, by essentially annihilating themselves and reappearing. That's how electrons really move. Now any questions about any of that? No questions at all?

OK, we're going to start taking this to the next level, which is obviously going to have to be more complexity. There are some constants that I'm just putting here. I'm not going to spend any time on it, but these are the constants you'll be using in the quantum world.

We have an electron volt. We have a Rydberg, which is 13.6 electron volts. And just to make it interesting, there's a Hartree, which is a half of that. And then the same with angstroms and Bohr. These are the kinds of unit-- do you say angstrom, do you say Bohr-- to-may-to, to-mah-to-- you can choose, but just keep track of it all.

Now, as we go to more complex-- so I've given you a particle in a box, and then I gave you a particle, actually, on Tuesday, in an oscillator. And then I give you a particle in 1 over r. And that got us a long way.

We explained spectral lines. We got hydrogen right. But if I just add a little bit more complexity, you see things get really messy.

Now, this was a problem. I wanted to show how messy things get with analytic solutions as a kind of motivational exercise. So I gave this on a homework problem in this class two years ago. And I'll admit that was probably a mistake.

I had a lot of people at office hours, because you see, this is the same thing. I'm throwing my quantum mechanical ball into a wall that has another wall behind it. So can't you just set it up?

Well, sure, you can. And this is what you get. And you put that into Mathematica, which every single student did, and it chokes-- can't do it. Too many for Matlab. I guess too many boundary conditions, or too many variables, or something, but nobody could get Mathematica to do this without some intelligent substitution of variables first, which was sort of the trick.

But my point in this was not to make students suffer. I don't like to do that, but it was just to convey how hard this equation gets to solve with just a little bit more complexity than one particle in a well or in 1 over r, or something like that. It gets really hard, and that's why we need computers. And that's what computation in the last 50 years has done. It has made this, together with some algorithms, some simplifications that you'll hear about-- it has made this equation solvable for much more complex systems.

So I can also say, well, let's not make the potential more complicated. Let's just add another electron. So now, I'm still with a 1 over r potential, but I've got two of them.

So now, all of a sudden, my potential term is these electrons interacting with the proton, but also those electrons interacting with each other. That's r12, the distance between the two electrons. And boy, does that make this equation hard to solve analytically.

You cannot use separation of variables. So even just one more electron, it's a deal breaker, basically. And now you think we want to do big molecules. We want to do fullerenes. We want to do silicon. We want to do thousands of electrons. Analytic approaches won't work.

So what can you do? Well, there are two different ways to go. You've got to do something. You've got to make it easier, because as you'll see, an exact solution, even with the most powerful computers in the world times squared are not going to do it.

You need to make approximations to the actual equation. And you'll hear about those next week. And one thing you can do is you can use perturbation theory to say that this Hamiltonian is actually some simpler Hamiltonian.

That Hamiltonian is some simpler Hamiltonian that you can solve easily plus some perturbation to it. We're not going to really do that. Has anybody used perturbation theory? So we're not going to do it much but, I'm just using it for reference.

And then, so you do something for something. Perturbation theory, what you do is you say, well, that's hard, so I'm not going to do that. But this is actually kind of related, and it's easy, and I know how to do this. So I'll do this and then add something to it. That's basically perturbation theory.

But what we're going to do is we're going to try to solve it using more of a matrix eigenvalue approach. And again, we are not going to go deep into the math here. And you will not be tested on the math.

As I said, my goal here is to have you guys applying these equations to real materials problems. But I do think that it's useful to know what's under the hood, to know what equations are being solved when you press "Simulate." So you'll hear more about this, and how you go about actually making these approximations, making the approximations you need to make in order to get an eigenvalue problem that can be solved on a computer.

There are a couple of different ways to do that. The way that we're going to settle on in this class is density functional theory. So we'll talk a little bit about that. And again, the only Nobel Prize in computation was given for that, the development of that theory.

Now, there's one more thing I need to talk about before I move to just a couple of examples online that I'd like to show you. And that is that there's something still missing here. So we've got-- let's see, we've got this 1s.

So now we know where these things come from. We really know where they come from, the solution to the hydrogen atom-- 2p, 3s, and so on. And then hydrogen would be what? How would I show hydrogen here?

Put an arrow there. What would helium be? One more. OK, tell me carbon-- I like carbon.

AUDIENCE:	[INAUDIBLE].
JEFFREY GROSSMAN:	Carbon is right here. It hits me in the heart every time. How many more?
AUDIENCE:	Four.
JEFFREY GROSSMAN:	And then what?
AUDIENCE:	Two up.
JEFFREY GROSSMAN:	Two up-- oh, why not like this? No? It just feels wrong-- exclusion. Now we're talking.

You guys already kind of have a feeling for this. But actually, you can have materials that violate someone's rule. Anyone know what that rule is called?

AUDIENCE: Pauli exclusions.

JEFFREY GROSSMAN: Well, actually, this doesn't violate Pauli exclusions.

AUDIENCE: Hund's rule.

JEFFREY GROSSMAN: Hund's rule-- very good, whoever pulled that one out. That was good. But this is how carbon usually looks.

Now, something that we've done here is we've already done what I'm about to tell you, which is we've put spin in there. We've put those electrons pointing up or down. But we also have those quantum numbers.

This is n. N equals 1. This is n equals 2, and this is l equals 0, l equals 0. And this is p.

So this is n equals 2, l equals 1. And each one of these is an m. m equals plus or minus 1 and 0. So that's why I have three p's. So those are those quantum numbers you get from quantizing the solution to the Schrodinger equation for an electron in the 1 over r potential.

But there's this one more thing, which was also very surprising at the time, which is that if you put a particle, in this case silver atoms, if you think about electrons as charges spinning, you should have a reaction to a magnetic field. They should have a magnetic moment.

But classically, you see, if you have charged spinning, you get a magnetic field. Classically, if you shoot this through a really large magnet, you should just get a whole range of lines of fields. But just like the double slit, it didn't turn out that way. You got two dots instead, only two dots.

And these are very famous. These are the Stern-Gerlach experiments, which were done all around the same time they were figuring all this out. And what it showed is that the spin can only be up or down. It can only be two things. There's only two values for the spin of an electron, the spin being the thing that's causing this thing to have a magnetic moment that's causing it to react to the external magnetic field.

You should get a line. You should get all this-- classically, electrons should have any spin they want. I don't know what that was, but it should be able to point in any direction. But no, it can only point this way or this way.

Now, is an electron really spinning? If a charge is spinning, it has a magnetic moment, but is an electron really spinning? How does it have a magnetic moment?

Let's talk. That's a really good one, too, but it does. And you think about it as spinning because that is our classical Maxwell sort of ENN framework. We think about charged spinning.

You've done it. You make current go through a wire, and you get a field. And that's why we use the word "spin."

It's sort of like "orbital." Should we really be using the word "orbital?" Is this electron orbiting? No.

And that's another ice-breaking question. You go to your friend, and you just say, do you think electrons are really orbiting? Just like that. And see how many people say yes.

They kind of are spinning in our minds. But the spin is up or down because of those experiments. Now then, the sort of end of the story-- so they have a magnetic moment, and it gives them up and down.

And they can only be up and down, only up and down, two values. And so what you have is sort of a new quantum number. You have spin, which is equal to plus or minus 1.

That's that and that. So now each of these-- and that's why with these collections of quantum numbers, you can get that many electrons into those shells. And I love this.

So somebody said "Pauli exclusion." Somebody tell me what the Pauli exclusion principle is. Yes.

AUDIENCE: Two fermions can't be in the same state.

JEFFREY GROSSMAN: OK, so two electrons, we'll just say, which are fermions, cannot be in the same state. And what do you mean by the "same state?"

AUDIENCE: That they can be in sort of the same energy shell with the same spin at the same time.

JEFFREY GROSSMAN:

OK, very good. Basically what it means is they cannot have the exact same quantum numbers. Pauli exclusion says you cannot do this.

Now, I mentioned you can violate Hund's rule. And you can violate Hund's rule by having degenerate orbitals with the same energy, and doing it there. But usually, you don't.

Pauli exclusion is an incredibly important aspect of quantum mechanics. It says that no two electrons, fermions, can occupy the same set of quantum numbers when you include spin. That is what gives us literally the periodic table and all of chemistry when you add that to quantum mechanics.

That is what gives us the rest, that plus the hydrogen atom. You don't need much more, except you do. But I love this letter from Thomas to Goudsmit in 1926.

"I think you and Uhlenbeck"-- because they're the ones that discovered this stuff in working out the theory-- "have been very lucky to get your spinning electron published and talked about before Pauli heard of it. It appears that more than a year ago, Kronig believed in the spinning electron and worked out something. The first person he showed it to was Pauli. Pauli ridiculed the whole thing so much that the first person became also the last, and no one else heard anything of it, which all goes to show that the infallibility of the deity does not extend to his self-styled vicar on Earth."

So Pauli had an interesting reputation. But that is amazing to me, because this is it. This is one of the foundations of the Pauli exclusion principle, so Pauli built his whole reputation and really made an important contribution because of what apparently he didn't really believe in at first.

So it goes to show-- keep an open mind. So that's what we just said, can't have the same quantum numbers. Got to mix up the quantum numbers, and that's it.

And that is it. You see, because now, we had all these levels from the hydrogen atom solution-- an electron a one electron in a simple 1 over r potential, and we got all those levels. And now all we need to do is fill them up. And with the Pauli exclusion principle, we know the rules.

We know the rules. We know we can only put two electrons here. We know we can only put two electrons in s and six electrons in p, so eight here. We know we can only put two, six, and how many in d?

10, because n goes from minus 2 to plus 2, so 5. I mean, d has that. So that's starting to sound a whole lot like this. That's it.

Essentially, with those fundamental principles that were worked out in the '20s, and the solution of the hydrogen atom, you get essentially all of the periodic table. It's really powerful. It's pretty darn cool. And you can connect, as I said, back to the spectral lines and all of that.

Now, what I want to spend the last couple of minutes on is I wanted to show you-- has anybody looked at the quantum part? You guys are still doing homework from the last part, right? So on the NanoHUB, there is-- so you go to the NanoHUB, and you go to-- sorry, I should check this out. There I am.

That's amazing. That's a picture from, like, I won't say how long ago. That's embarrassing.

So you go. This is my personal thing. But anyway, the tool you want is this one, and it has a little star next to it. That's so exciting.

It's called the "MIT Atomic Scale Modeling Toolkit," formerly known as the Berkeley Atomic Scale Modeling Toolkit, because I developed it at Berkeley. So much for that, but it's now at MIT. And if you click that, these are actually tools I developed for a class I made up when I was at Berkeley, when I valued sunshine over science. It doesn't say that.

And you can launch it, and you'll see that-- and you can rate it a 10. Don't rate it anything else. But please rate it, or don't rate it. Everybody is so star driven these days, number of stars. What was that?

There was an NPR piece the other day about how there's this whole business, opportunity sprouting up, of people who have companies, where all they do is they get your number of stars for your products high. So they have people around the world, because you've got to do it from different places, and you've got to write fake reviews of products, and have different fake Google email addresses-- blowing me away, the so-called internet.

Now, you look here, and you see that actually in this MIT Atomic Scale Modeling Toolkit, there are many things. There are many things. We will be using two tools from this, and both are quantum mechanical tools.

One is going to be GAMESS, which is a quantum chemistry package. It's free. You can download it and run it on your laptop, actually. And it's for molecules and atoms.

And another is going to be called SIESTA. So you play games, you take a siesta. And this one, we're going to use when we do solids. Both of them are going to use an approximation called "density functional theory" to solve the Schrodinger equation for real materials.

So let's just take, in the last few minutes of class, let's take a look at GAMESS. And you can see-- why isn't it letting me-- it's not letting me scroll down. Seriously? Oh, there's my scrollbar there.

OK, so the input is actually pretty straightforward. So you can calculate the energy or you can optimize it. The method is going to be DFT, Density Functional Theory. The basis set is something you'll learn about on Tuesday, what that is, but pick Medium.

And then I want to not have a solvent, but I want to plot these orbitals. And then, I think it disappeared again. Don't you guys love the NanoHUB? It's so bug free. And now it's not dragging. It's great.

So what you can do is you can do New, and let's do the carbon atom, my favorite one. And I'm going to-- do you guys know about XYZ coordinates? So you put the number of atoms in the top line. You leave the next line blank or you write whatever you want.

And, well, don't let me see some of the things you might write. I don't know. And then you put the atoms with their XYZ positions. So carbon is going to be at the origin, and we click "Simulate."

And it's doing it. That's it. It just solved the Schrodinger equation for carbon, something you couldn't do for a million years-- no, for 50 years-- analytically. And it just did it. And now it's still executing a script, which is very frustrating. Is it this slow for you guys? This is one atom. Man.

Well, so we go back to here. One thing you got right there is you got those energy levels, which I can't scroll down to look at. This is so amazingly frustrating.

So now, what I'm going to do, since it's not working, is I'm going to try it again. And I'll pick a different basis, low. See if that works. And I just did the Schrodinger equation for carbon.

You've got to be kidding me. You've got to be kidding me. Really? Seriously? Let's try a different atom. Let's try-- somebody give me an atom.

AUDIENCE: Boron.

JEFFREY GROSSMAN: All right, this is going to be lucky. This is going to do it. Oh, yeah, It's not able to do it-- unbelievable.

Let me just try one more thing. I'm going to try putting two atoms in. Let's see if that helps. And we'll optimize it.

Yeah, now it is a party. Oh, OK, but did it give me the orbitals? No. Hang on. Sorry, guys. Oh, it's still here.

Let's just see if it gave me the orbitals. OK, there they are. OK, this is it. It was Firefox, which I never use, but it came to the rescue for this one.

So look at this, just really quickly, because if you want to play with this, this will just take one minute to show. OK, there, I did the carbon dimer. That's a lot of electrons, and it just solved it. Because of what you're going to learn on Tuesday, the approximations, it just solved it.

And look-- if you right click on top of the image, you get surfaces, and then you get orbitals. And look at that-- that is actually-- what do you think those two are? There are two carbon atoms here-- the s's. Those are those 1s's together in the dimer.

And these are now the 2s and p's, all bonding together. And you want to know how they look? Well, here's one of those s's. There it is.

It's an S orbital in the dimer, though. And it looks very much like the atomic s orbital, which it should. Why? Remember, those are the ones we don't care about. They don't really do anything when you bond.

It's all about the other ones, like for example, one of these p's. That's it. That's the solution to the Schrodinger equation for the carbon dimer. And that's where that p-type orbital-- that's where the electron in that level sits.

And this is no longer an atom. You can do it for the carbon atom, and see the p orbitals and the s orbitals, but now when you make a molecule, things get more complicated, and more and more complicated. So that'll be the tool we use for our molecule things, assuming it actually works. And if anyone has any questions, email me. And remember, class next Tuesday, but not next Thursday.